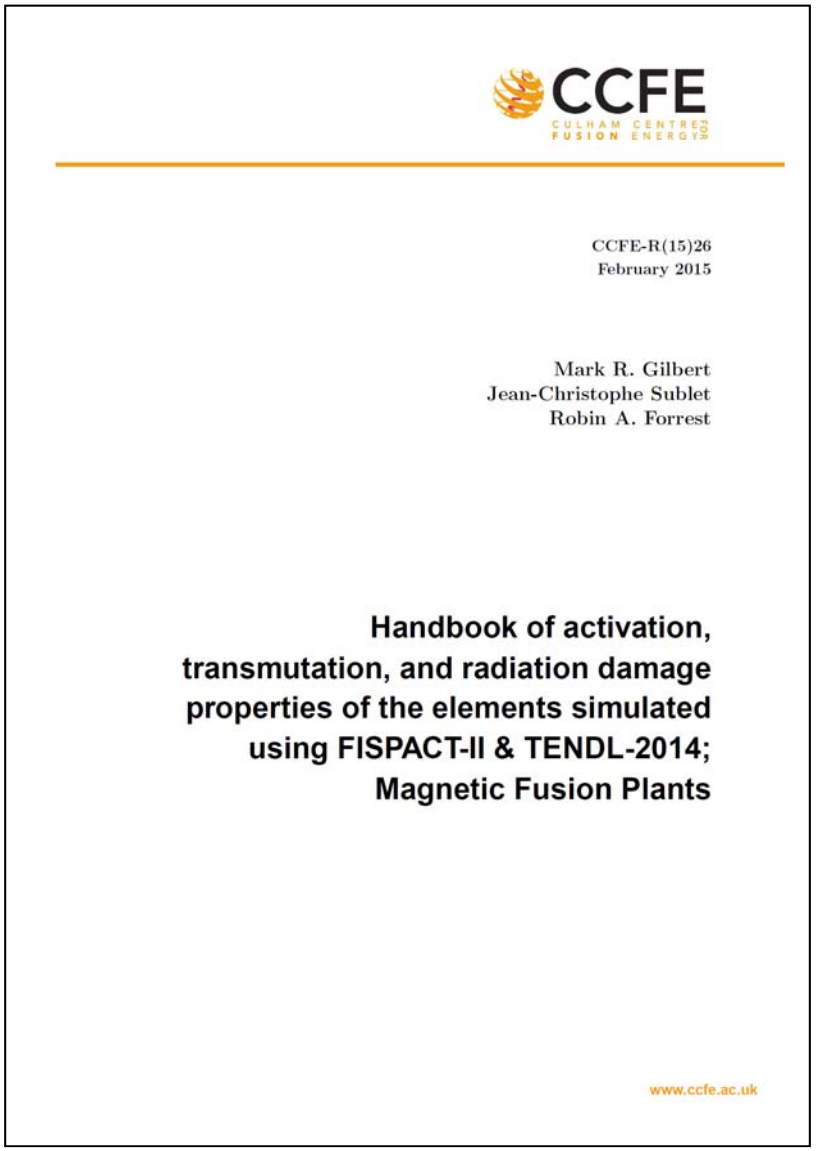
Chapter 4. Applications: Scoping studies

Scoping of material response

- FISPACT-II can be easily incorporated into an automated infrastructure for scoping inventory simulations
- A reference document of typical responses of the elements to neutron irradiation is a useful tool during material selection exercises for reactor design, etc.
- Automated processing is vital if such a document is to be produced regularly (varying libraries, conditions, etc.)

Materials inventory handbooks


CCFE
CULHAM CENTRE FOR FUSION ENERGY

CCFE-R(15)26
February 2015

Mark R. Gilbert
Jean-Christophe Sublet
Robin A. Forrest

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

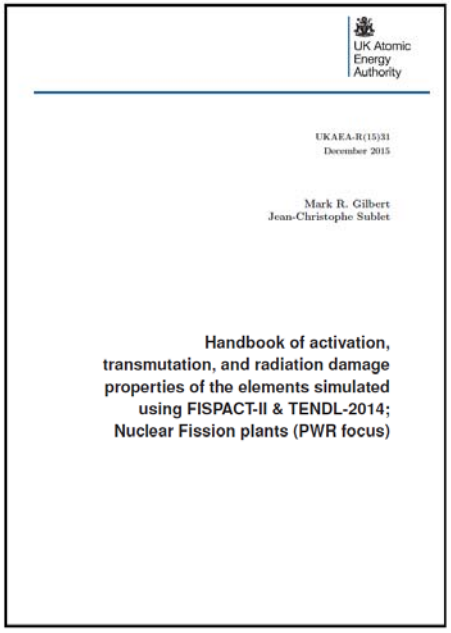
Handbook format

1. Tabulated activation response
   - % contributions of important radionuclides to various radiological quantities as a function of cooling time
2. Graphs of activation response
   - Decay evolution of total activity, heat and γ-dose under different spectra & compared to Fe + indicative 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. Transmutation response
   - Time evolution under irradiation of initially-pure elemental composition
   - Nuclide concentration map at 2 full power years (fpy)

Handbook format

5. 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

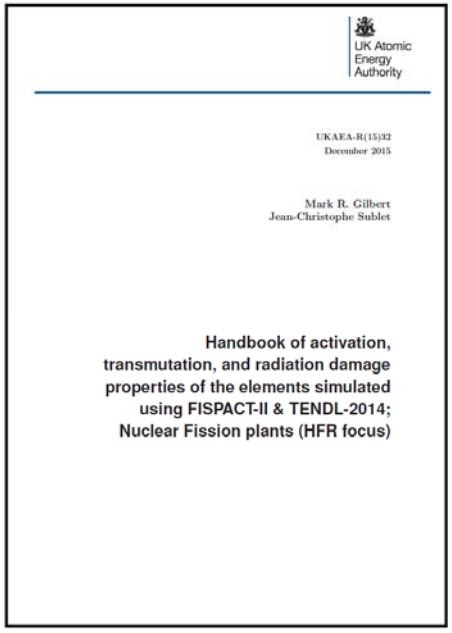
The automated system makes the production of additional handbooks straightforward…


UK Atomic Energy Authority

UKAEA-R(15)31
December 2015

Mark R. Gilbert
Jean-Christophe Sublet

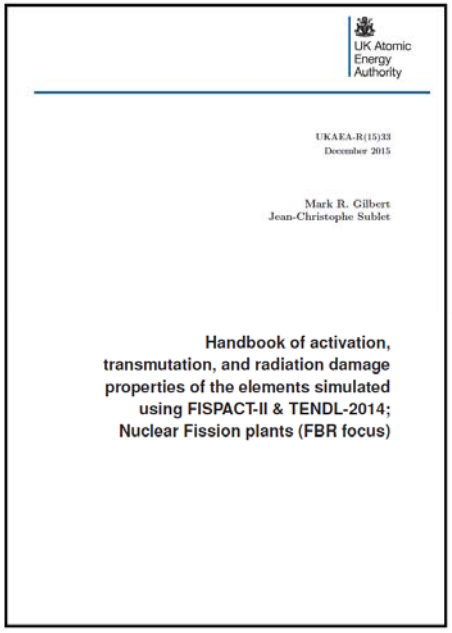
Handbook of activation, transmutation, and radiation damage properties of the elements simulated using FISPACT-II & TENDL-2014; Nuclear Fission plants (PWR focus)


UK Atomic Energy Authority

UKAEA-R(15)32
December 2015

Mark R. Gilbert
Jean-Christophe Sublet

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

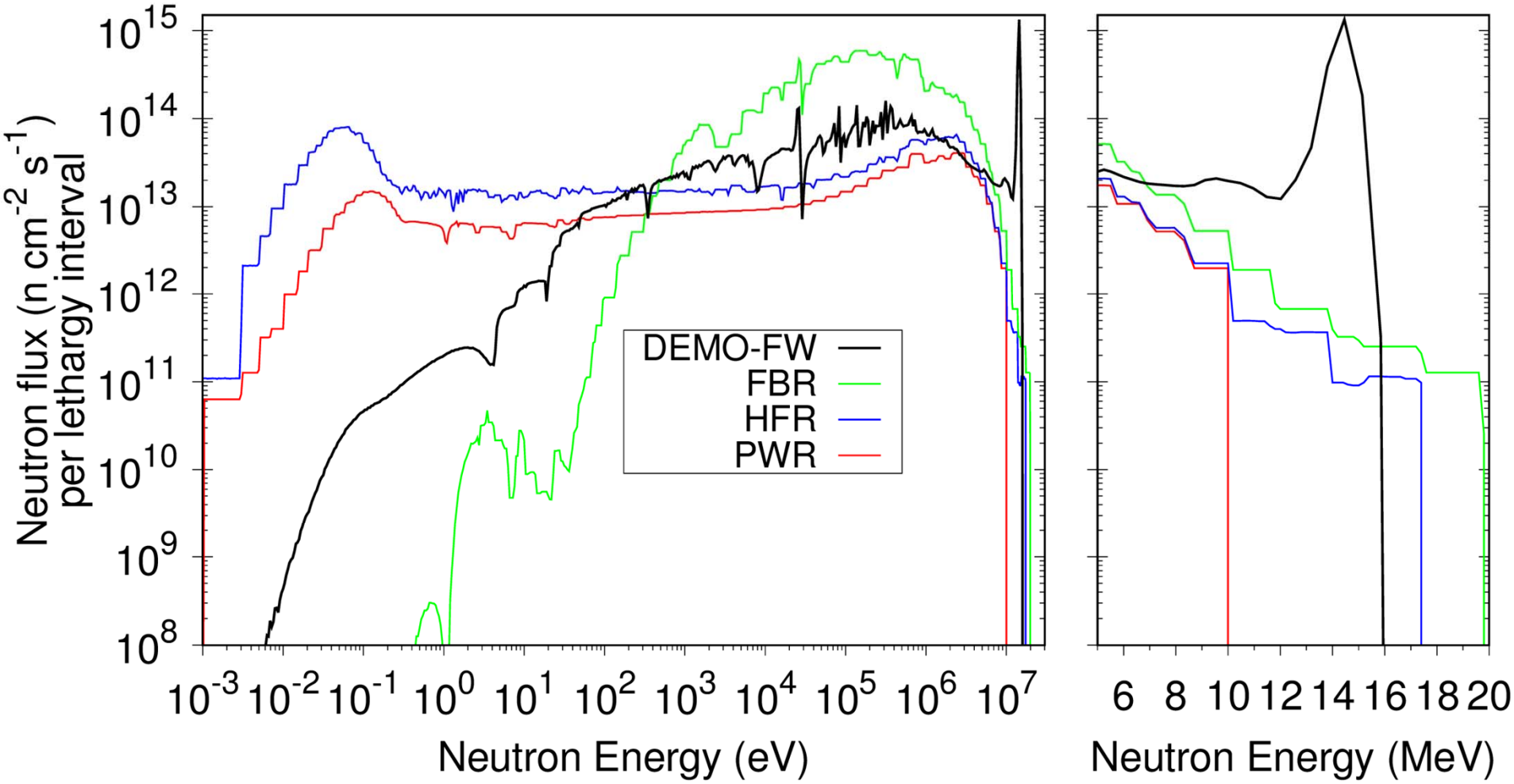
Mark R. Gilbert
Jean-Christophe Sublet

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

Three other handbooks for typical fission environments: PWR, FBR, HFR

UK Atomic Energy Authority

Handbooks Neutron spectra



- All 4 TENDL reports have also been reproduced with other international nuclear libraries (JEFF, JENDL, ENDF/B)
- Almost 250,000 separate FISPACT-II calculations in total

(1) Activation tables

- Activation response after 2 fpy (full power years)
- Table for 6 radiological quantities, with nuclide % contributions at different cooling times
- Using inventory break-down in FISPACT-II output (also available from dominant nuclide lists) **Aluminium DEMO-FW**

Act	0s	5.3m	3.7d	1y	100y	10^4y
Bq kg^{-1}	4.59E+14	3.86E+14	4.18E+12	1.16E+11	4.90E+08	4.51E+07
Na24	56.5	66.9	97.1			
Mg27	39.9	32.3				
Al28	3.4	0.8				
H3			2.9	99.7	90.7	
Al26					9.3	100.0

Heat	0s	5.3m	3.7d	1y	100y	10^4y
kW kg^{-1}	2.49E-01	2.27E-01	3.04E-03	2.30E-07	2.28E-08	2.22E-08
Na24	78.0	85.3	100.0			
Mg27	18.8	14.0				
Al28	3.0	0.7				
H3				46.0	1.8	
Na22				44.3		
Al26				9.7	98.2	100.0

Dose	0s	5.3m	3.7d	1y	100y	10^4y
Sv h^{-1}	3.89E+05	3.67E+05	5.29E+03	1.80E-01	3.39E-02	3.36E-02
Na24	86.8	91.7	100.0			
Mg27	10.9	7.9				
Al28	2.2	0.5				
Na22				81.2		
Al26				18.8	100.0	100.0

Ing	0s	5.3m	3.7d	1y	100y	10^4y
Sv kg^{-1}	1.15E+05	1.13E+05	1.75E+03	5.88E+00	1.78E-01	1.58E-01
Na24	96.7	98.0	99.6			
Mg27	2.9	2.0				
H3			0.3	82.8	10.5	
Na22			0.1	14.5		
Al26				2.7	89.5	100.0

Inh	0s	5.3m	3.7d	1y	100y	10^4y
Sv kg^{-1}	7.20E+04	7.09E+04	1.13E+03	3.14E+01	1.03E+00	9.01E-01
Na24	97.2	98.3	97.1			
Mg27	2.3	1.6				
H3			2.8	96.0	11.3	
Al26			0.1	2.9	88.7	100.0
Na22				1.1		

Clear	0s	5.3m	3.7d	1y	100y	10^4y
	4.74E+11	3.89E+11	4.07E+09	3.95E+06	1.27E+05	1.22E+05
Na24	54.8	66.4	99.9			
Mg27	38.7	32.1				
Al28	6.4	1.5				
Na22			0.1	67.5		
H3				29.3	3.5	
Al26				3.1	96.5	100.0

(1) Activation tables

- For some materials such tables can be very complex

Total activity and decay heat tables for zirconium (DEMO FW):

Act	0s	5.3m	3.7d	1y	100y	10^4y
Bq kg^{-1}	7.43E+14	4.79E+14	2.37E+14	2.07E+12	5.60E+08	2.93E+08
Zr90m	32.3					
Y89m	25.2	37.2	34.6			
Zr89	24.1	37.3	34.7			
Zr95	4.3	6.7	12.9	29.7		
Nb95	4.3	6.6	13.4	64.1		
Zr89m	3.3	2.2				
Y90	1.6	2.5	2.0	0.1	22.9	
Nb97	1.0	1.5	0.1			
Zr97	1.0	1.5	0.1			
Nb97m	0.9	1.4	0.1			
Y91	0.4	0.6	1.2	1.9		
Y88	0.1	0.2	0.3	3.3		
Zr93					26.6	50.6
Nb93m					25.4	49.1
Sr90				0.1	22.9	
H3				0.1	2.0	

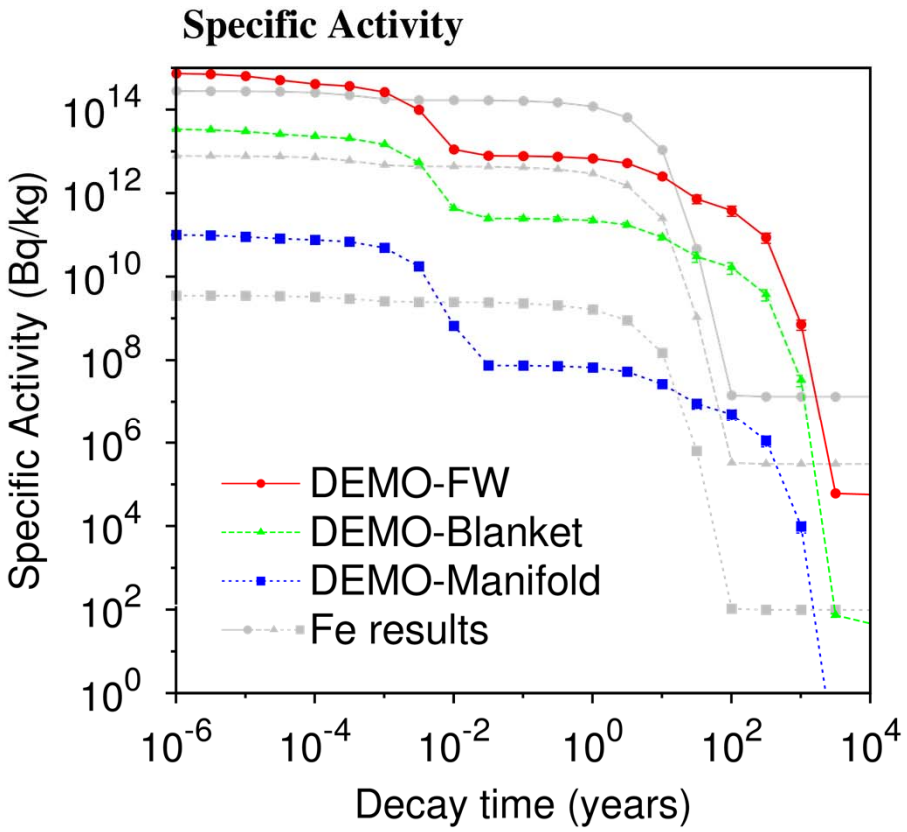
Heat	0s	5.3m	3.7d	1y	100y	10^4y
kW kg^{-1}	1.45E-01	5.28E-02	2.64E-02	2.91E-04	2.43E-08	1.38E-09
Zr90m	61.6					
Y89m	18.8	49.2	45.4			
Zr89	6.9	18.8	17.3			
Zr95	3.0	8.3	15.9	28.9		
Nb95	2.9	7.8	15.6	59.1		
Zr89m	1.8	2.1				
Y90	1.2	3.3	2.6	0.1	79.2	
Nb97	0.9	2.5	0.1			
Zr97	0.7	1.9	0.1			
Nb97m	0.6	1.5	0.1			
Y92	0.4	1.2				
Y88	0.2	0.6	1.2	10.3		
Y91	0.2	0.6	1.1	1.3		
Sr90					14.8	
Nb93m					2.9	51.6
Zr93					1.9	33.0
Nb94					1.2	15.4

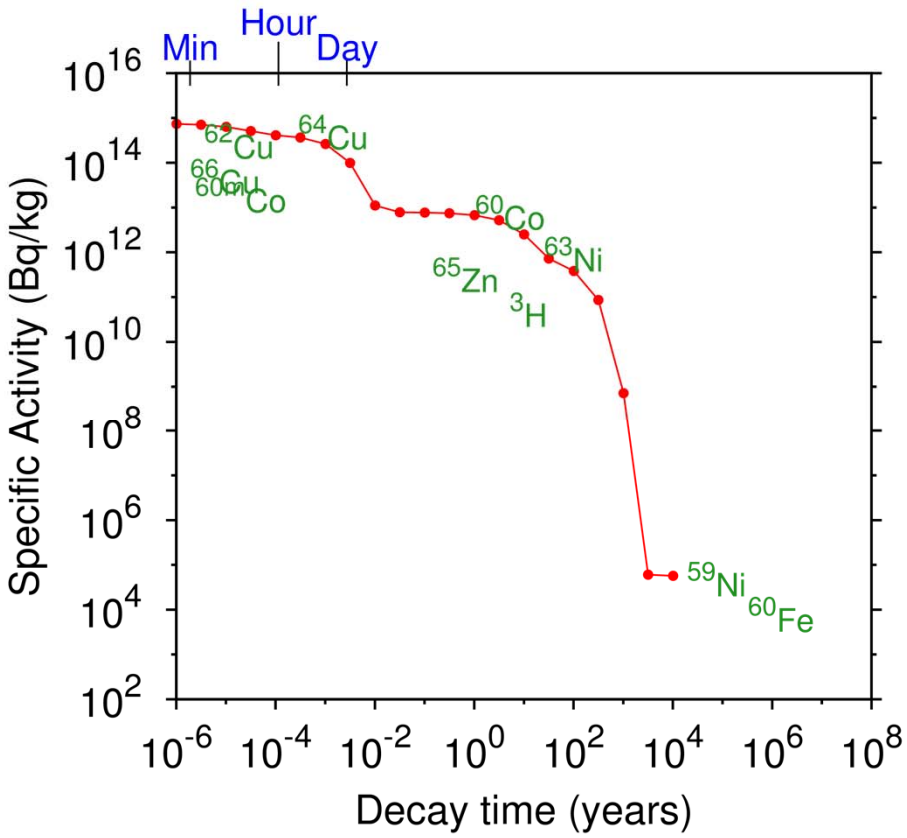
(2) Activation graphs

- Decay curves following 2 fpy irradiations under 3 spectra
- Specific (total) activity, γ-dose rate and decay heat output
  - Iron curves included for (standard) comparison & 2nd plot shows indicative nuclide contributions for primary spectrum
  - Plotted directly from .gra FISPACT-II files (and using provided GNUPLOT plotting templates)
    - "GRAPH 5 2 1 1 2 3 4 5"

(2) Activation graphs

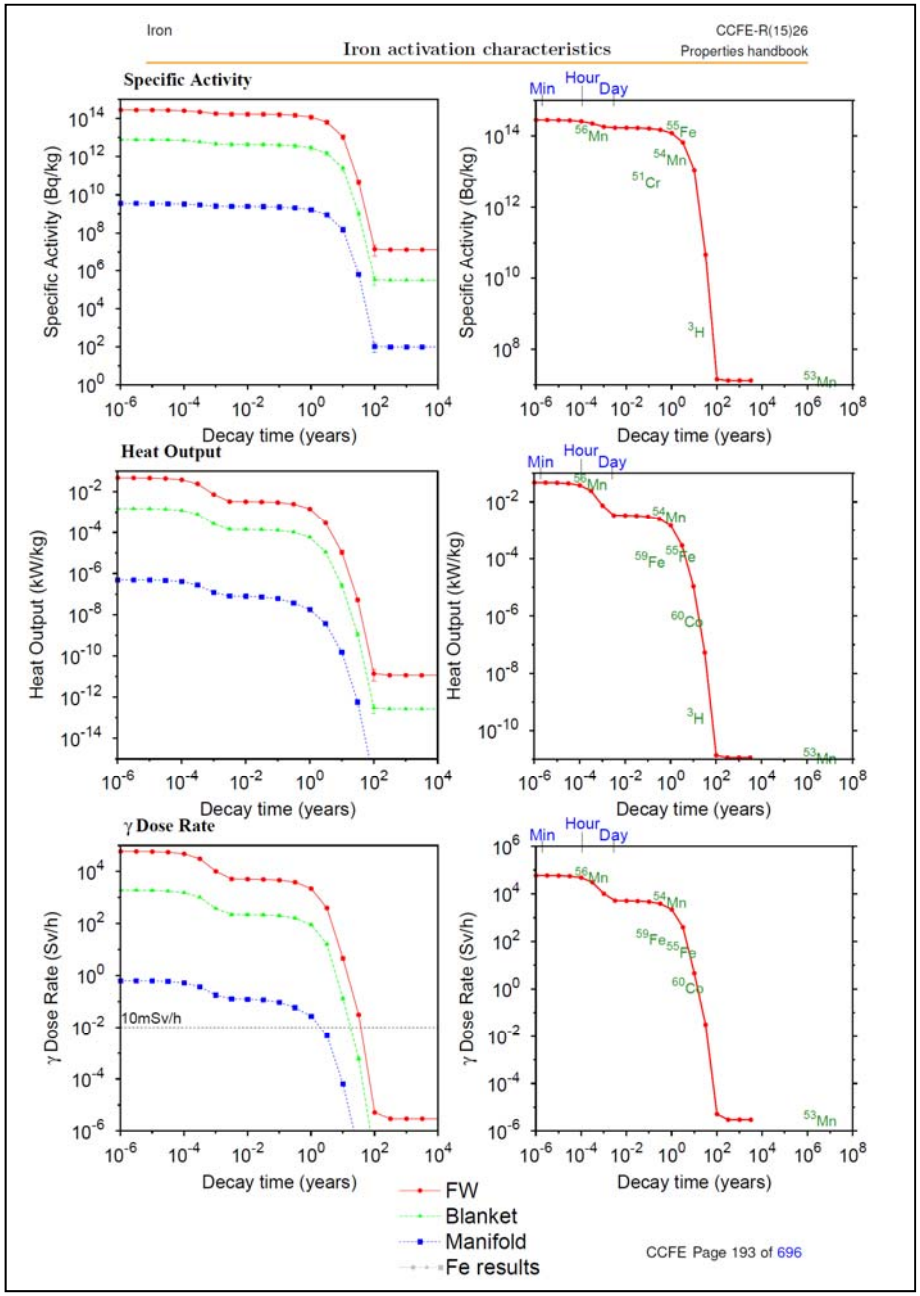
- E.g. copper total activity





- Right-hand plot shows the important nuclides, when they are likely to be important, & their maximum contribution

(2) Activation graphs



One page per element

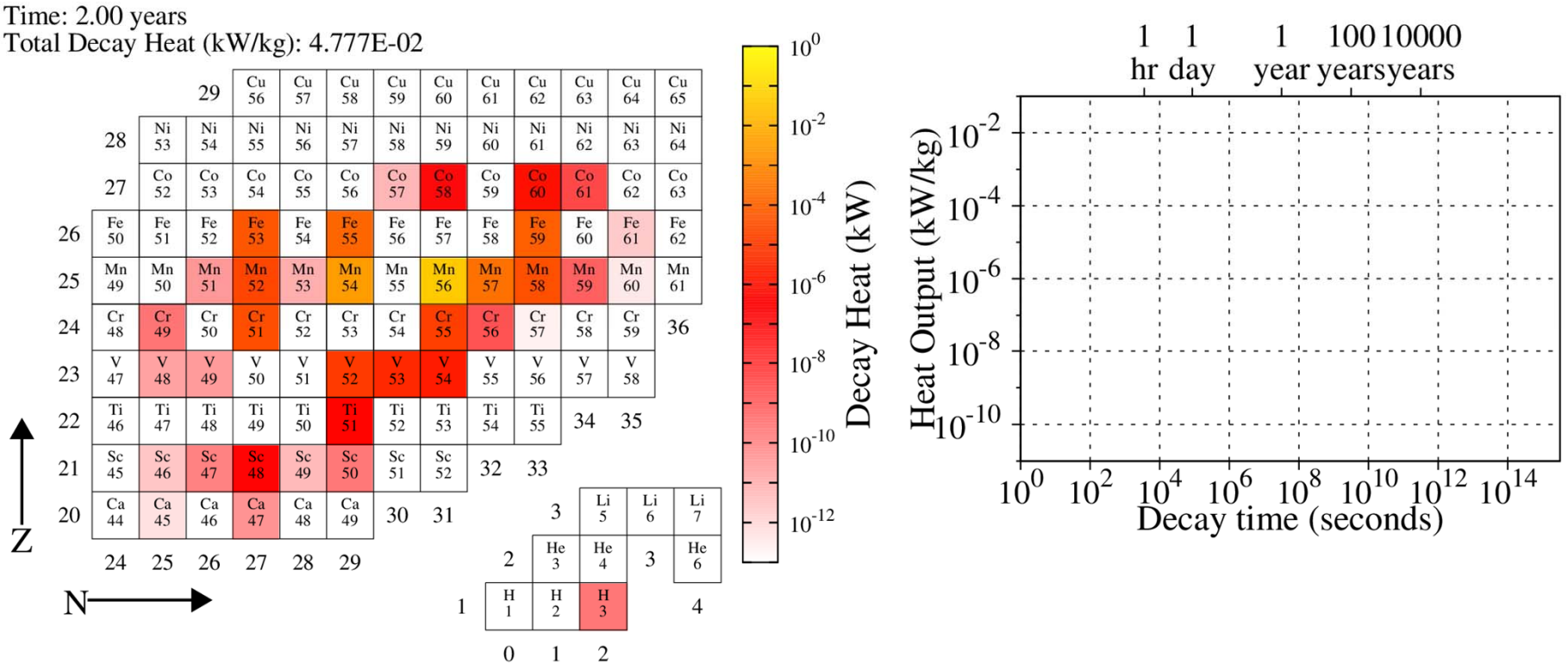
E.g. Fe:

- ^{56}Mn important at short timescales (< 1 day)
- ^{53}Mn dominates at very long cooling times

(2) Activation graphs

*Gilbert et al. *Nucl. Sci. Eng.* ***177*** *(2014) 291-306*

- Decay heat output from Fe:



- (right) Animated nuclide chart* tracks contributions to decay heat
- (left) Total heat output plot from .gra file can also be animated
  - Nuclides appear at ($T_{1/2}$, heat at shutdown) coordinates

(2) Activation graphs

*Gilbert et al. *Nucl. Sci. Eng.* ***177*** *(2014) 291-306*

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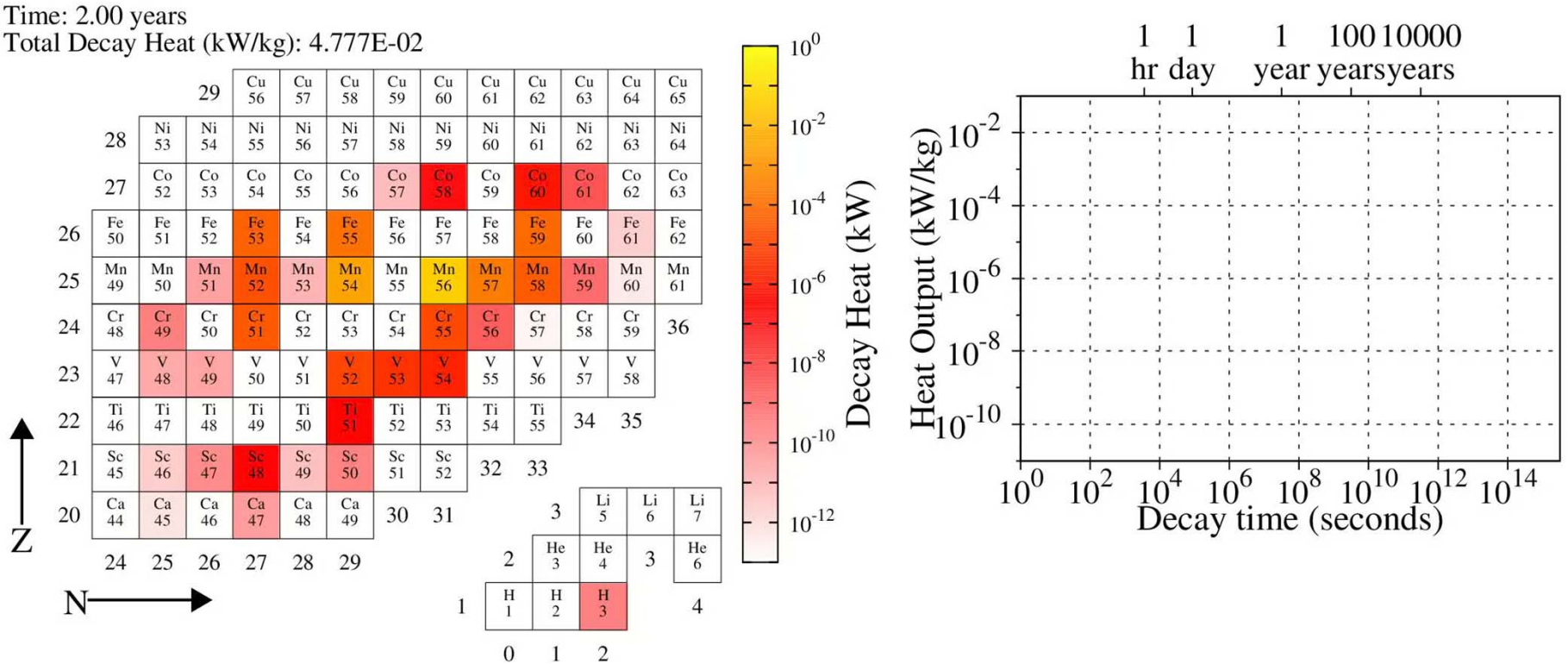

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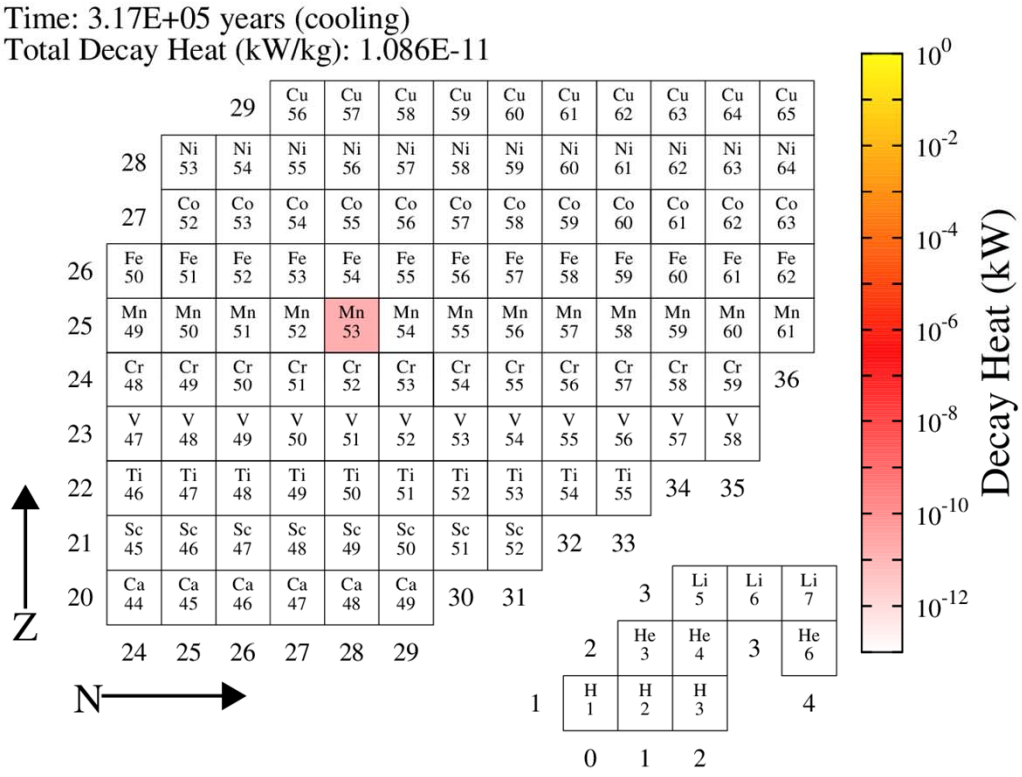

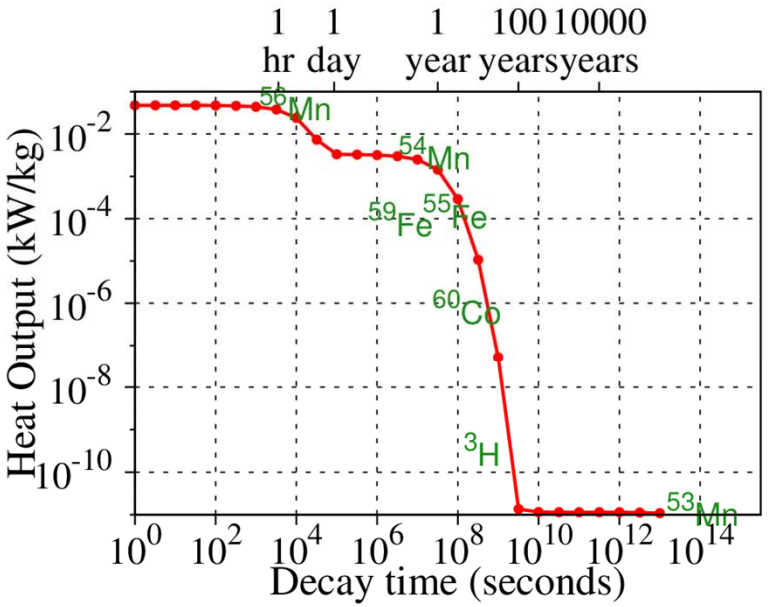

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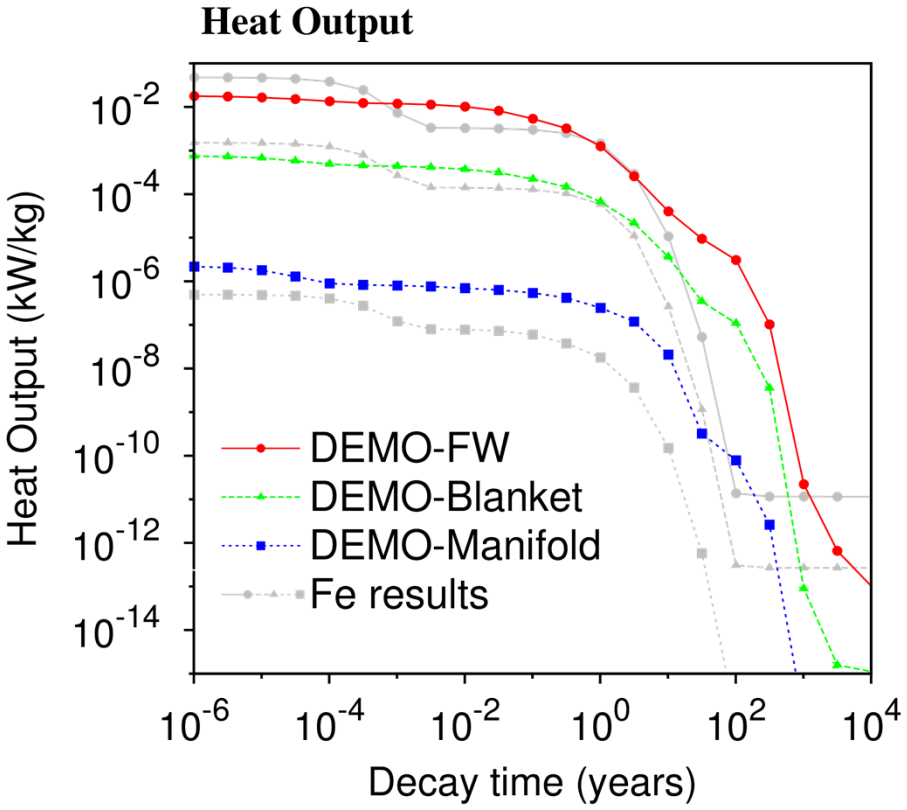
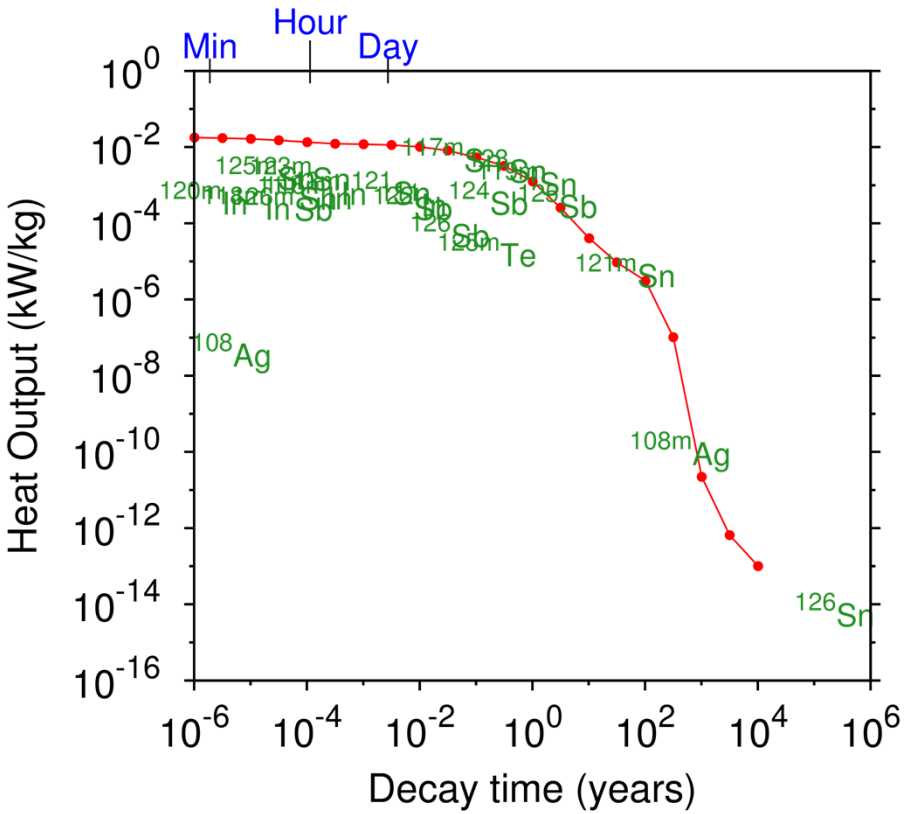
- (left) Total heat output plot from .gra file can also be animated
  - Nuclides appear at ($T_{1/2}$, heat at shutdown) coordinates

(2) Activation graphs

- The nuclide curves can be very complex for some elements, with overlapping contributions from many nuclides

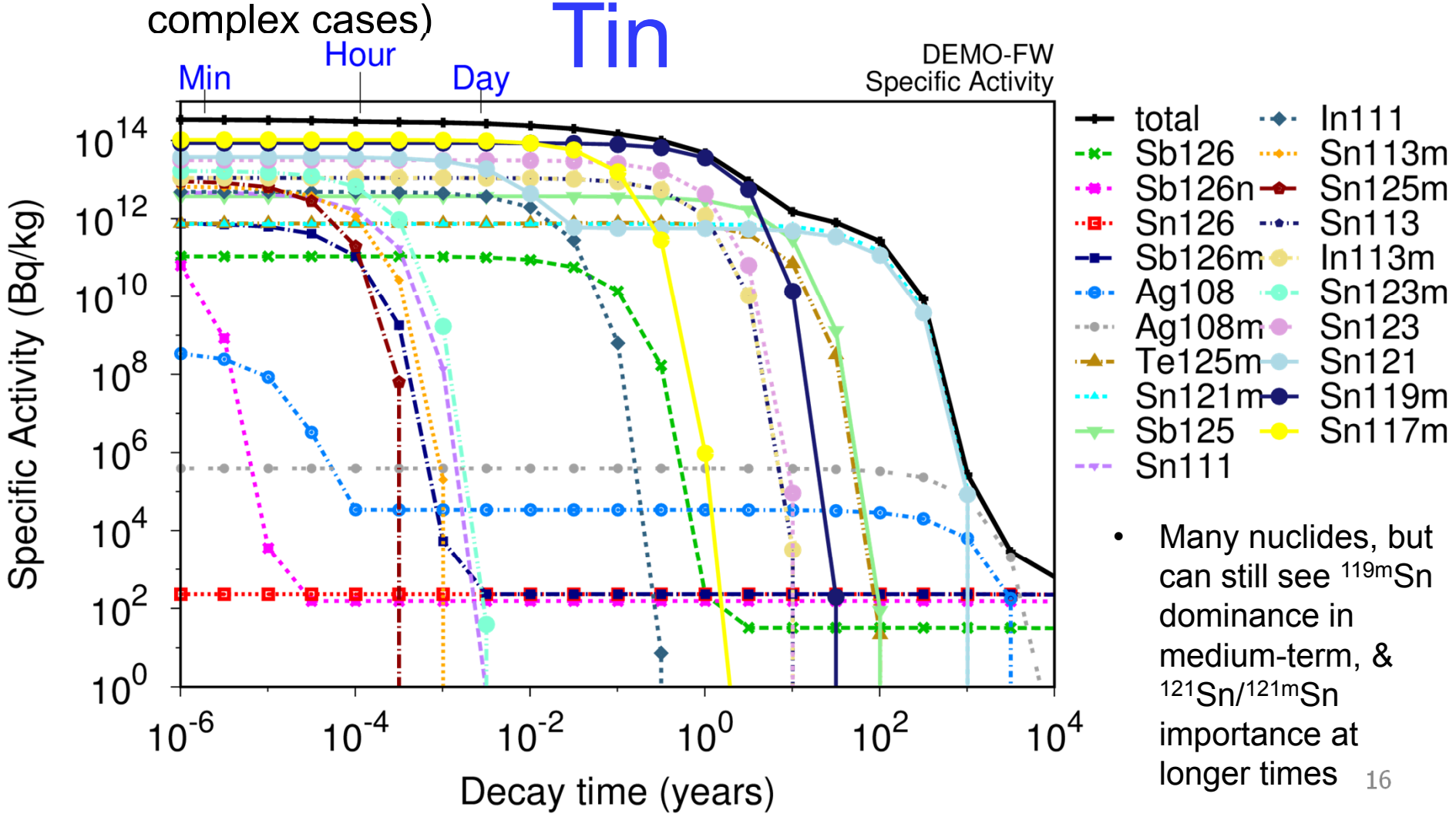
Tin (decay) heat output:





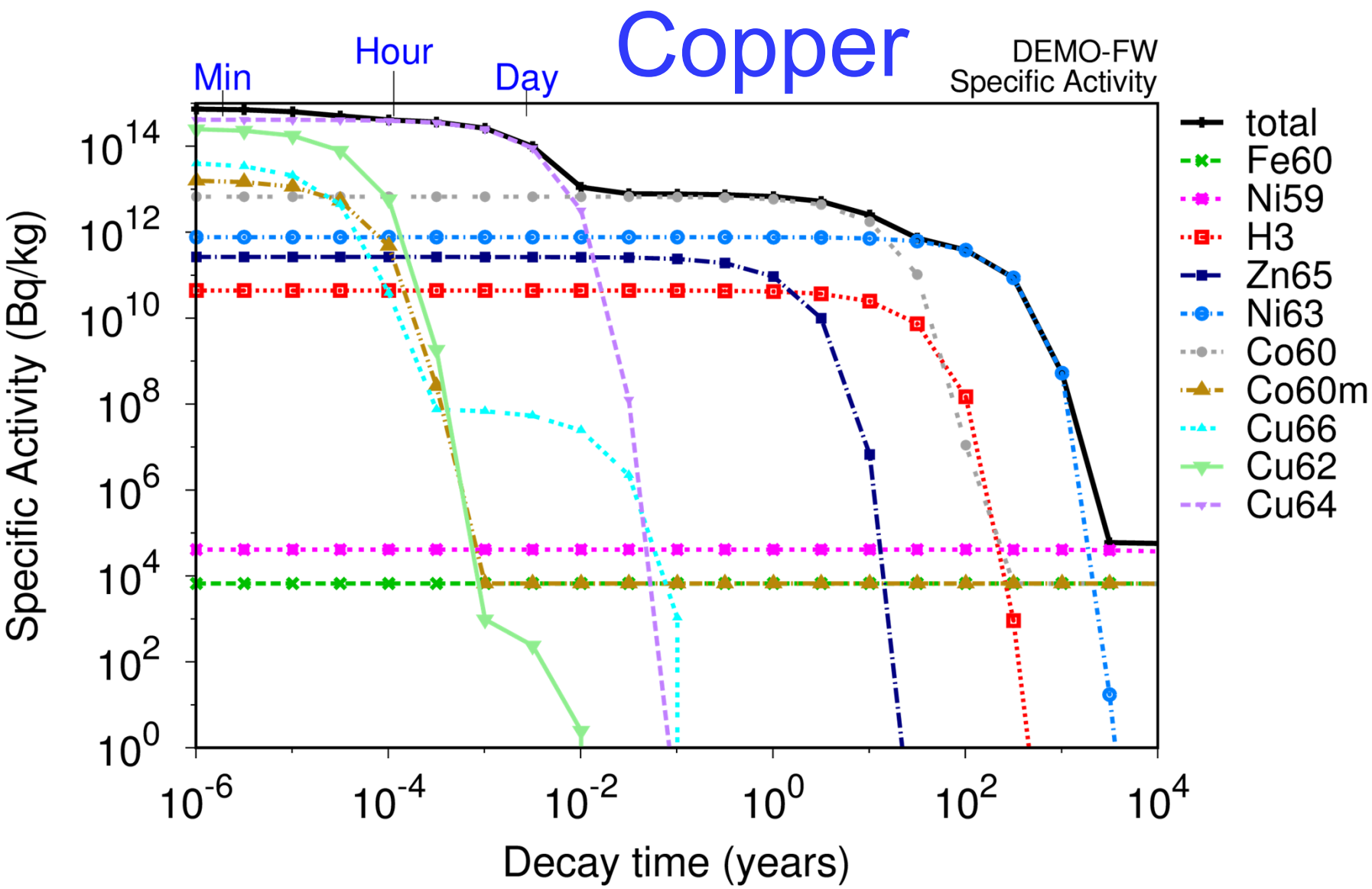
(2) Activation response – full nuclide contributions

- An alternative, newly developed automation using full inventory output
  - Plot of time evolution of dominant nuclide contributions
  - allowing nuclide contributions to be more easily viewed (even in complex cases)



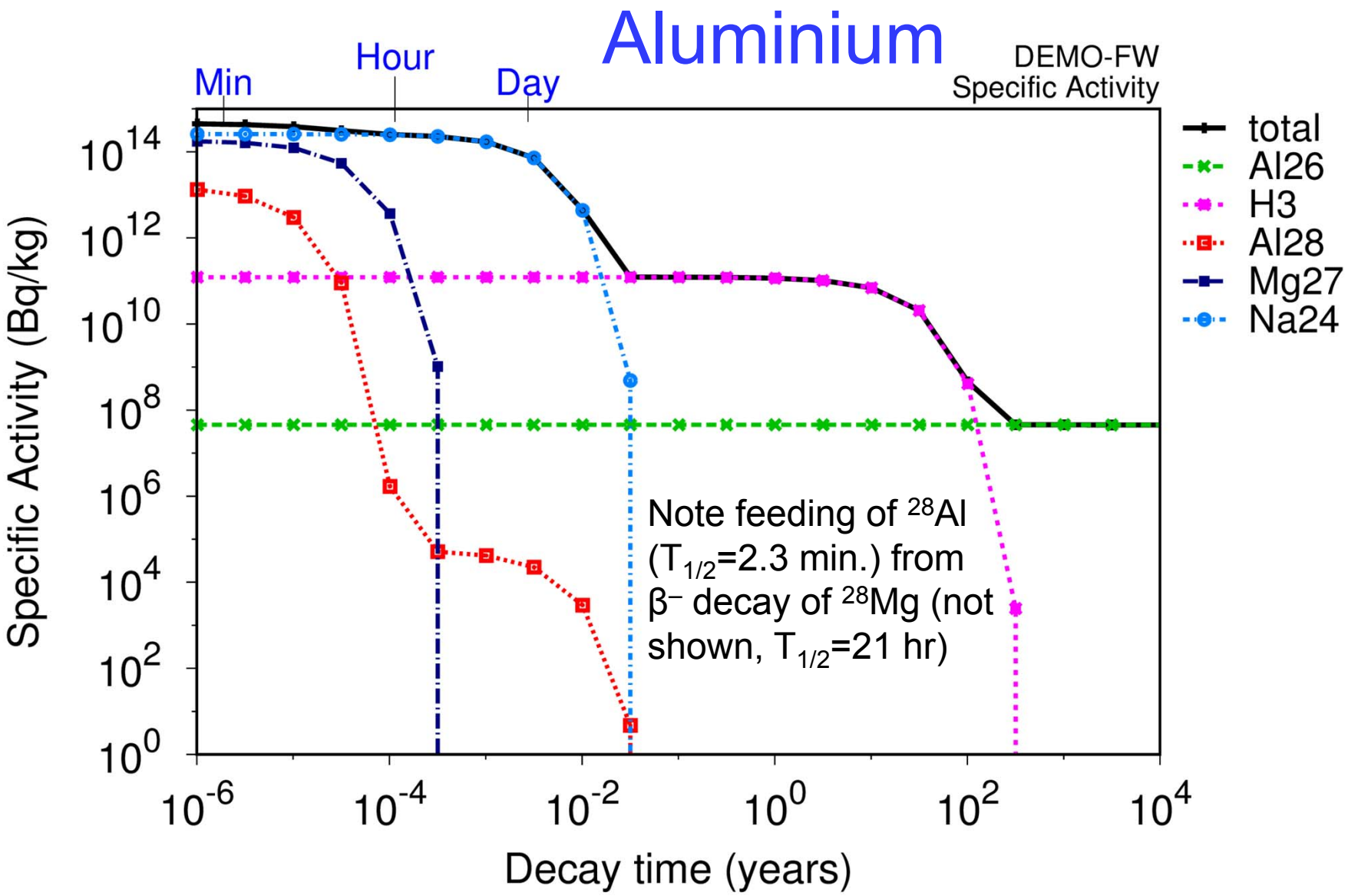
- Many nuclides, but can still see ^{119m}Sn dominance in medium-term, & ^{121}Sn/^{121m}Sn importance at longer times

(2) Activation response – full nuclide contributions



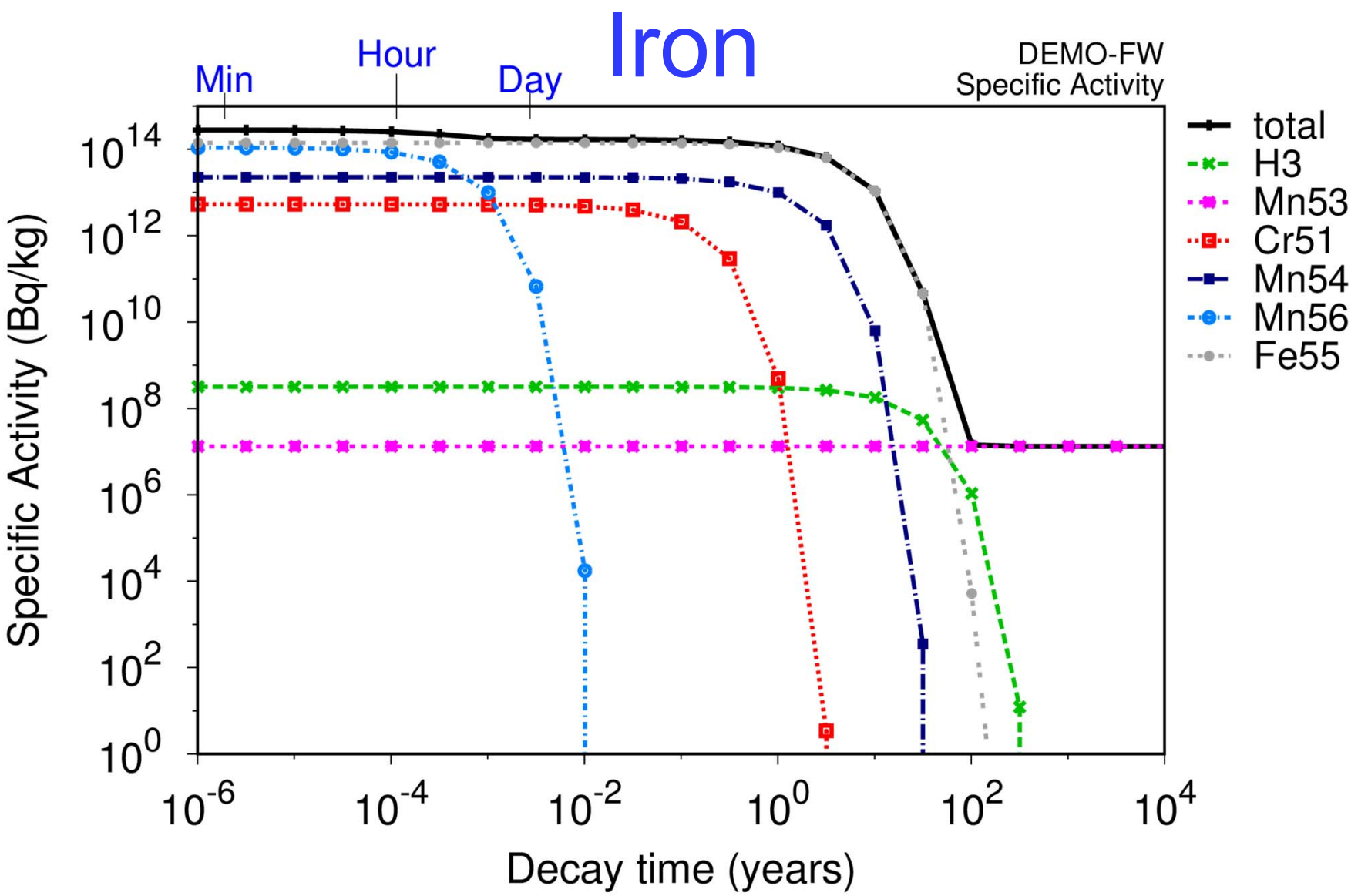
Short-term: ^{64}Cu; Medium term: ^{60}Co; Long-term: ^{59}Ni & ^{63}Ni

(2) Activation response – full nuclide contributions



Short-term: ^{24}Na; Medium term: ^{3}H; Long-term: ^{26}Al

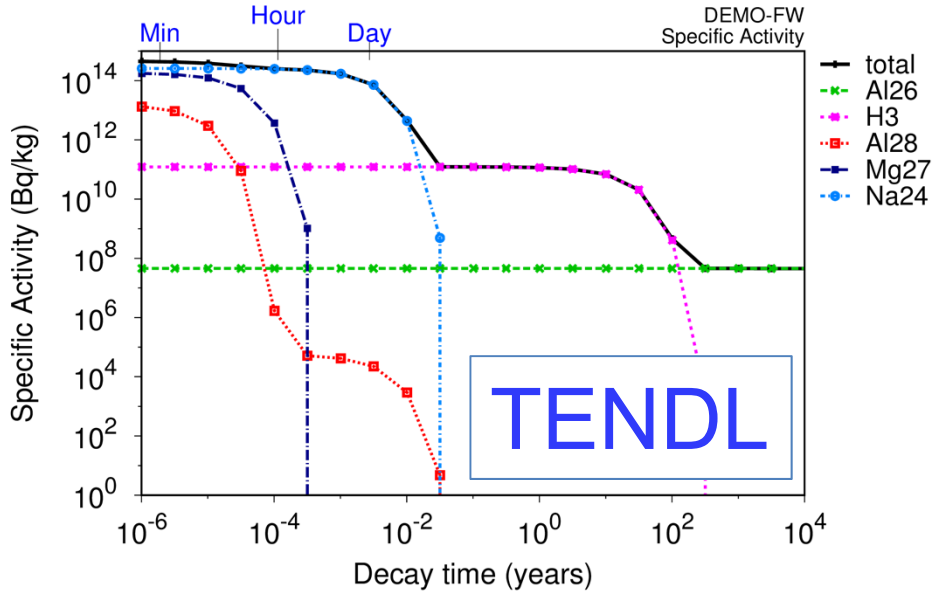
(2) Activation response – full nuclide contributions

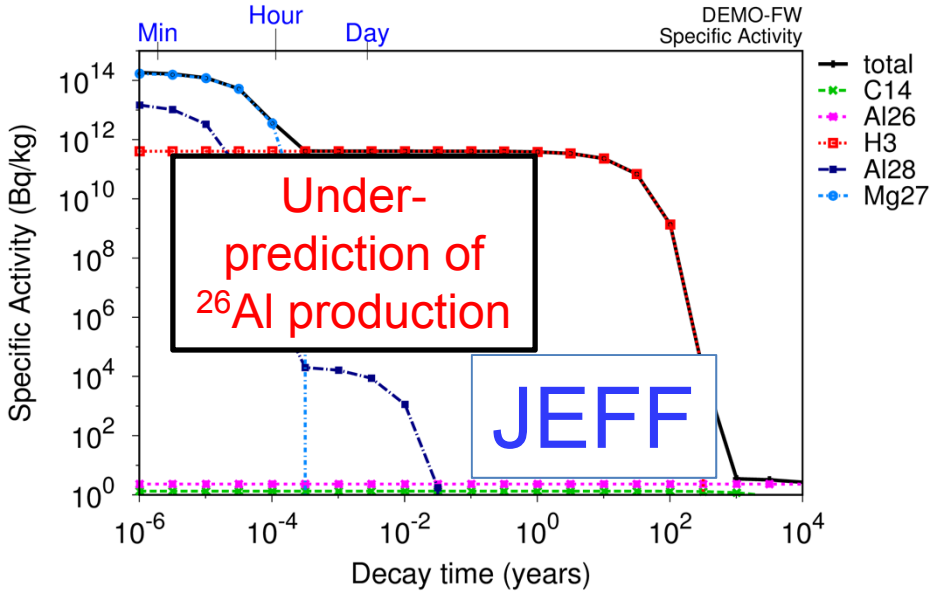


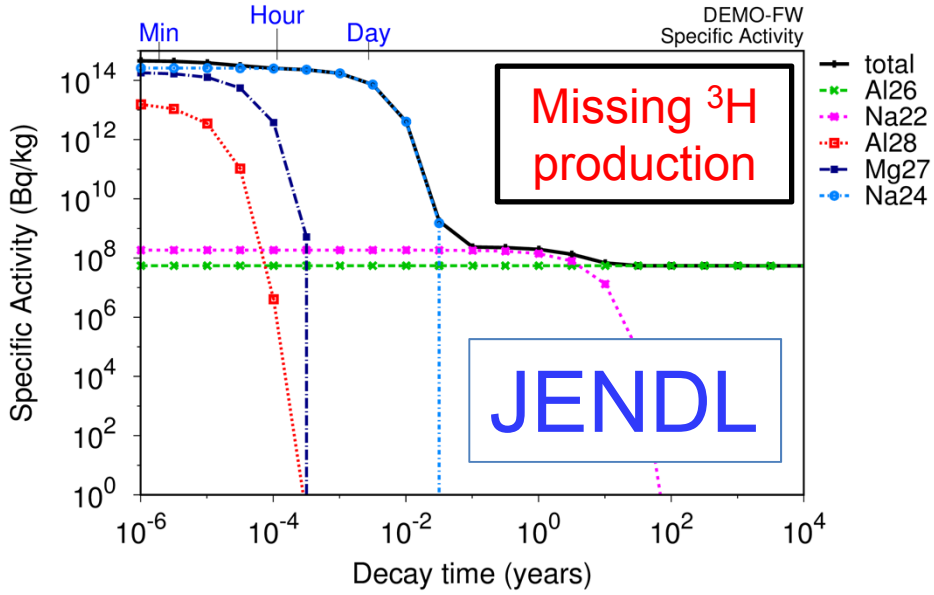
Short & Medium term: ^{55}Fe; Long-term: ^{53}Mn

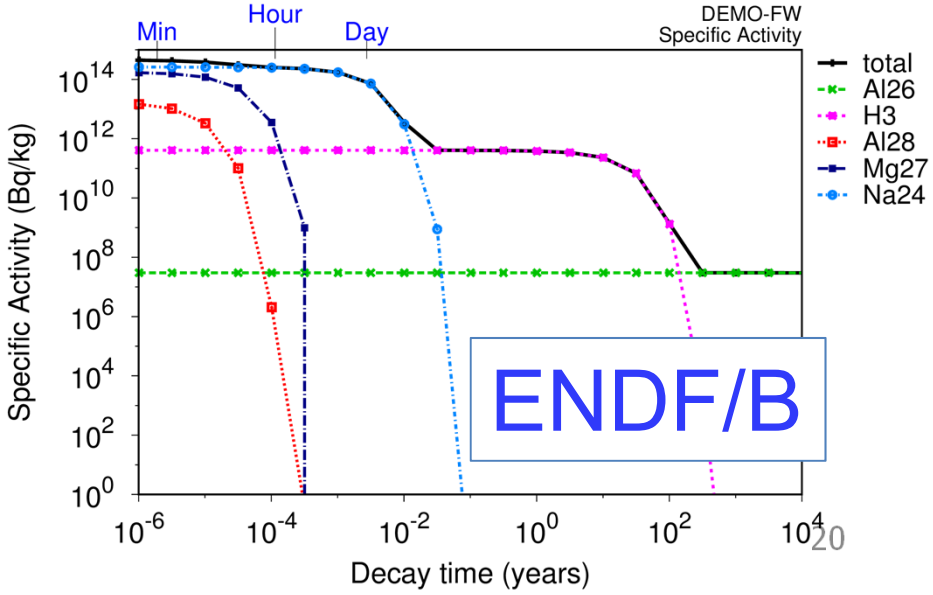
(2) Activation response: variation with library

Aluminium



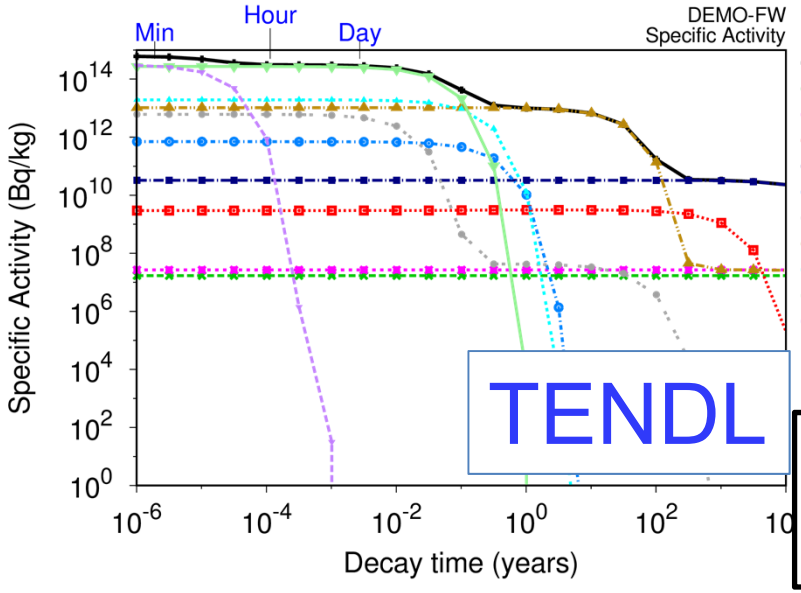


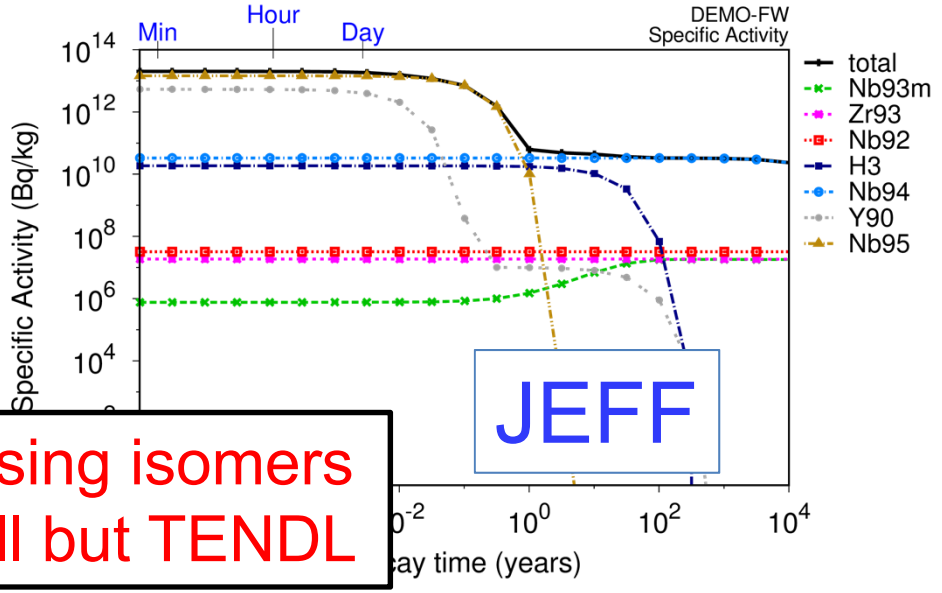




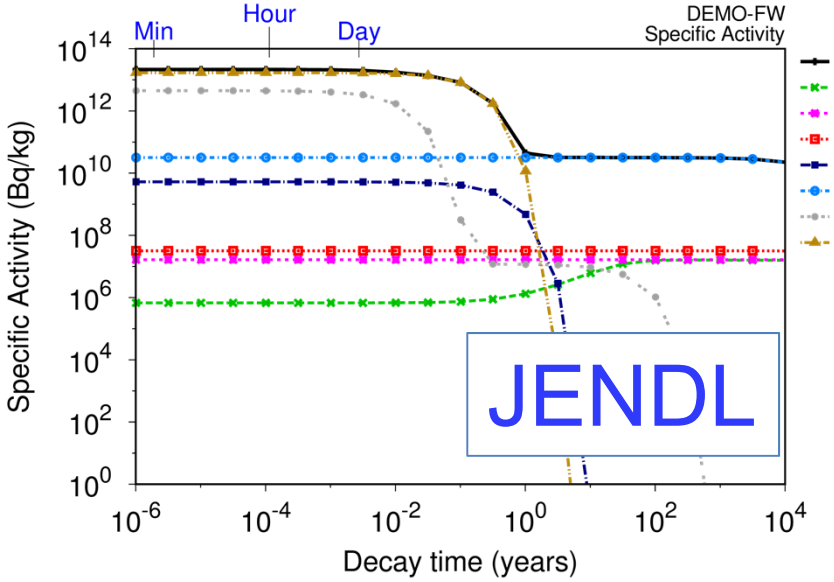
(2) Activation response: variation with library

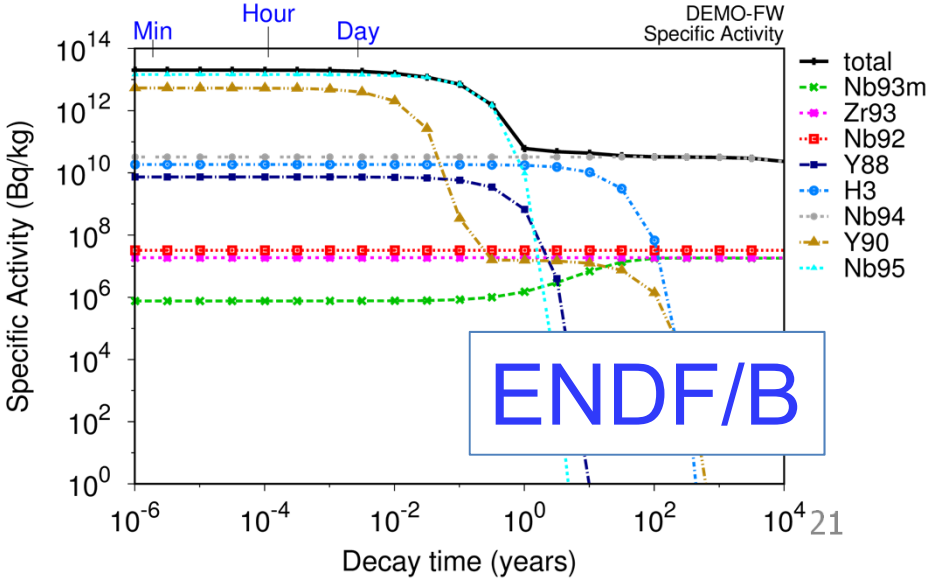
Niobium





Missing isomers in all but TENDL

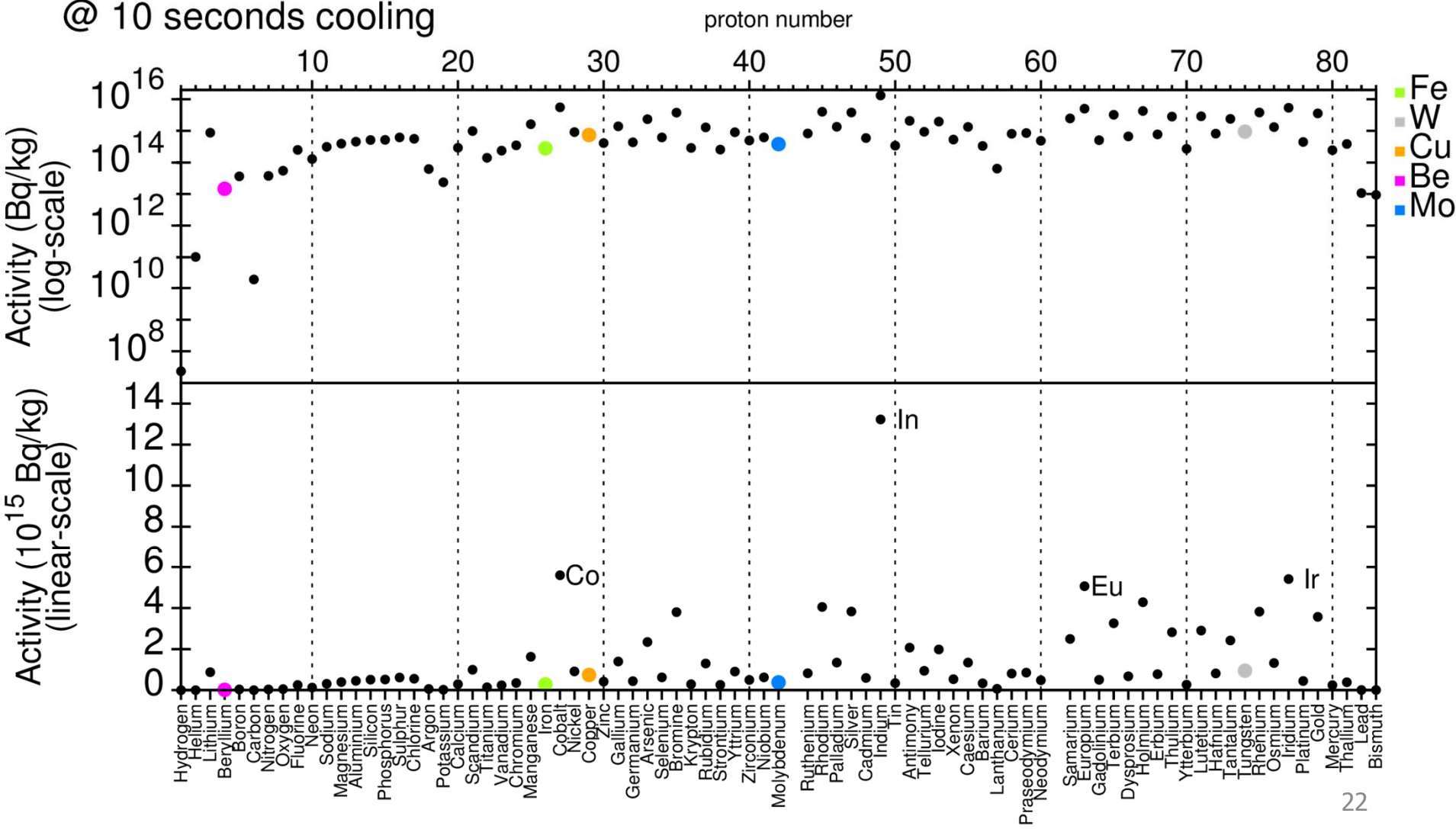




(2) Activation response – global results

- FISPACT-II output has fixed format, making it easy to extract equivalent results from many different files:

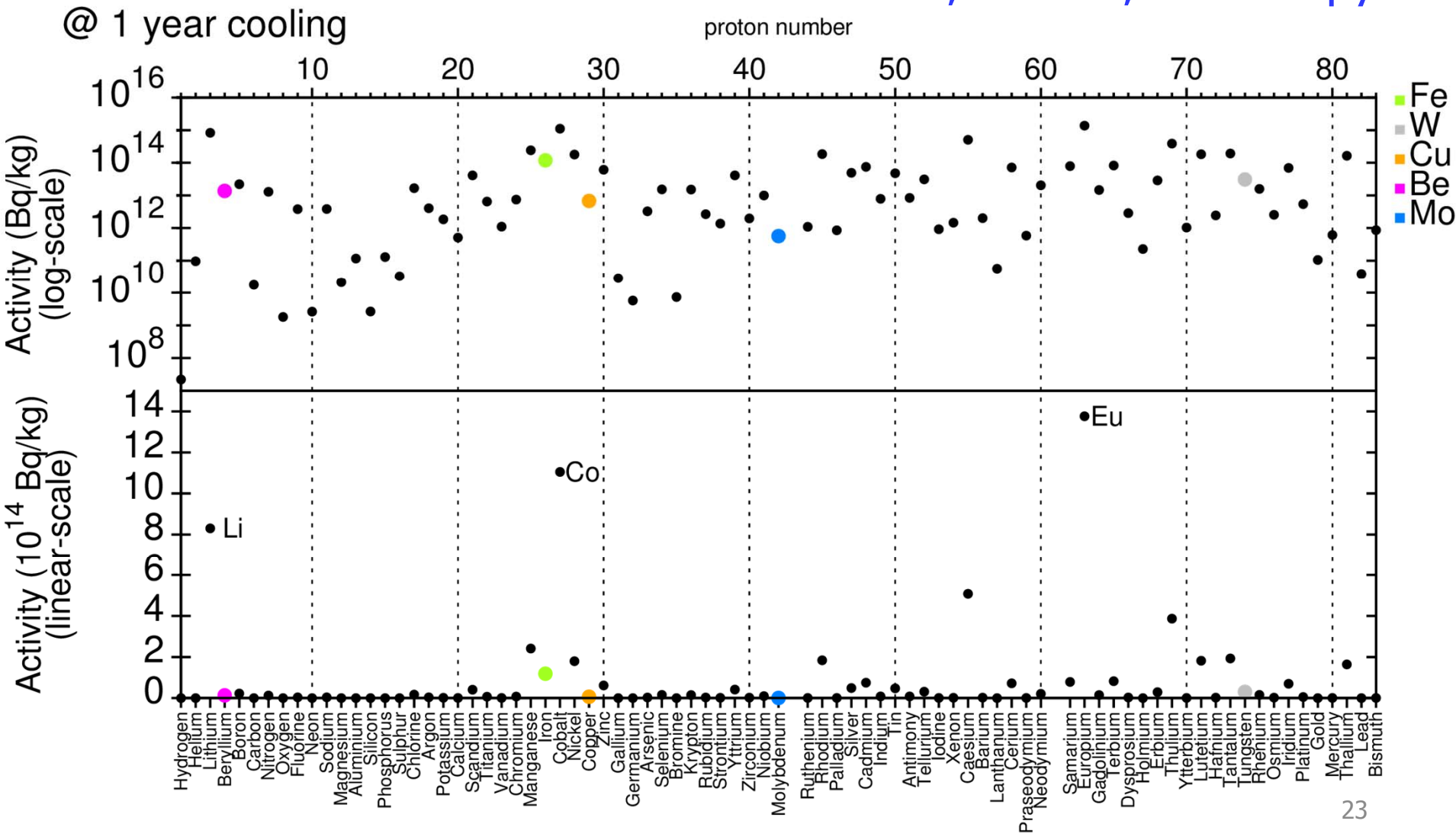
DEMO-FW, TENDL, after 2 fpy



(2) Activation response – global results

- … and as a function of time – showing order of magnitude fall-offs in activity at later cooling times

DEMO-FW, TENDL, after 2 fpy



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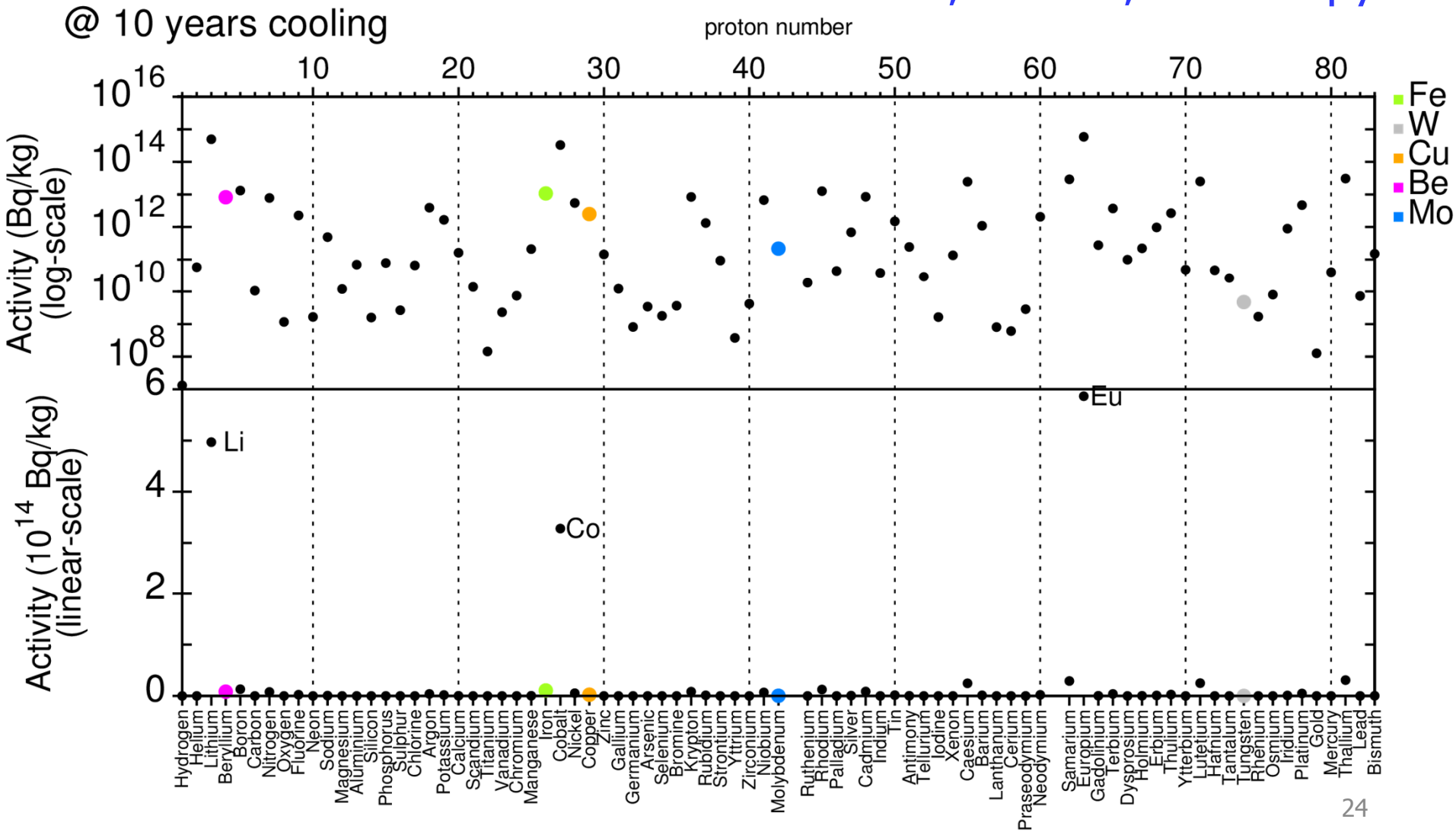

(2) Activation response – global results

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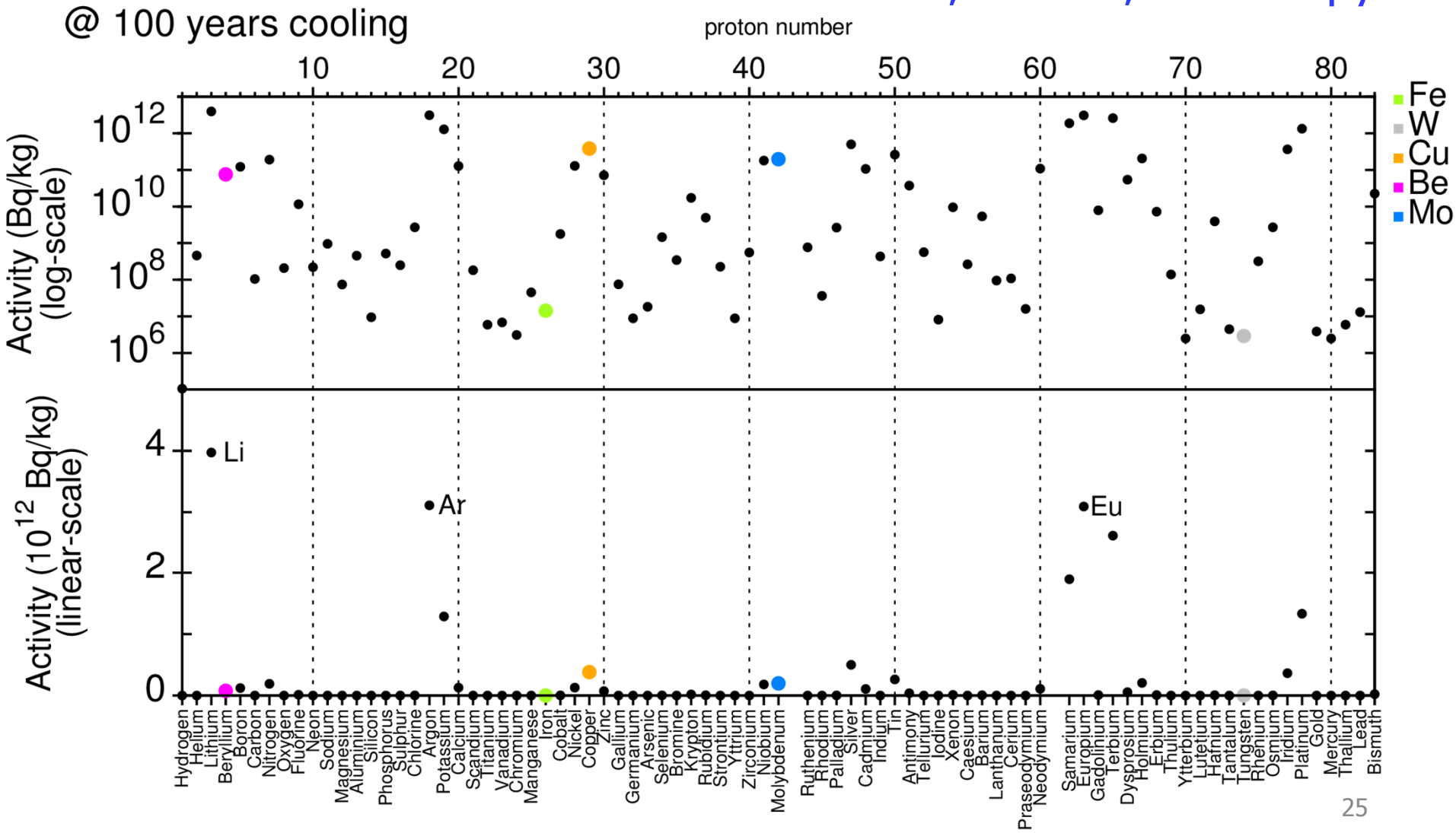
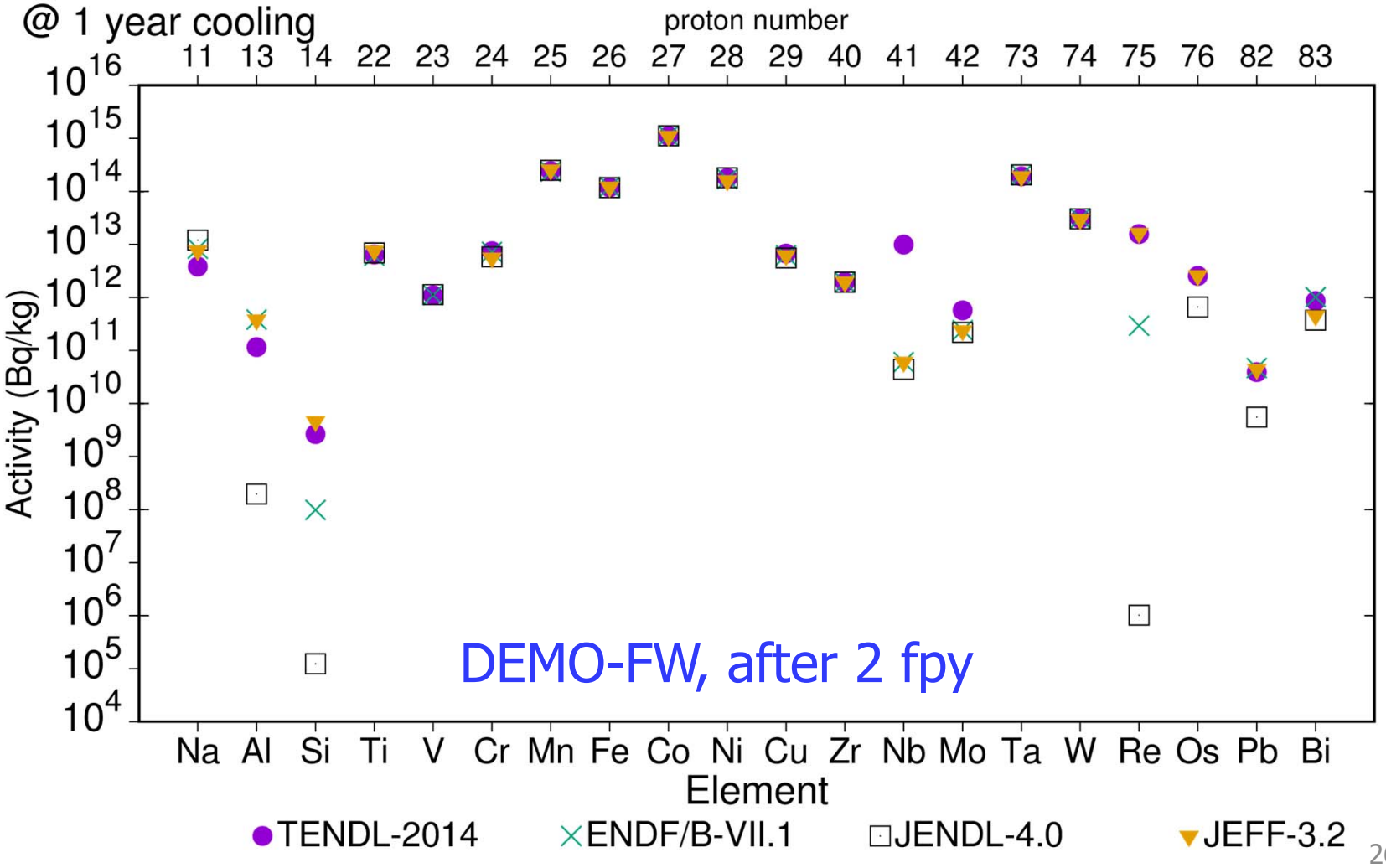


(2) Activation response – global results

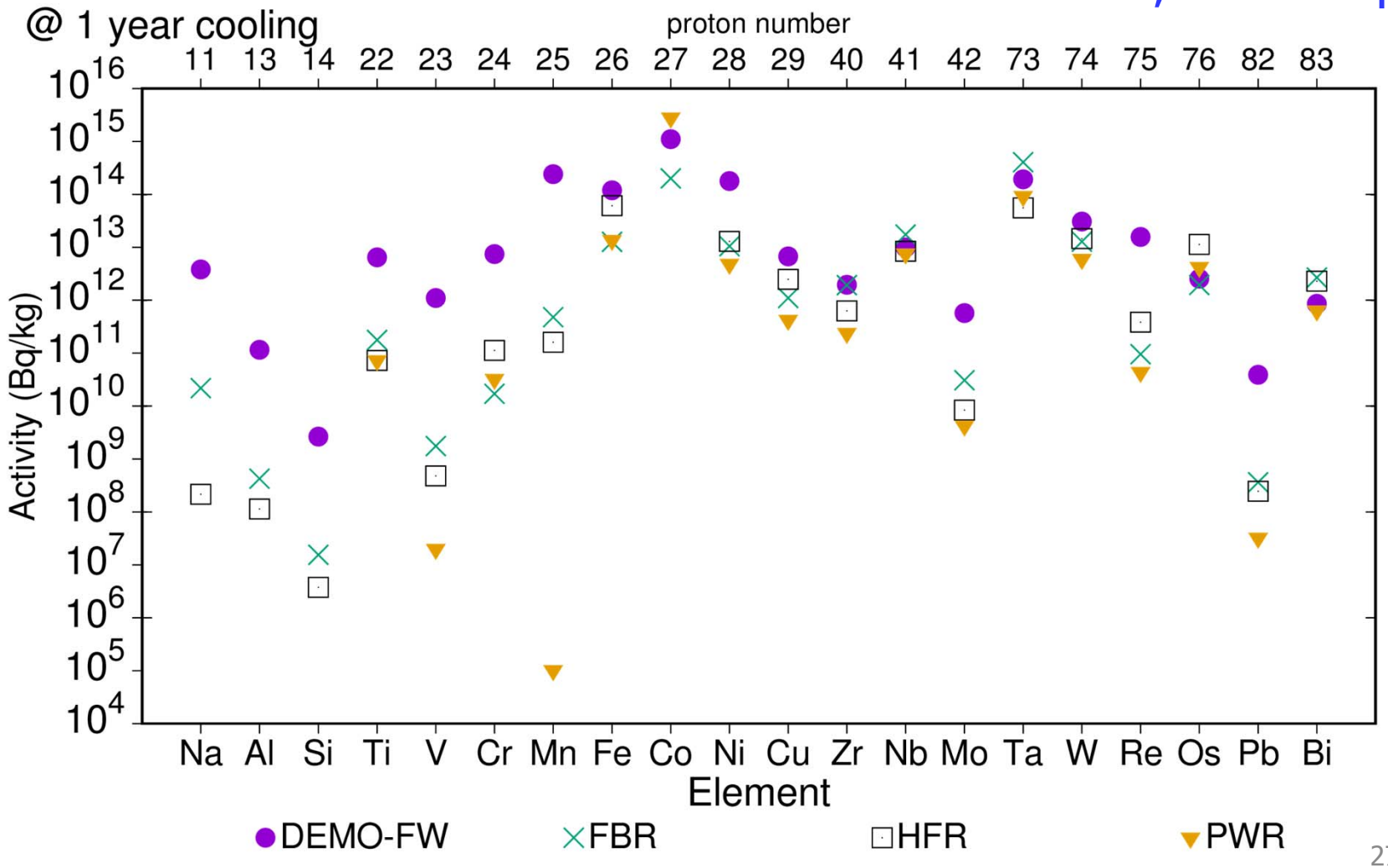
- For only selected (nuclear relevant) materials:
- Variation with library highlighting the need for careful choice of library, potentially varying with application



(2) Global results – fusion vs. fission

- For only selected (nuclear relevant) materials:
- Fusion generally produces more active materials

TENDL, after 2 fpy



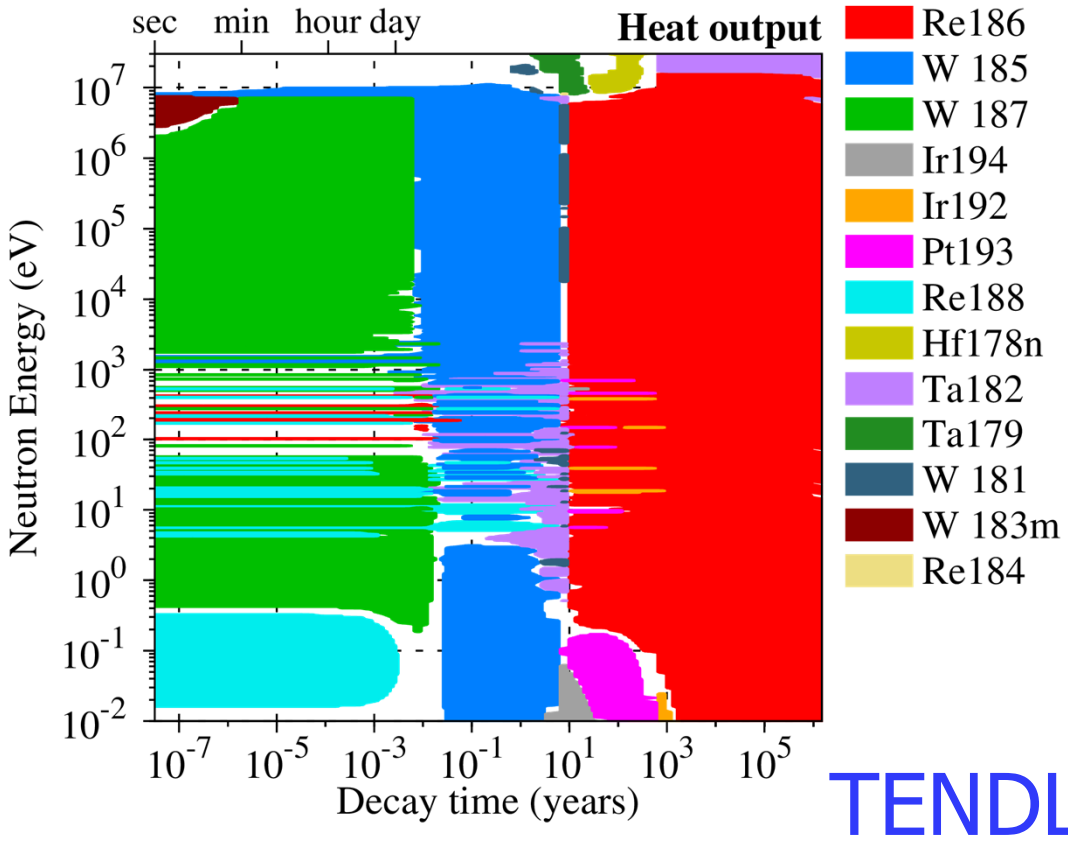
(3) Importance diagrams

- Dominant nuclides for a radiological quantity in the neutron-energy vs. decay-time space*
- Requires a sequence of “mono-energetic” neutron FISPACT-II calculations
  - i.e. using a fluxes files with only one non-zero entry
  - For each element in the handbook, 709 separate calculations are required (meaning almost 58,000 calculations in total for 81 elements)
  - Each inventory run has a fixed irradiation (2 fpy at 1 x 10^{15} $ncm^{-2}s^{-1}$ in handbooks)
  - Followed by a sequence of cooling times (at a high-enough resolution to populate the decay-time space)
  - Extensive post-processing (not currently part of the official FISPACT-II distribution) to define regions of dominance (> 50% contribution) and plot results

*Gilbert et al. *Nucl. Sci. Eng.* ***177*** *(2014) 291-306*

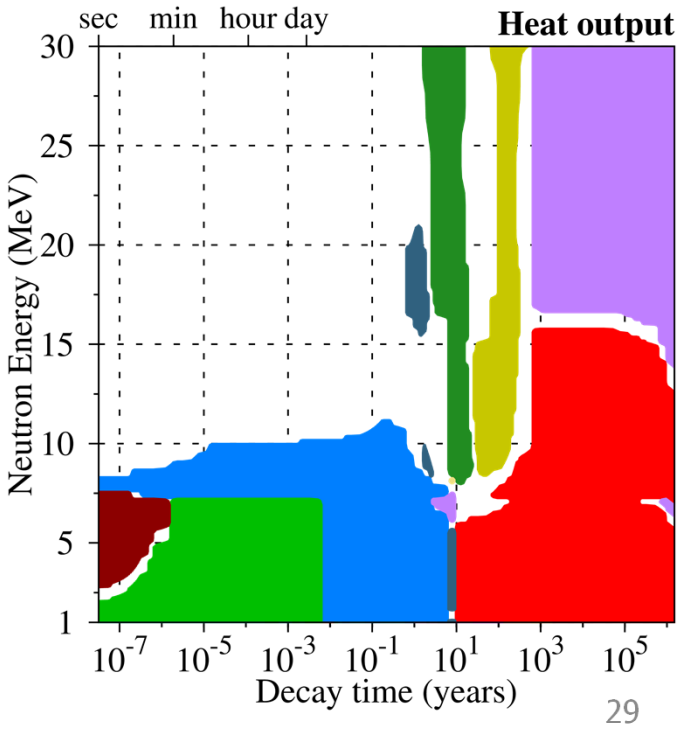
(3) Importance diagrams

- Handbook presentation gives two plots:
  - Log-log plot showing full energy range of interest (from thermal to MeV range of primary fusion/fission neutrons)
  - + lin-log plot showing the important MeV range in focus



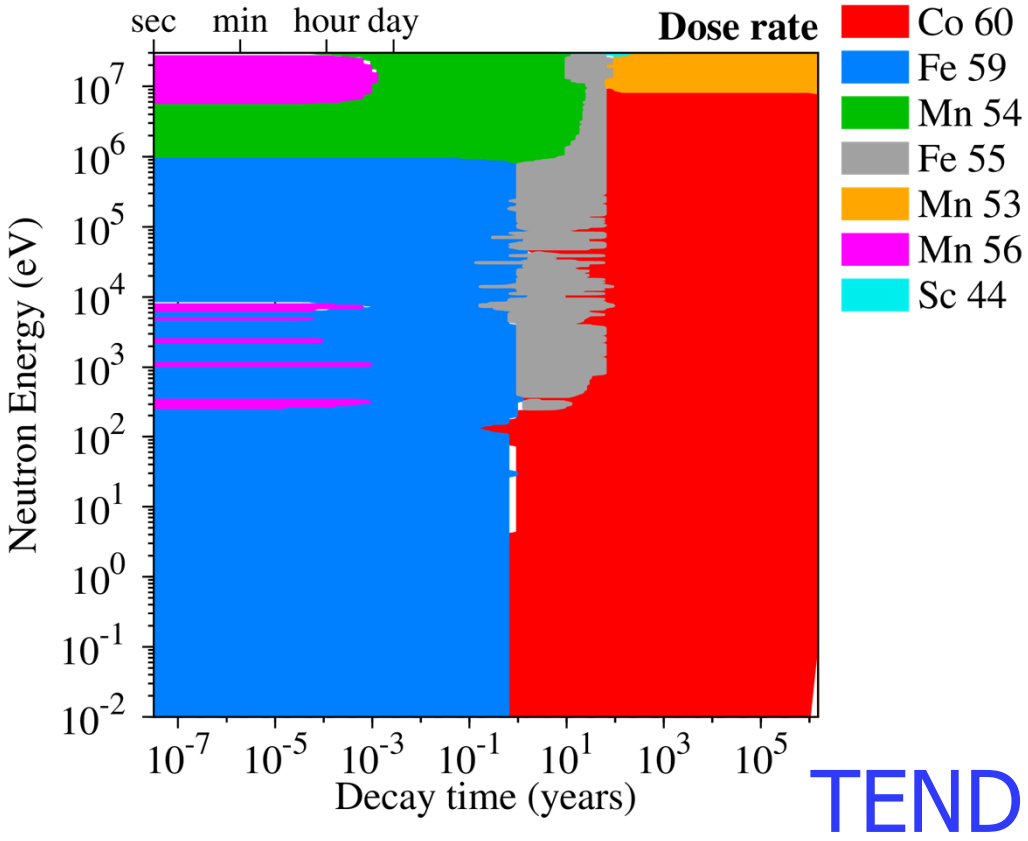
TENDL

Tungsten



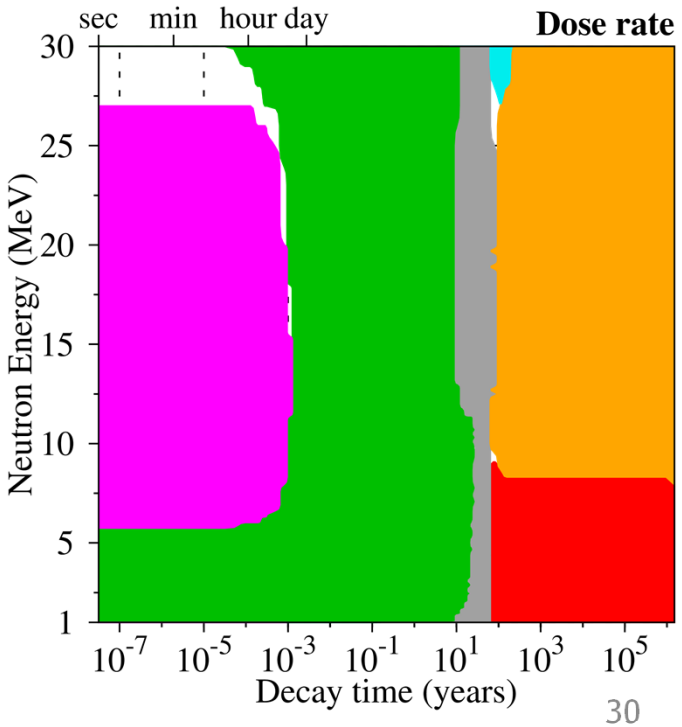
(3) Importance diagrams

- Diagrams for each of total Becquerel activity, decay heat, and (contact) γ-dose rate in handbooks, but can easily be produced for others (ingestion/inhalation, clearance, etc.)



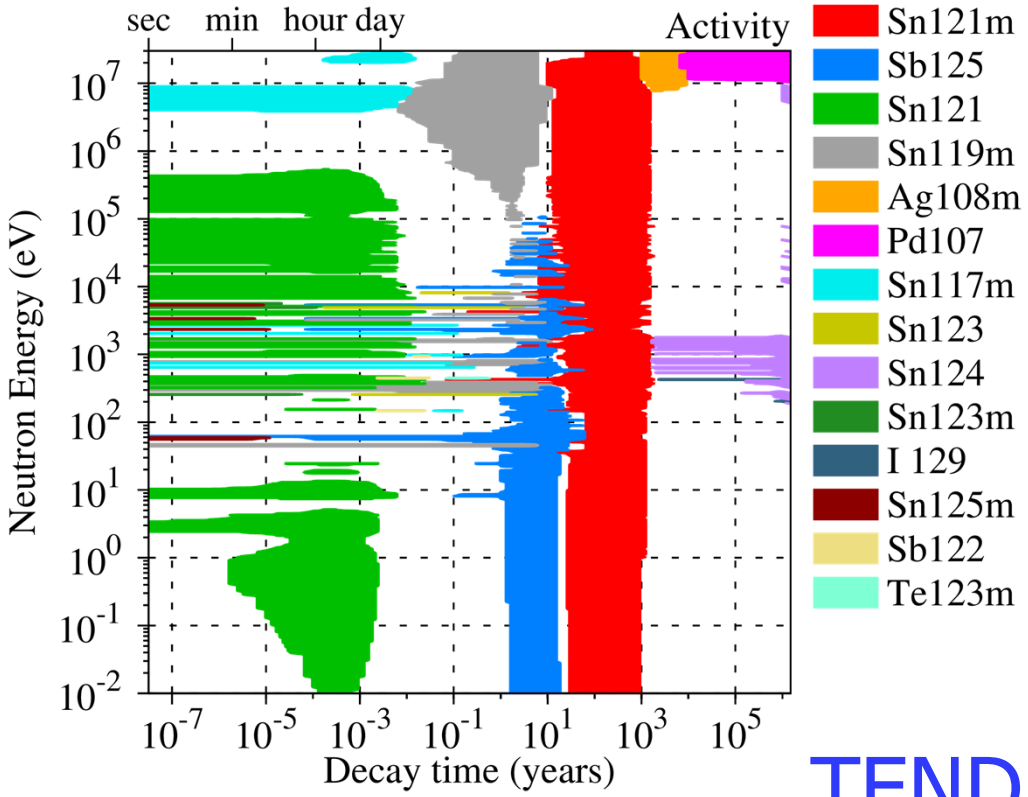
TENDL

Iron



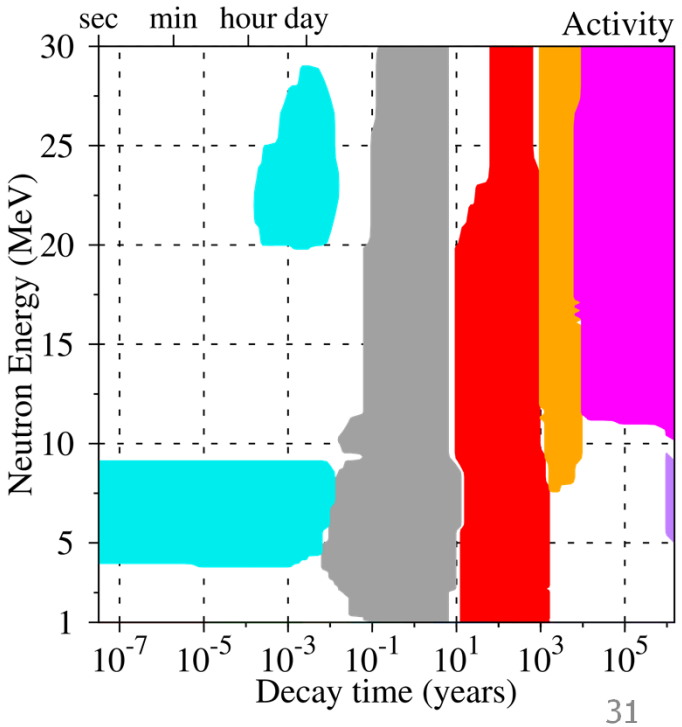
(3) Importance diagrams

- Significant empty space appears in materials with a complex activation response
  i.e. many nuclides contributing means no (>50%) dominance
- The high resolution group structure allows horizontal resonance bands to be seen



TENDL

Tin



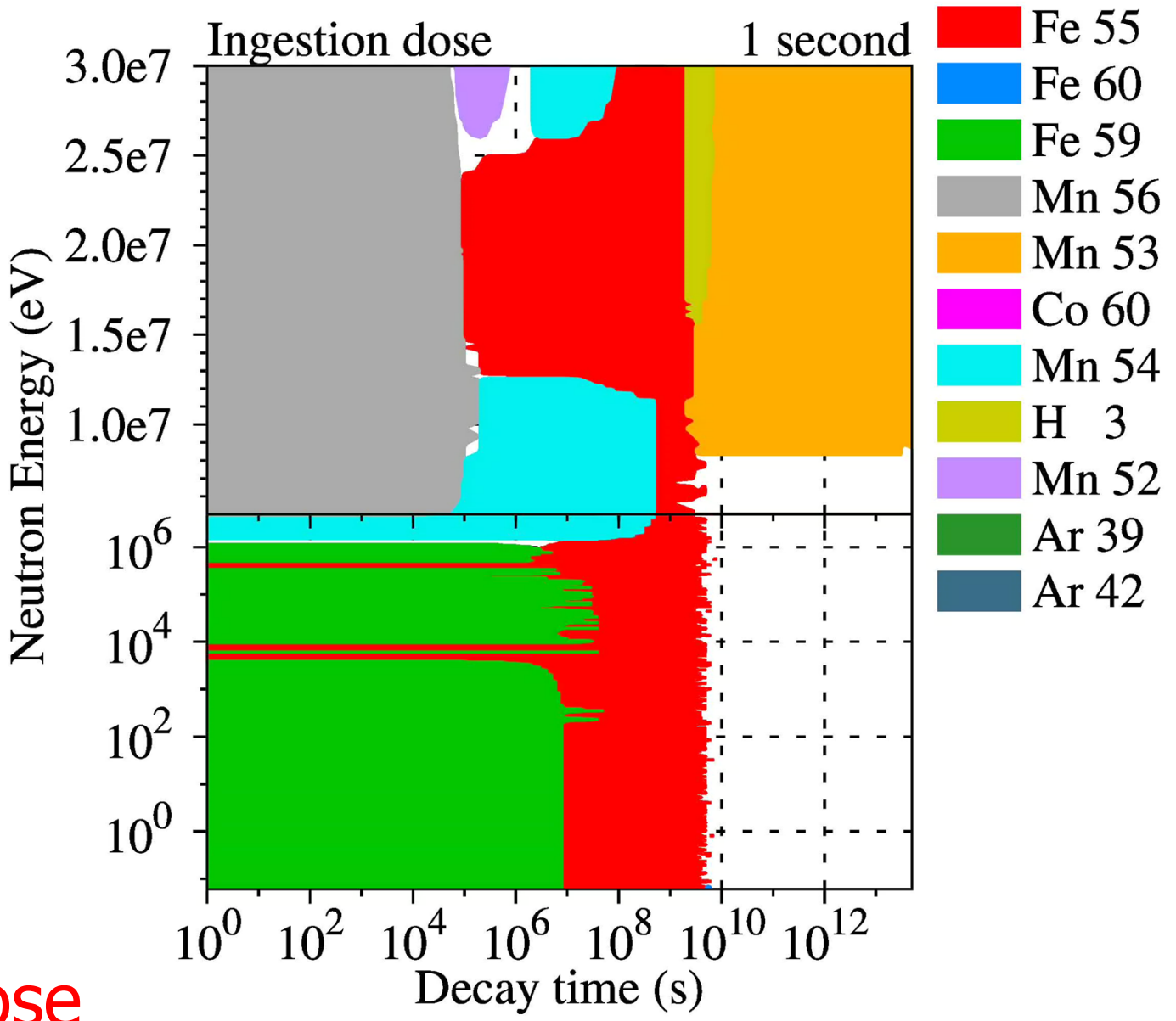
(3) Importance diagrams: animated

- Can be used to explore (via animation) variation with parameters
- E.g. as a function of:

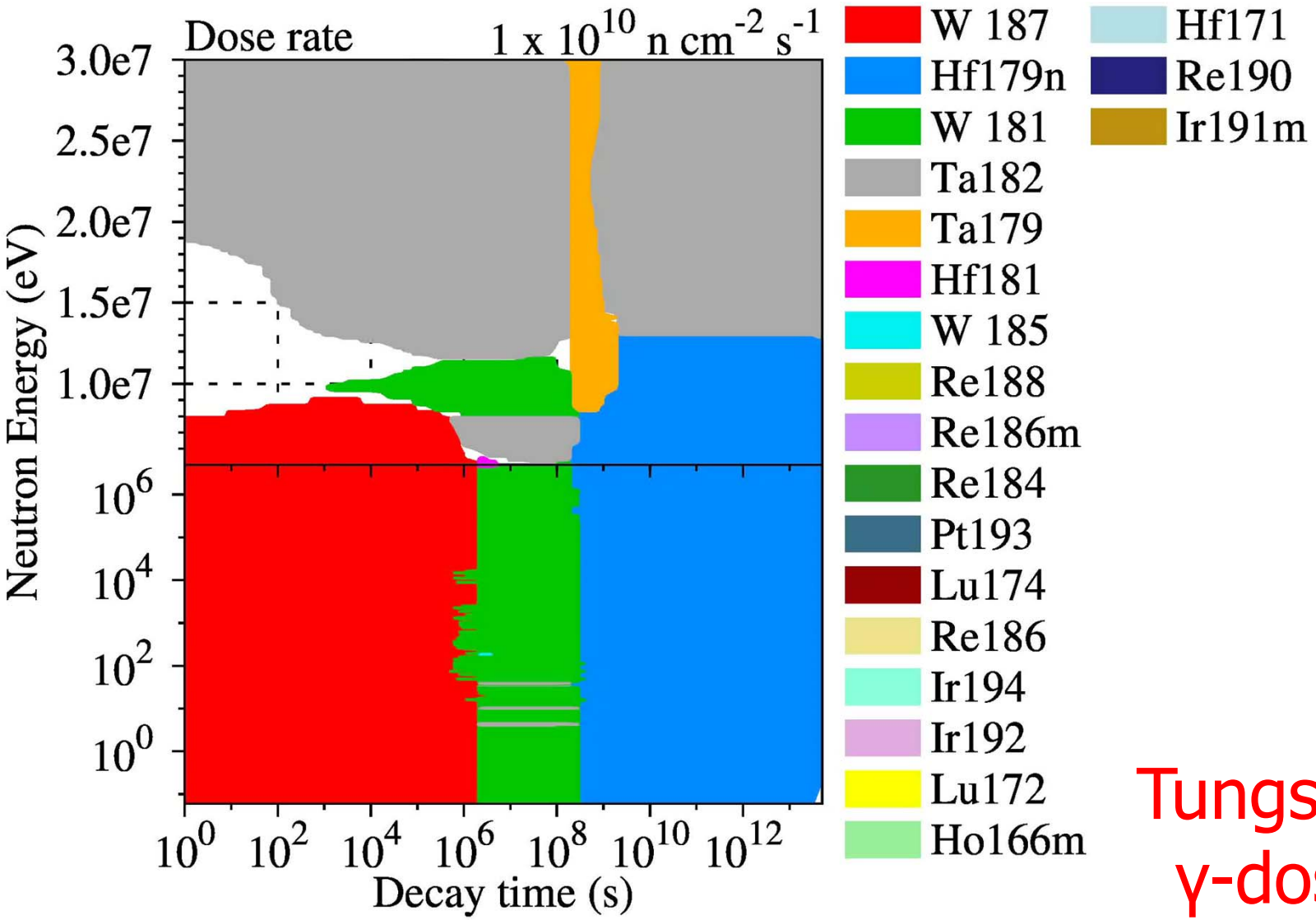
irradiation time

Iron

Ingestion dose

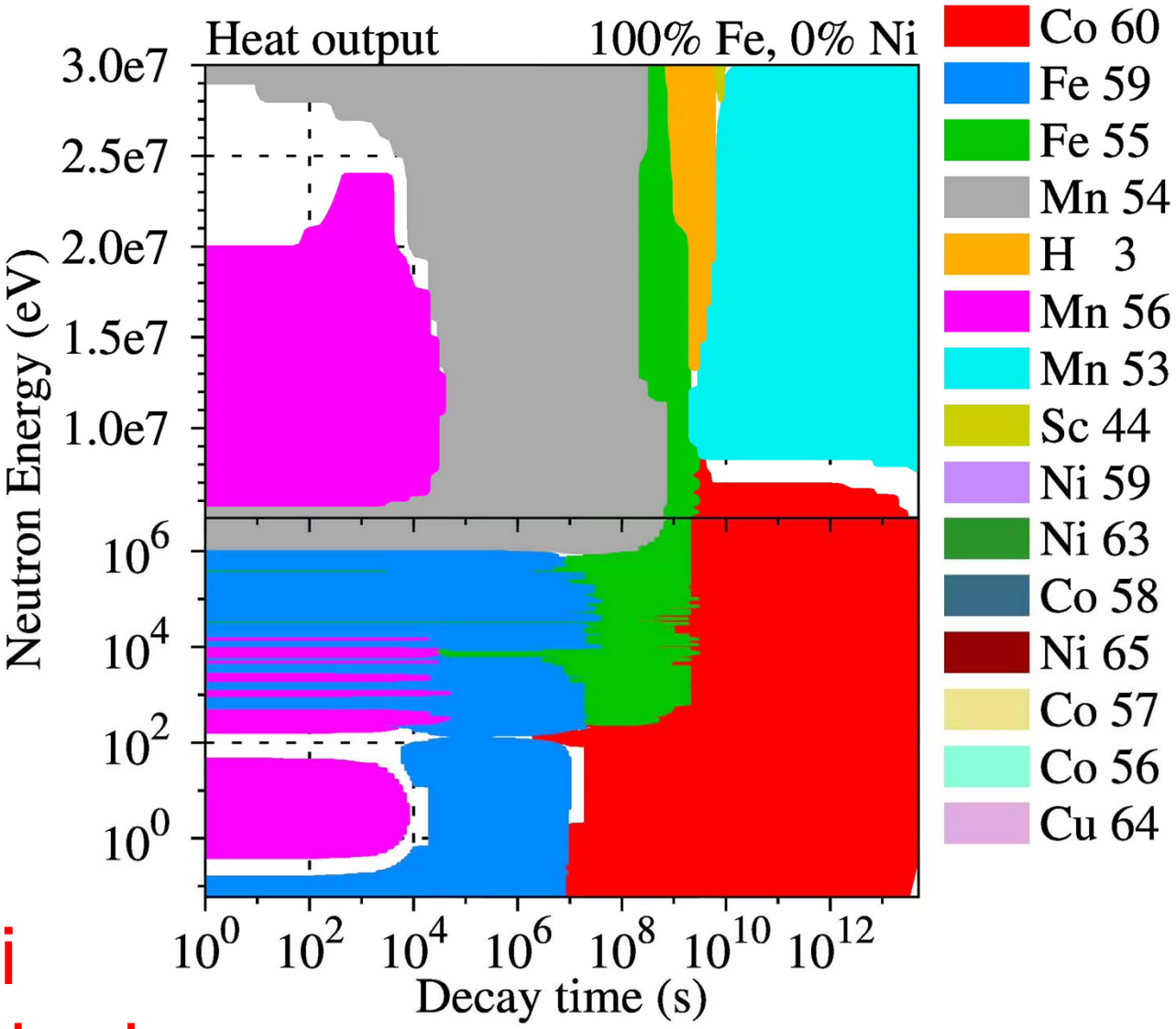


(3) Importance diagrams: variation with flux



Tungsten γ-dose

(3) Importance diagrams: variation with composition



FeNi

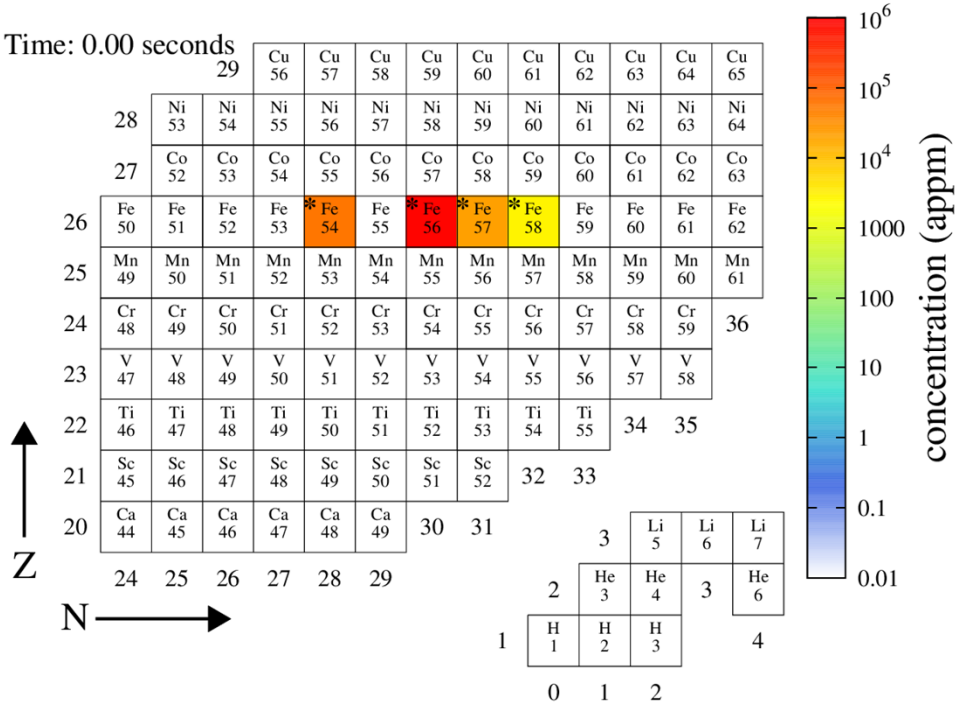
Heat output

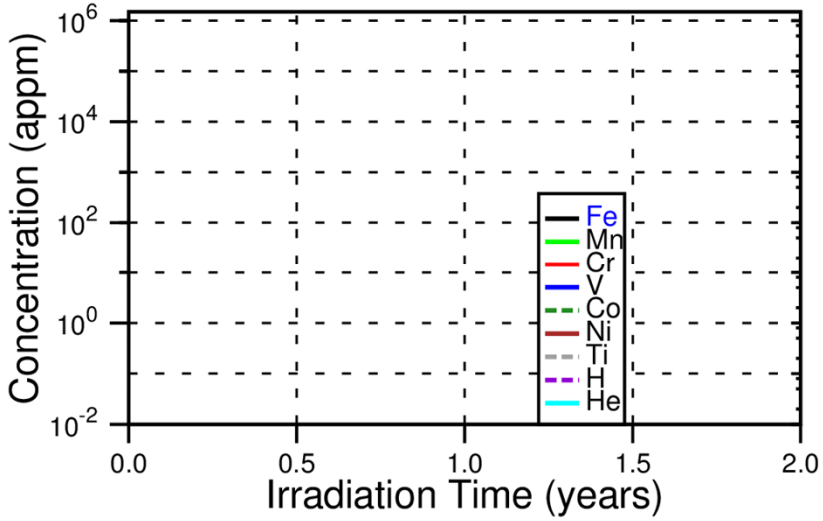
(4) Transmutation

- FISPACT-II output gives detailed, isotopically-separated break-down of the composition as a function of time
  - .tab1 file (`TAB1` command in input deck) provides the inventory composition output in an easily adaptable file for plotting
- Can be processed & plotted to observe the transmutation-induced evolution
  - At both the elemental (line chart) & isotopic (nuclide chart) level
  - Useful to identify problem impurities that may alter the mechanical & structural properties of a material

(4) Transmutation - animated

- Evolution in composition of pure Fe during 2 fpy in DEMO (TENDL results)

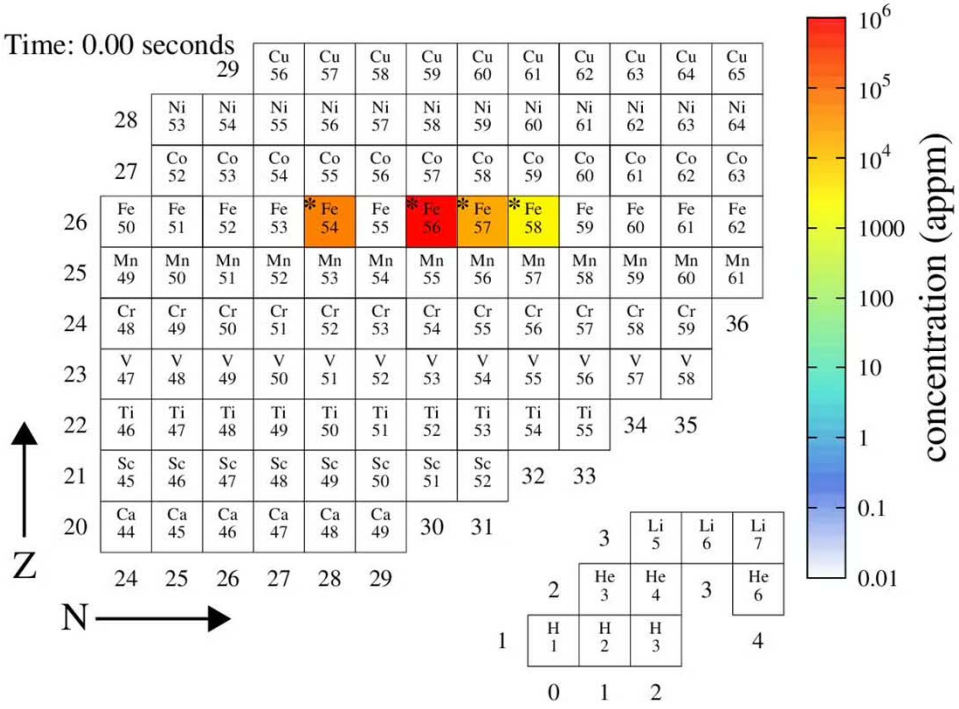


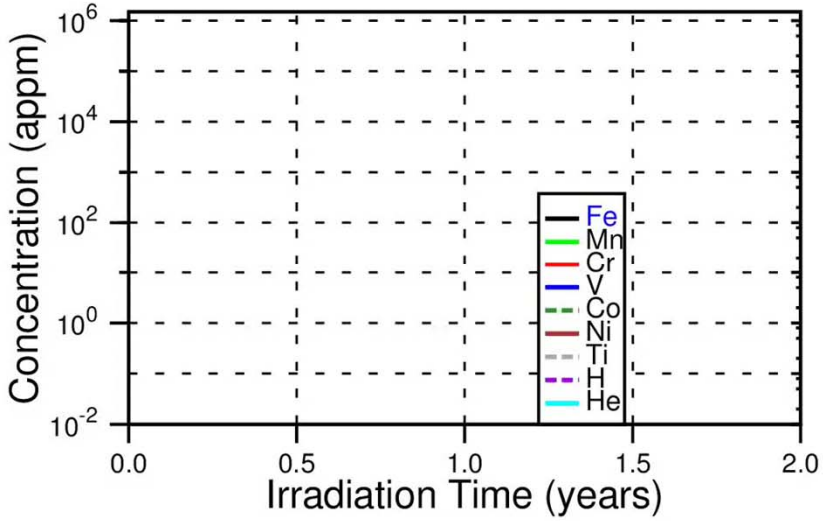


- Initial composition – four natural isotopes of Fe

(4) Transmutation - animated

- Evolution in composition of pure Fe during 2 fpy in DEMO (TENDL results)

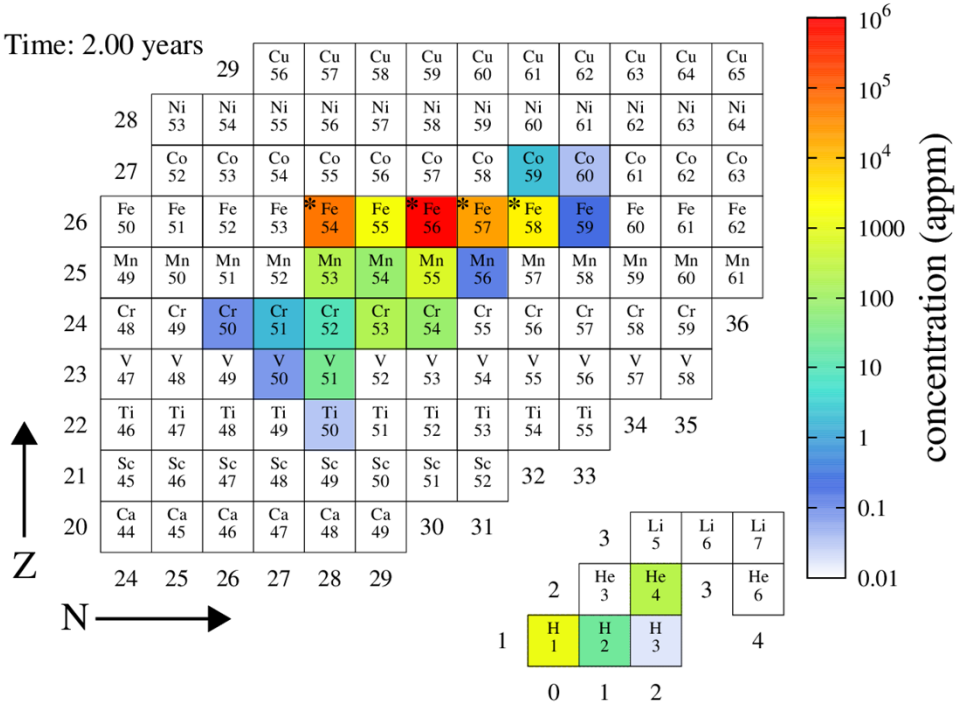


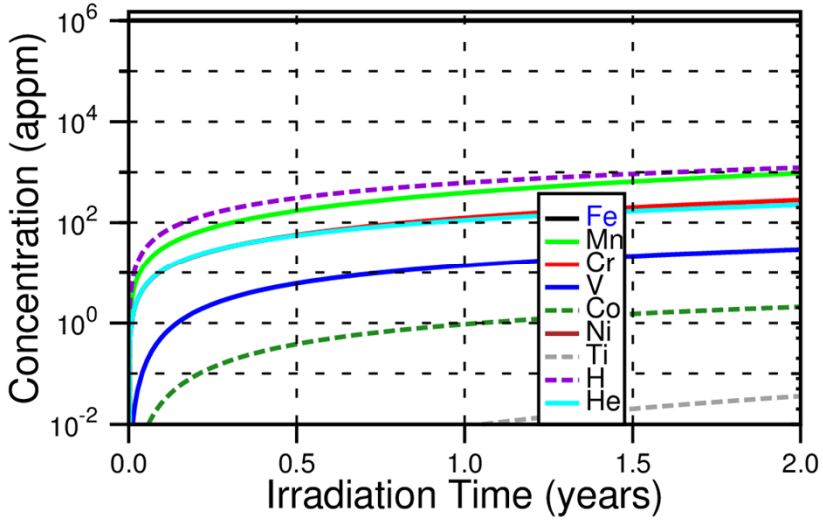


- Nuclear reactions create many new isotopes – both Fe and non-Fe

(4) Transmutation - animated

- Evolution in composition of pure Fe during 2 fpy in DEMO (TENDL results)



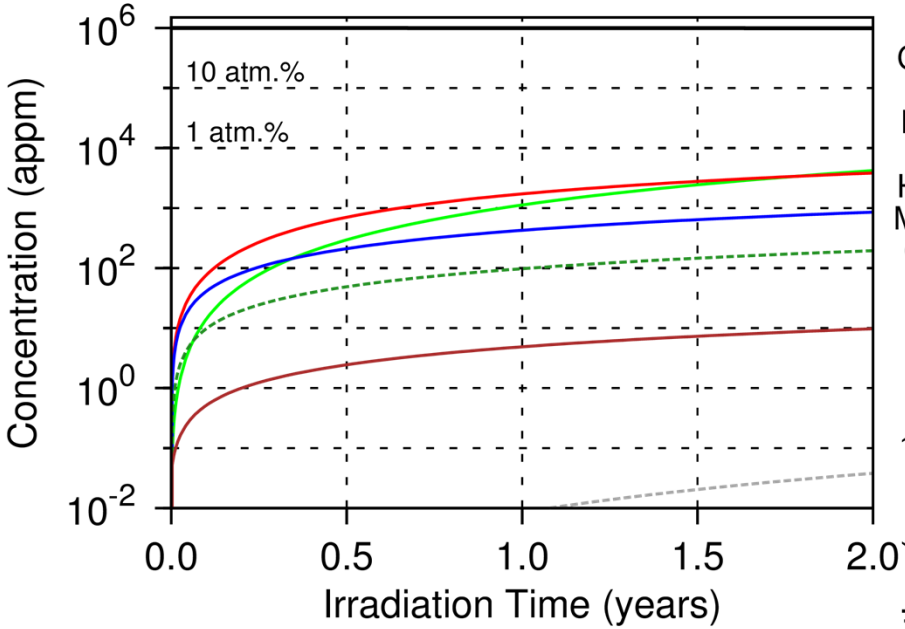


- Final composition is complex, includes gases, but is still dominated by original Fe isotopes
  (may not always be true)

(4) Transmutation

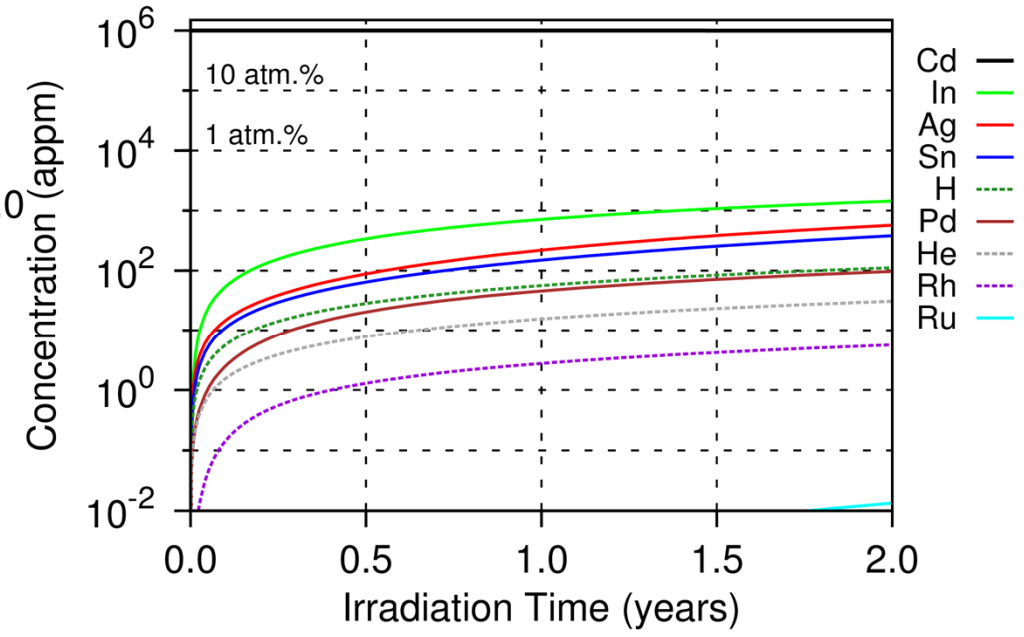
- Handbook presentation includes the elemental picture @ 2 fpy

Cobalt



97 appm He & 427 appm H after 1 year

Cadmium

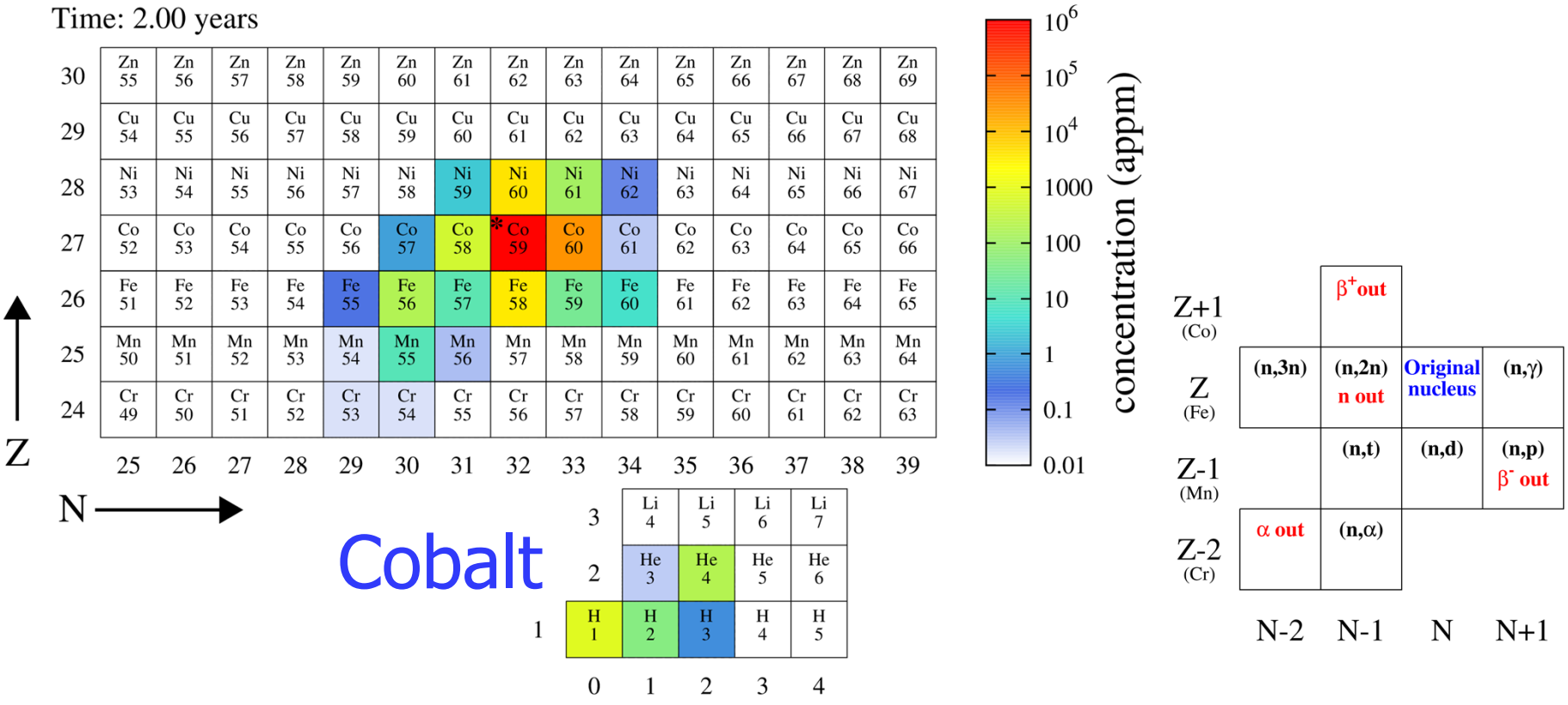


15 appm He & 56 appm H after 1 year

- He and H concentrations at 1 fpy given explicitly (lead to embrittlement at high concentrations)

(4) Transmutation

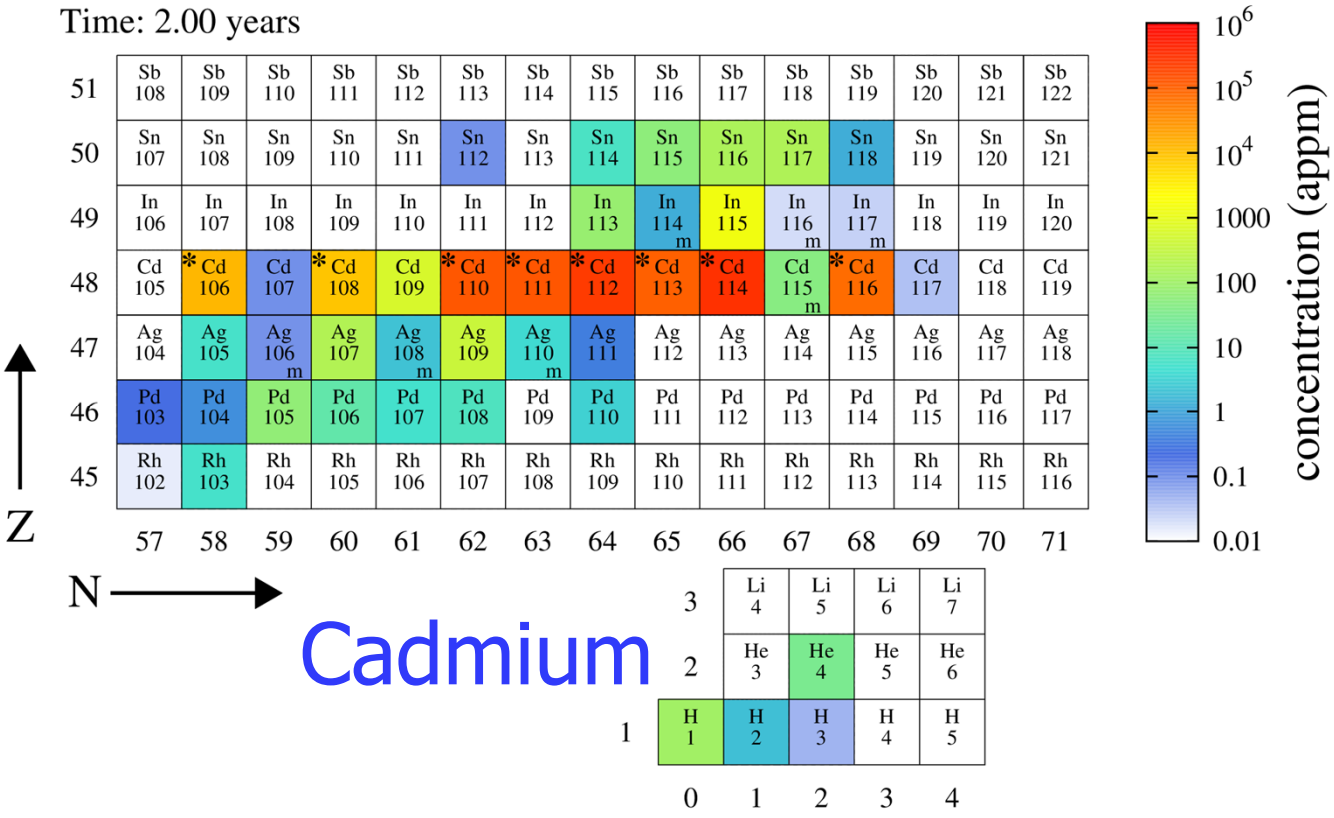
- & nuclide-chart snapshot at end of 2 fpy, showing full isotopic break-down

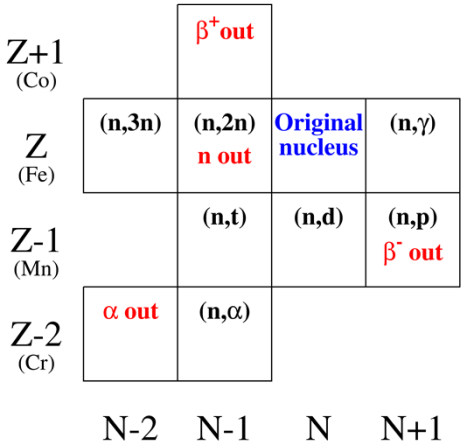


- Can be used to identify reaction pathways (more later)

(4) Transmutation

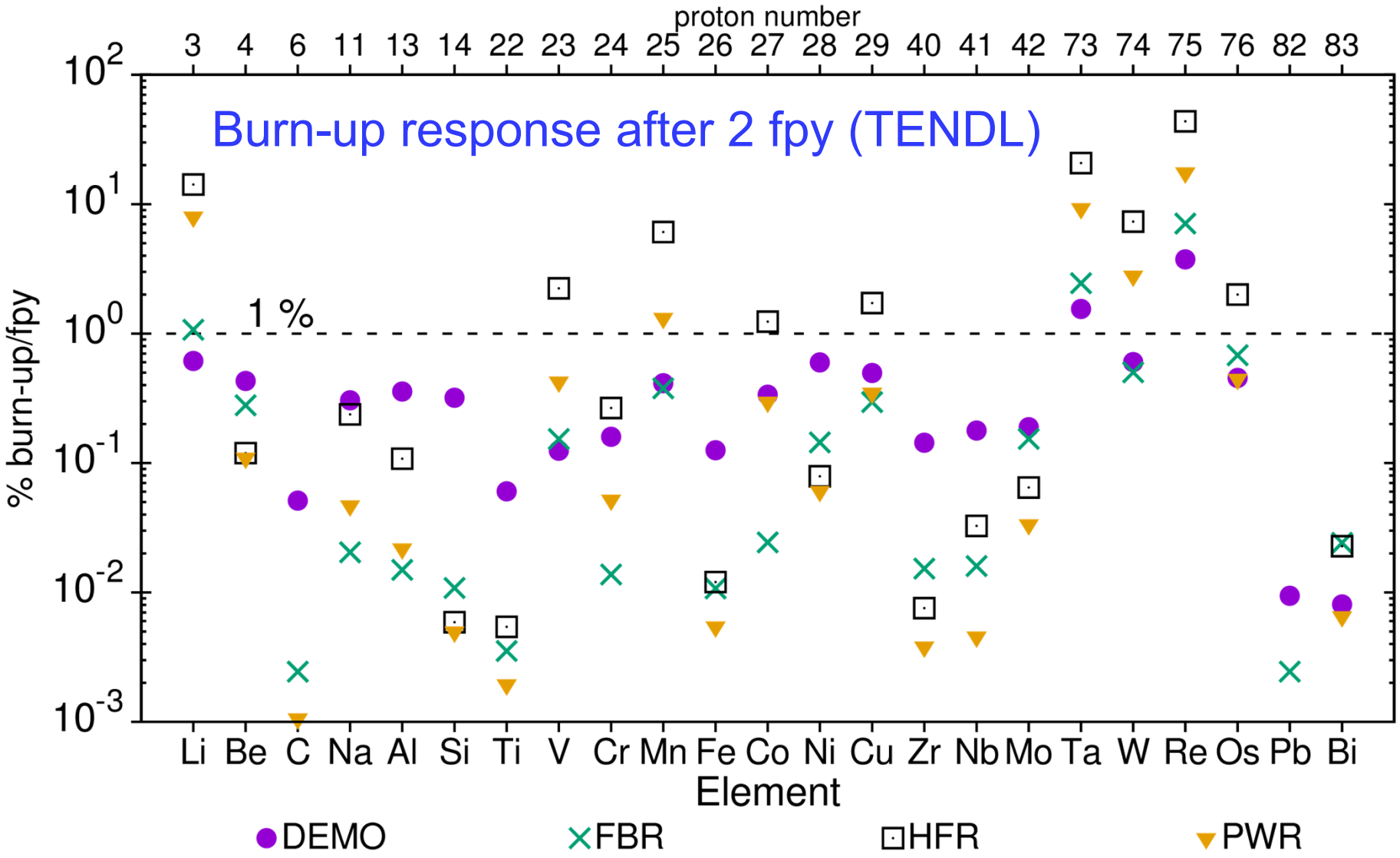
- & nuclide-chart snapshot at end of 2 fpy, showing full isotopic break-down





- Can be used to identify reaction pathways

(4) Transmutation global results: fusion vs. fission



- Fission spectra are moderated (“softer”) than fusion & combined with high-flux in HFR produces greater burn-up rates (mostly)

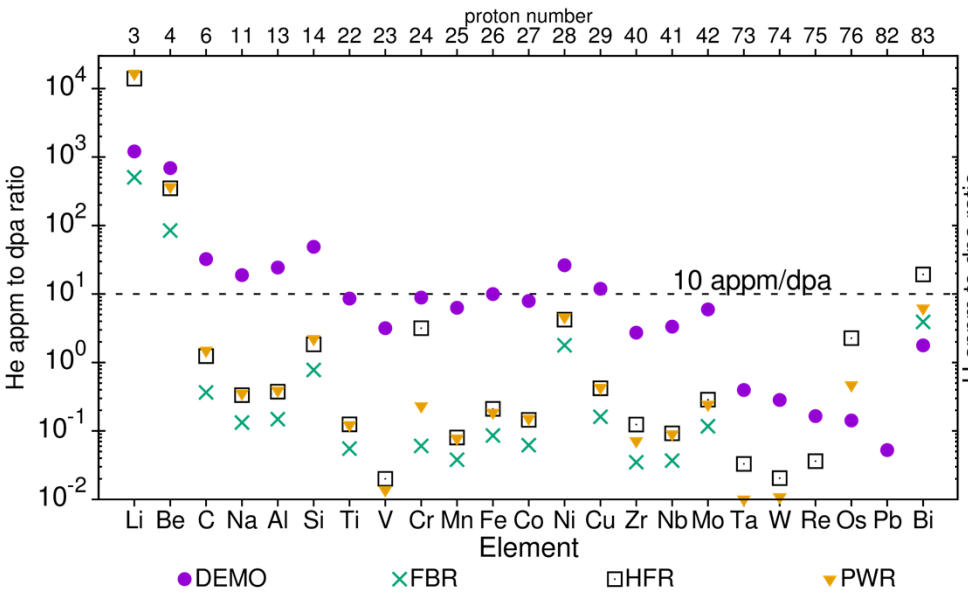
(4) Transmutation: Gas production

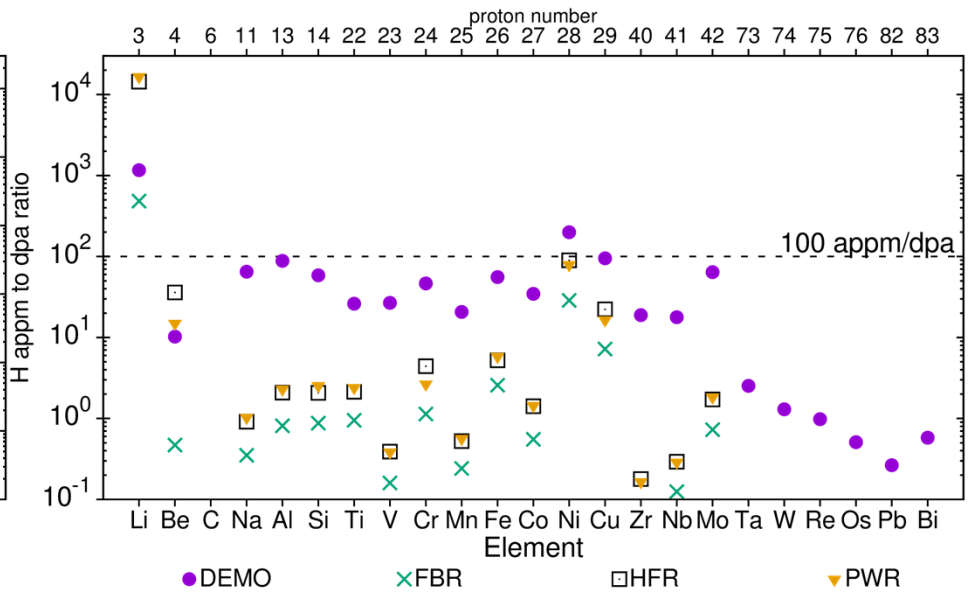
- Gas production is treated specially in the output for each time interval in FISPACT-II
  - Important for predicting and modelling material embrittlement
- Estimate of damage rate – the “displacements per atom” (dpa) measure also included

```
0  Total Displacement Rate (n,Ddiss)= 1.19503E+13 Disp./sec = 3.64814E-12 Disp.Per Atom/sec = 1.15127E-04 DPA/year
   Total Displacement Rate (n,Dinel)= 9.08836E+16 Disp./sec = 2.77446E-08 Disp.Per Atom/sec = 8.75554E-01 DPA/year
   Total Displacement Rate (n,Del  )= 7.08317E+16 Disp./sec = 2.16233E-08 Disp.Per Atom/sec = 6.82378E-01 DPA/year
   Total Displacement Rate (n,Dtot )= 1.62935E+17 Disp./sec = 4.97403E-08 Disp.Per Atom/sec = 1.56968E+00 DPA/year
0  KERMA RATE (n,Kktot) =  1.45096E+23 eV/sec = 2.32469E+01 kW/kg = 4.48666E-01 kW/cm^3
   KERMA RATE (n,Kphot) =  1.45067E+23 eV/sec = 2.32423E+01 kW/kg = 4.48576E-01 kW/cm^3
   KERMA RATE (n,Kfiss) =  0.00000E+00 eV/sec = 0.00000E+00 kW/kg = 0.00000E+00 kW/cm^3
   KERMA RATE (n,Kinel) =  1.25683E+21 eV/sec = 2.01366E-01 kW/kg = 3.88637E-03 kW/cm^3
   KERMA RATE (n,Knone) =  1.45530E+23 eV/sec = 2.33166E+01 kW/kg = 4.50009E-01 kW/cm^3
   KERMA RATE (n,Kel  ) =  1.21903E+19 eV/sec = 1.95310E-03 kW/kg = 3.76949E-05 kW/cm^3
   KERMA RATE (n,Ktot ) =  1.45543E+23 eV/sec = 2.33185E+01 kW/kg = 4.50047E-01 kW/cm^3
0  GAS   RATE (n,Xa   ) =  3.34046E+09 atoms per sec =  1.01976E-09 appm/sec
   GAS   RATE (n,Xh   ) =  0.00000E+00 atoms per sec =  0.00000E+00 appm/sec
   GAS   RATE (n,Xt   ) =  8.73363E+06 atoms per sec =  2.66617E-12 appm/sec
   GAS   RATE (n,Xd   ) =  6.28774E+07 atoms per sec =  1.91950E-11 appm/sec
   GAS   RATE (n,Xp   ) =  8.51293E+08 atoms per sec =  2.59880E-10 appm/sec
0  GAS   RATE (a decay) =  1.66048E-01 atoms per sec =  5.06906E-20 appm/sec
```

- The combined gas/dpa ratio is a useful measure
  - Particularly when designing experiments to mimic (fusion) reactor conditions

(4) Transmutation: gas/dpa ratios





- Fusion trend is lower gas production and hence lower ratios as element mass increases
- The difference between fusion and fission gas-to-dpa ratios (NRT* dpa) is high
- Makes it difficult to realise the correct rates for fusion using fission conditions

TENDL results

*Norgett, Robinson, Torrens, *Nucl. Eng. Des.* **33** (1975) 50-54

(5) PKA spectra

- The term primary knock-on atoms (PKA) refers to the initial recoil atom(s) created by neutron (or proton, electron, etc.) interactions with the constituent atoms of a material
- These PKAs can initiate cascades of displacements, leading to the accumulation of structural damage
  - Life-limiting consequences for materials
- A full description of the PKAs generated under neutron irradiation is a necessary source term input to modelling and simulation of the creation & evolution of radiation damage
  - Can also be used to design experiments to mimic neutron damage

(5) PKA spectra

- Complete description of PKAs requires all possible nuclear reaction channels to be considered
  - More than scattering
  - non-elastic reactions
  - & including all recoiling species of a reaction (secondary emitted, light particles)
- The resulting energy.vs.flux spectra of PKAs provides a much richer data-set
  - More detail than simpler damage measures (e.g. DPA)
  - uses more of the information available from particle transport and inventory simulations

(5) PKA spectra

Computational methodology:

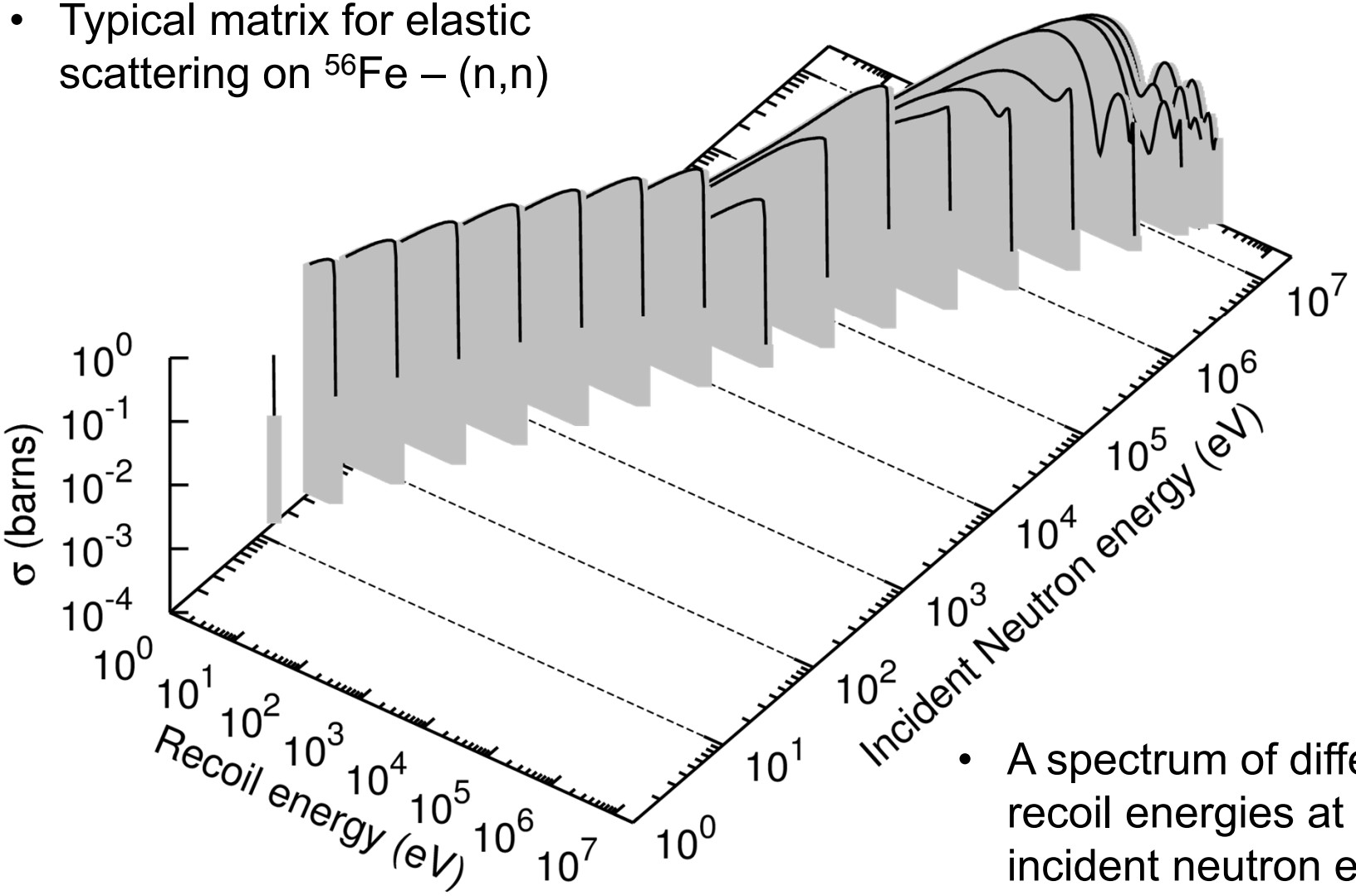
- NJOY processes the raw point-wise nuclear data and calculates neutron-interaction recoil matrices:

$$M^{x \to y} \equiv \left\{ m_{ij}^{x \to y} \right\}$$

  - $m_{ij}^{x \to y}$ 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
  - Derived from reaction cross sections and angular distributions
  - For each parent target isotope (e.g. ^{56}Fe) there will be a set of $M^{x \to y}$
    - & perhaps more than one matrix for a given nuclear reaction e.g. (n,α) will produce a heavy recoil and a ^{4}He

(5) PKA spectra – recoil matrices

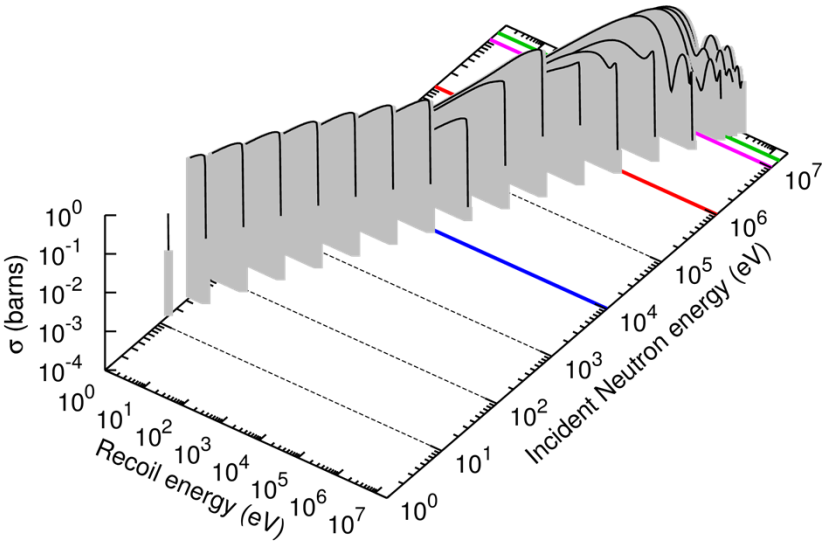
- Typical matrix for elastic scattering on ^{56}Fe – (n,n)

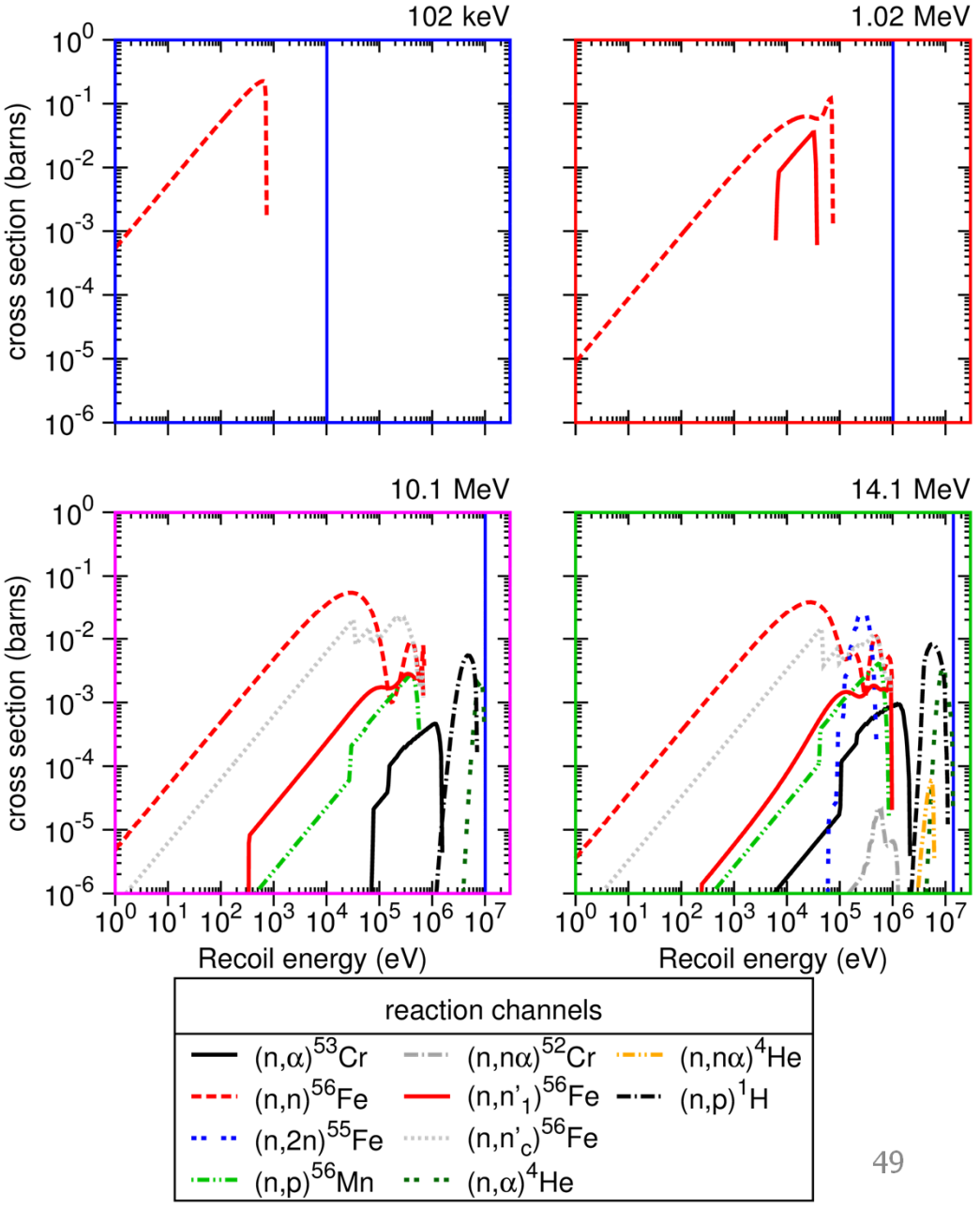


- A spectrum of different recoil energies at each incident neutron energy

TENDL results

(5) PKA spectra – recoil matrices & vectors



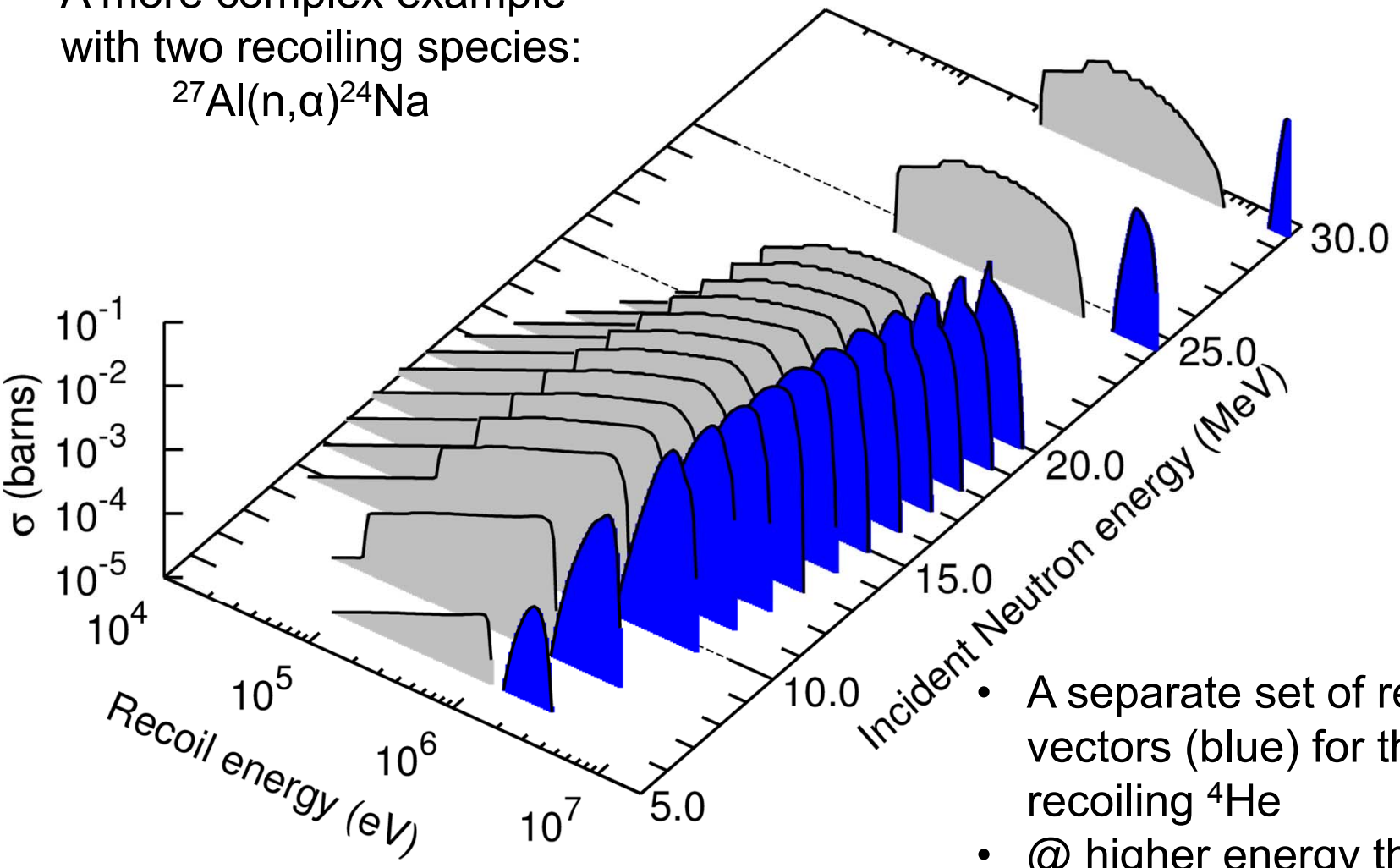


- In ^{56}Fe: at low incident energy only elastic and inelastic channels are open
- Number of contributing channels increases dramatically at higher energies (MeV range)

TENDL results

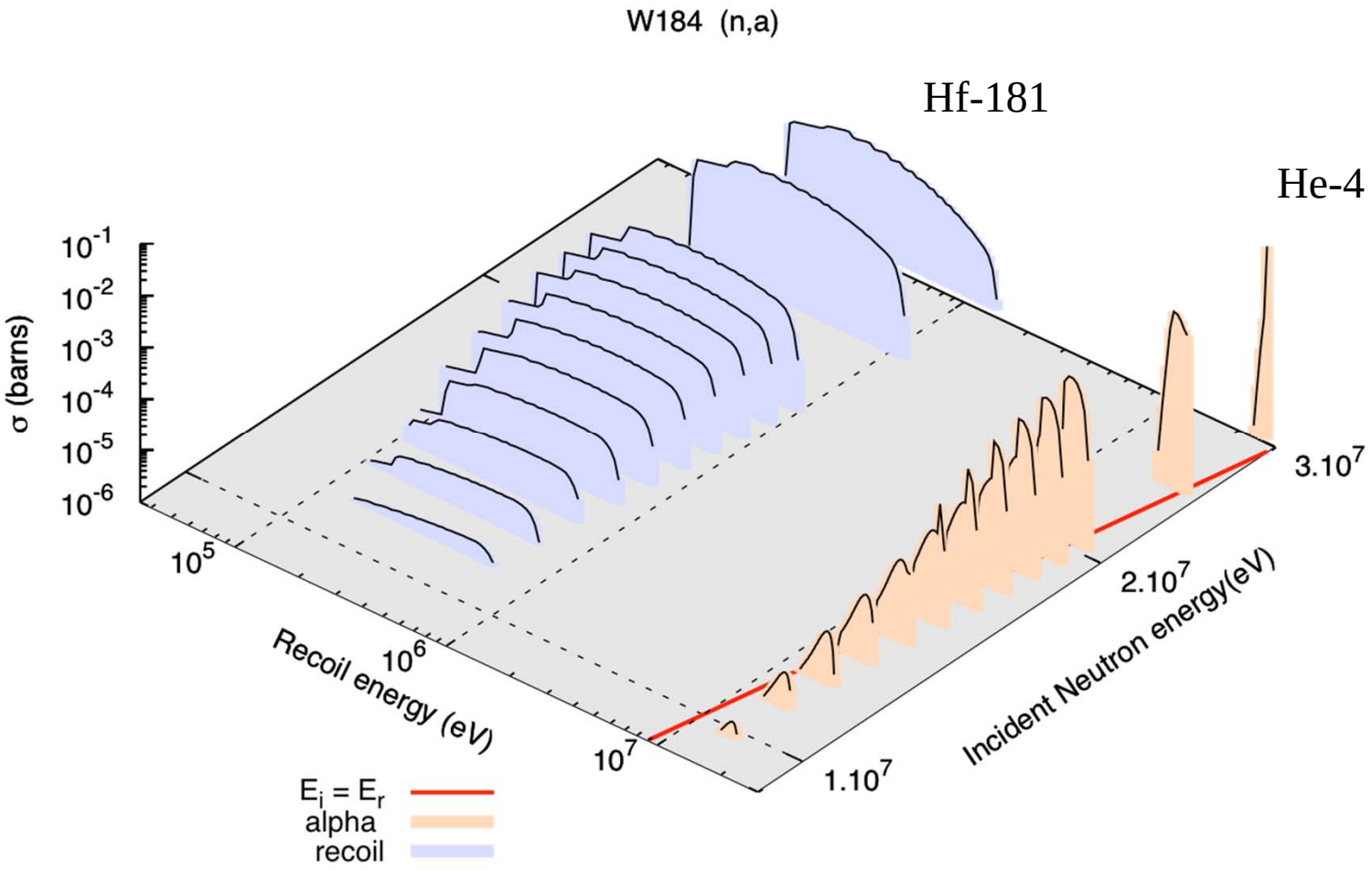
(5) PKA spectra – recoil matrices

- A more complex example with two recoiling species:
  $^{27}Al(n,\alpha)^{24}Na$



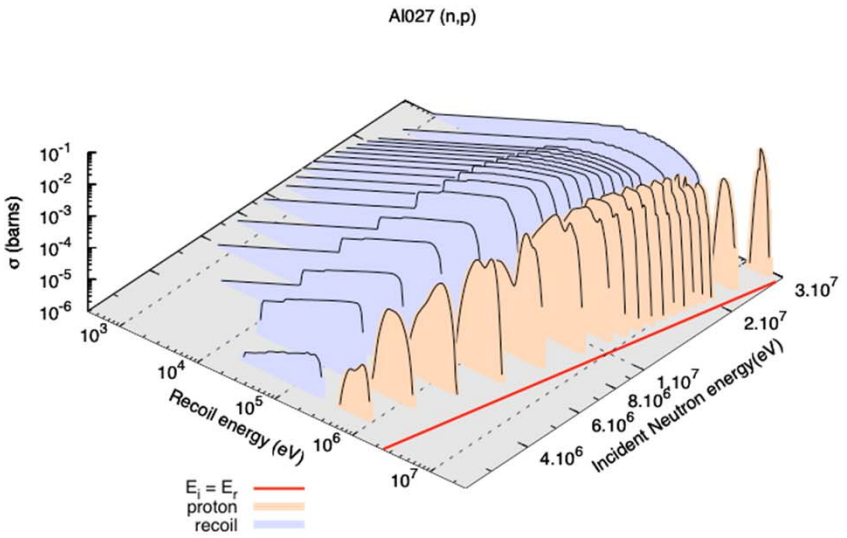
- A separate set of recoil vectors (blue) for the recoiling ^{4}He
- @ higher energy than heavy ^{24}Na recoil (mass partition)

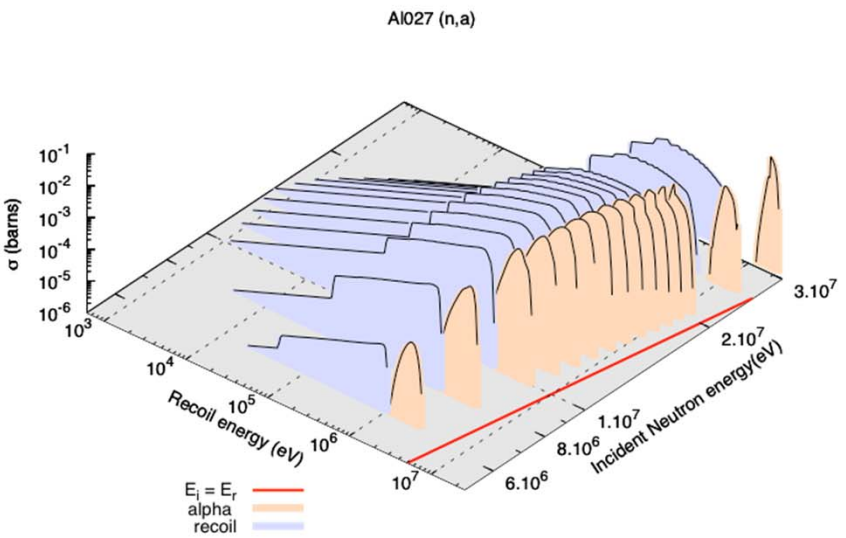
W-184 TENDL example

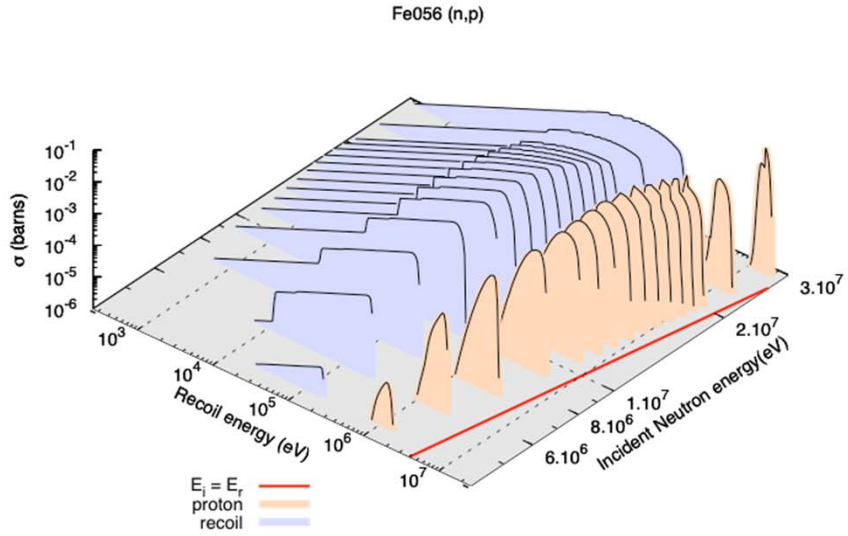


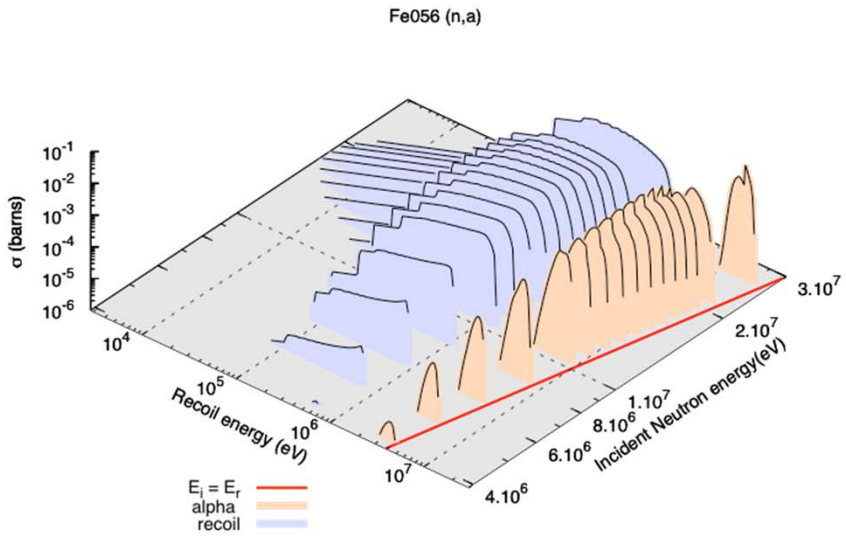
Q positive (7.3 MeV) means that the alpha energy can be much higher than the energy of the incident neutron

TENDL Al-27 and Fe-56









(5) PKA spectra

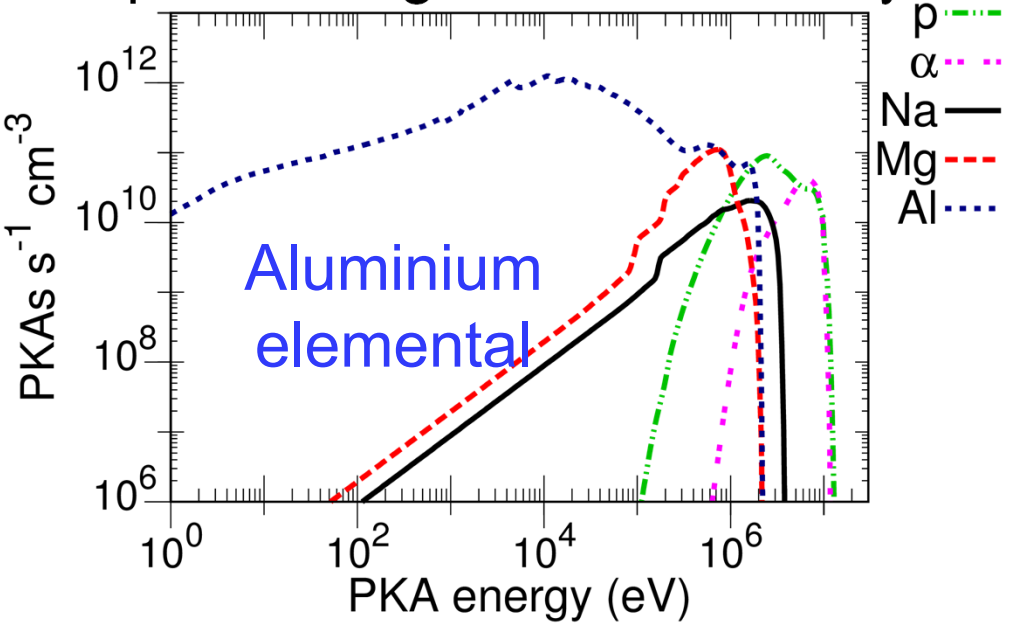
Computational methodology (b): *Gilbert et al., *JNM* **467** (2015) 121-134

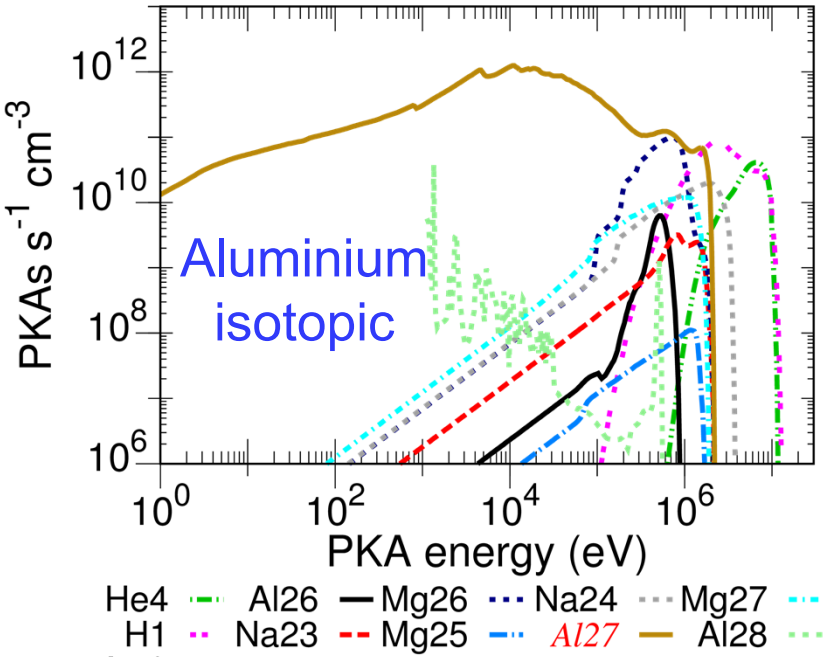
- Collapsing each matrix with a neutron flux spectrum gives the recoil (PKA) spectrum $R^{x\rightarrow y}(E)$:

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

where ϕ_j is the neutron flux at energy E_j for a given neutron field

- processing done with newly written SPECTRA-PKA*

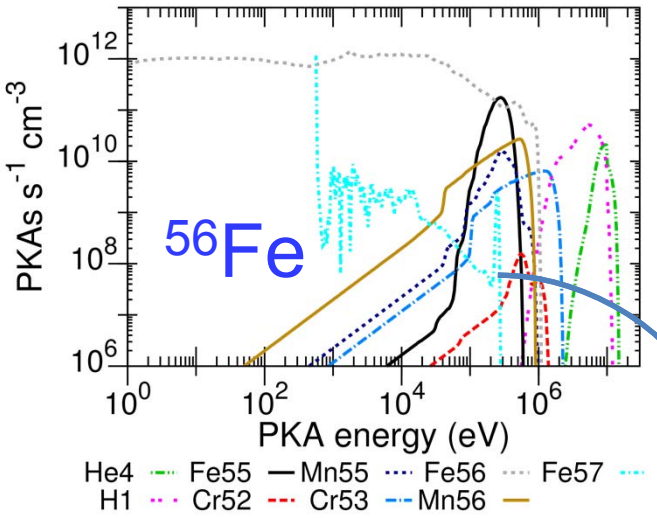


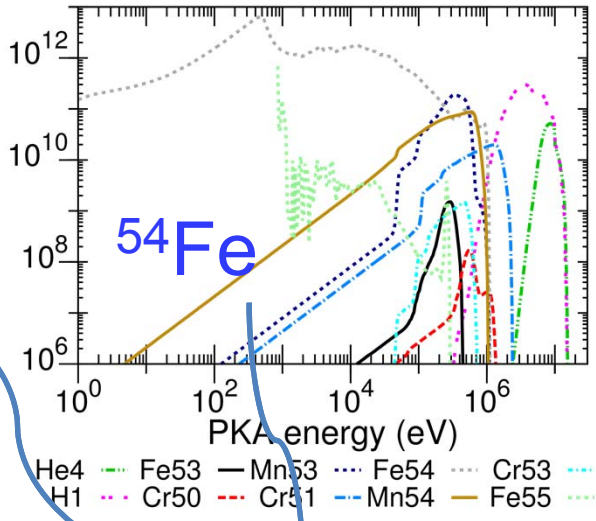


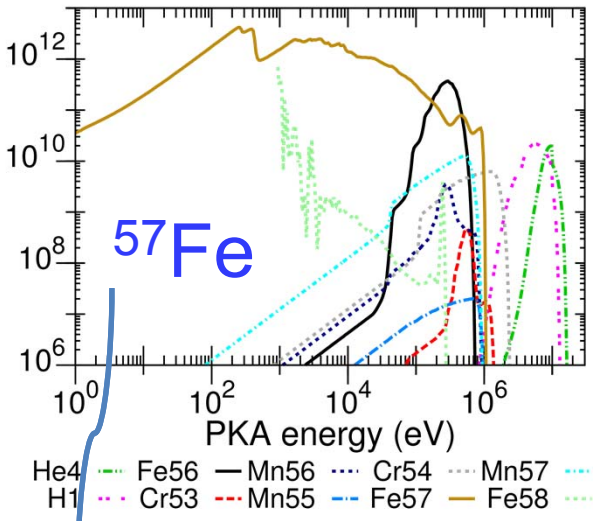
- Al under DEMO first wall conditions (TENDL results)
- Even with only one target (^{27}Al), there are many different recoiling species

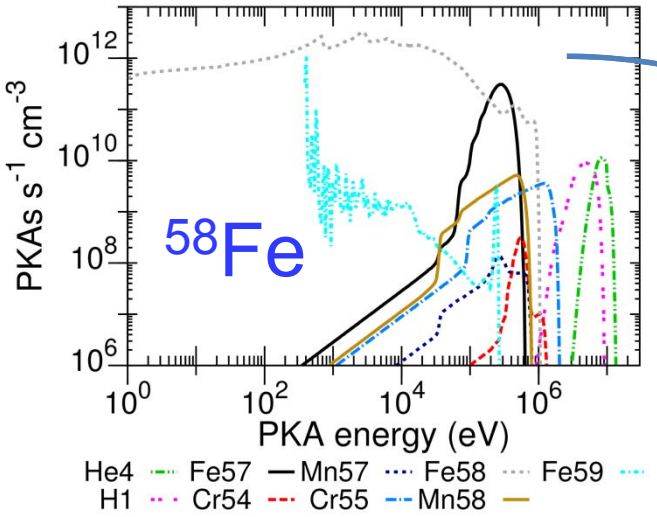
(5) PKA spectra – a multi-target (isotope) material

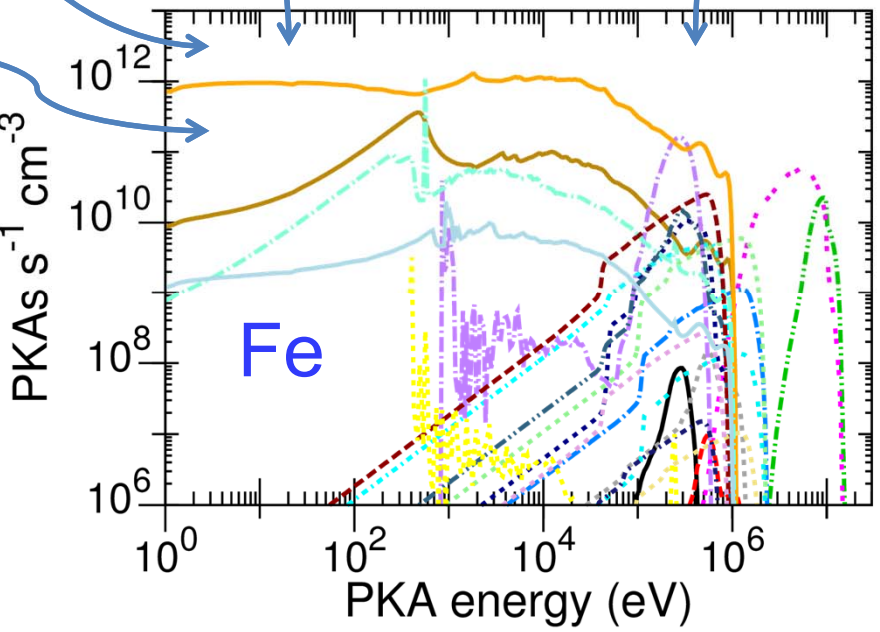
- In most cases, results must be weighted and merged for multiple targets











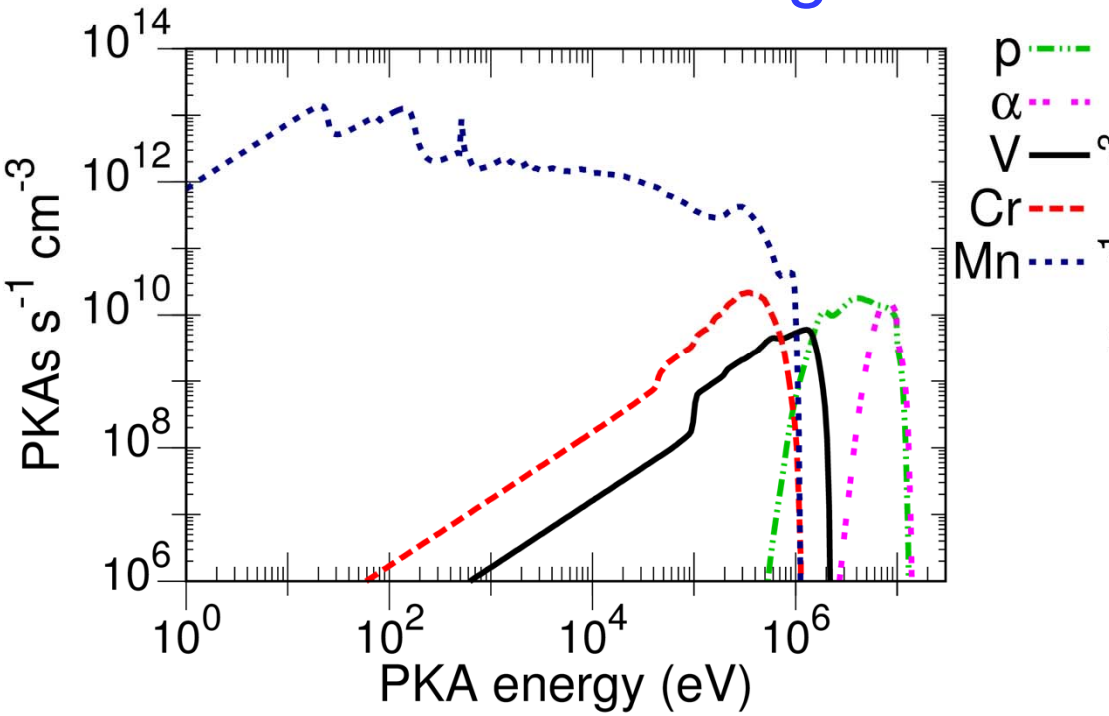
- SPECTRA-PKA module handles all the necessary processing

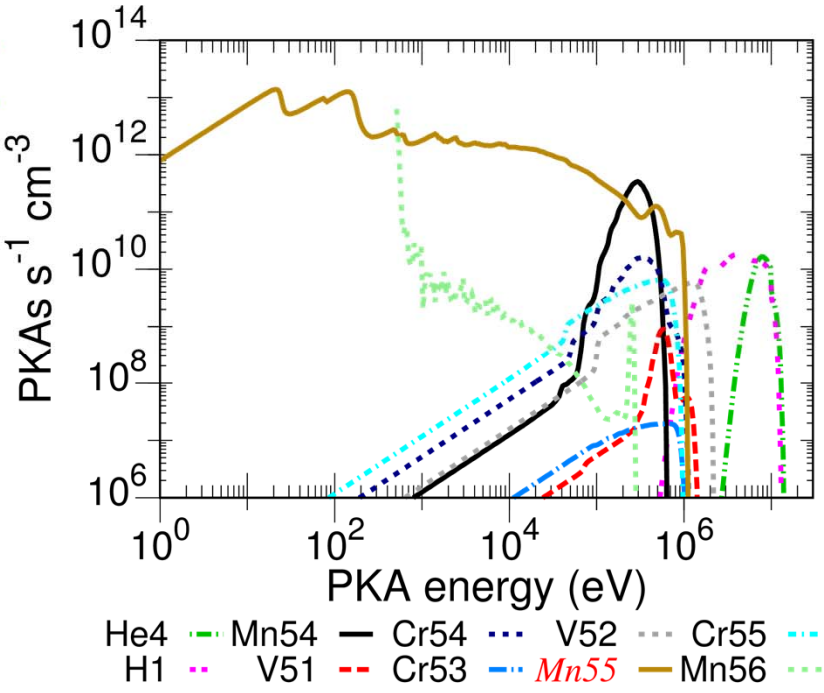
Fe - 5.845% ^{54}Fe, 91.754% ^{56}Fe, 2.119% ^{57}Fe, 0.282% ^{58}Fe

(5) PKA spectra

- Handbooks present elemental and isotopic PKA spectra for each element under relevant neutron irradiation
  - A t=0 snapshot (before any transmutation)

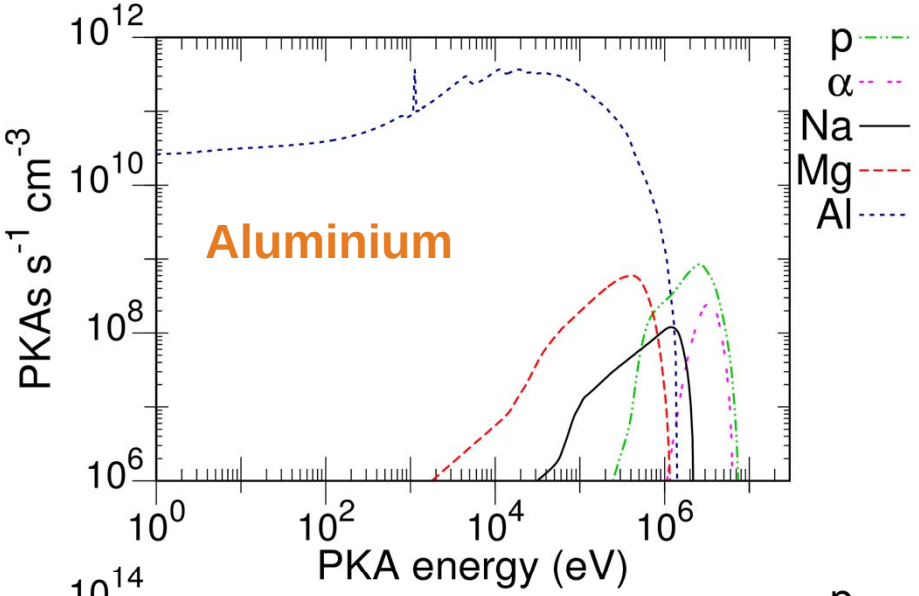
Manganese

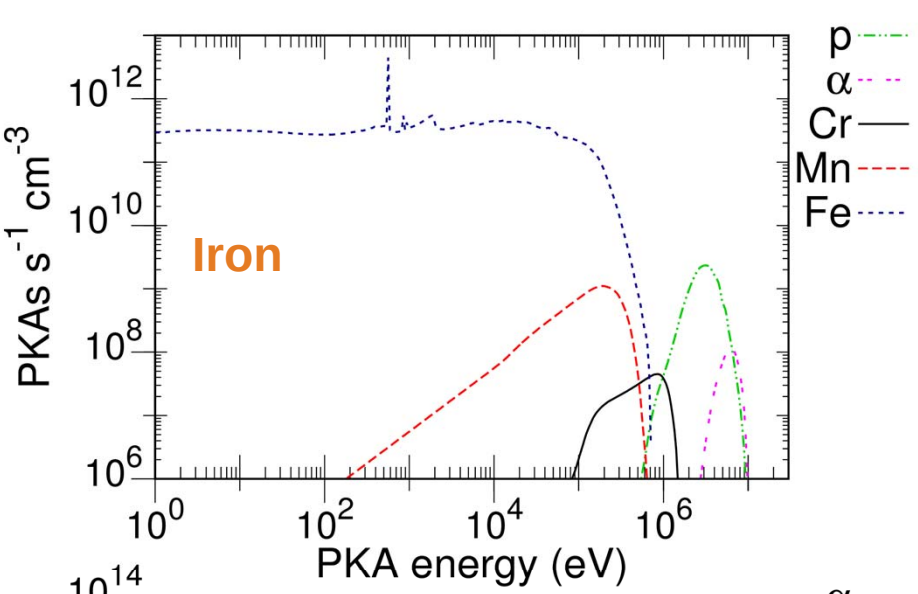


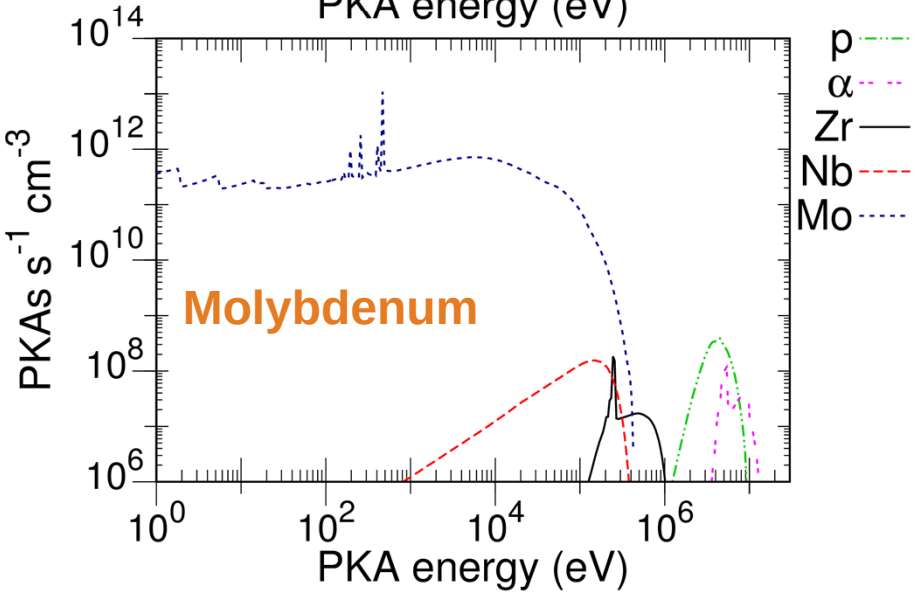


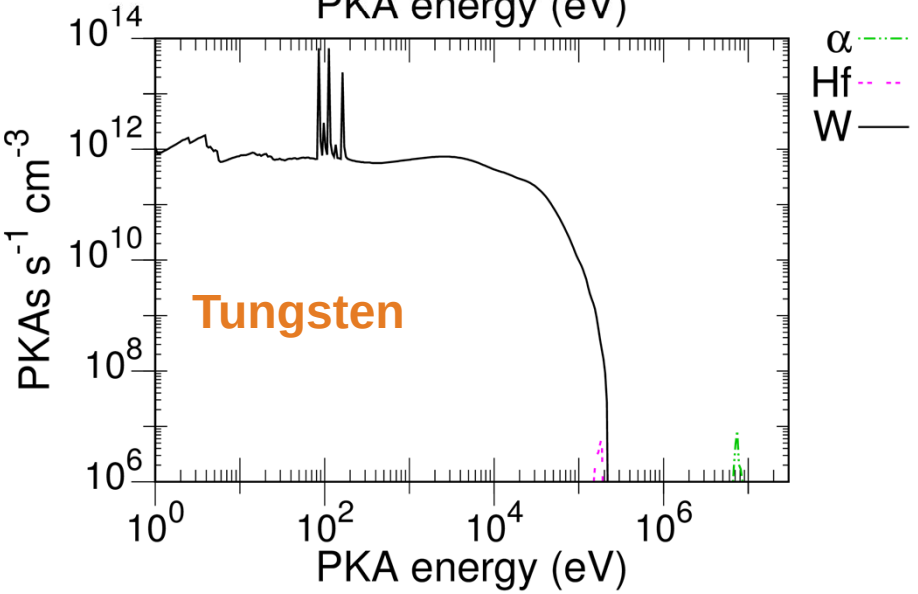
(5) PKA spectra

- PKAs in **different elements** under PWR conditions:



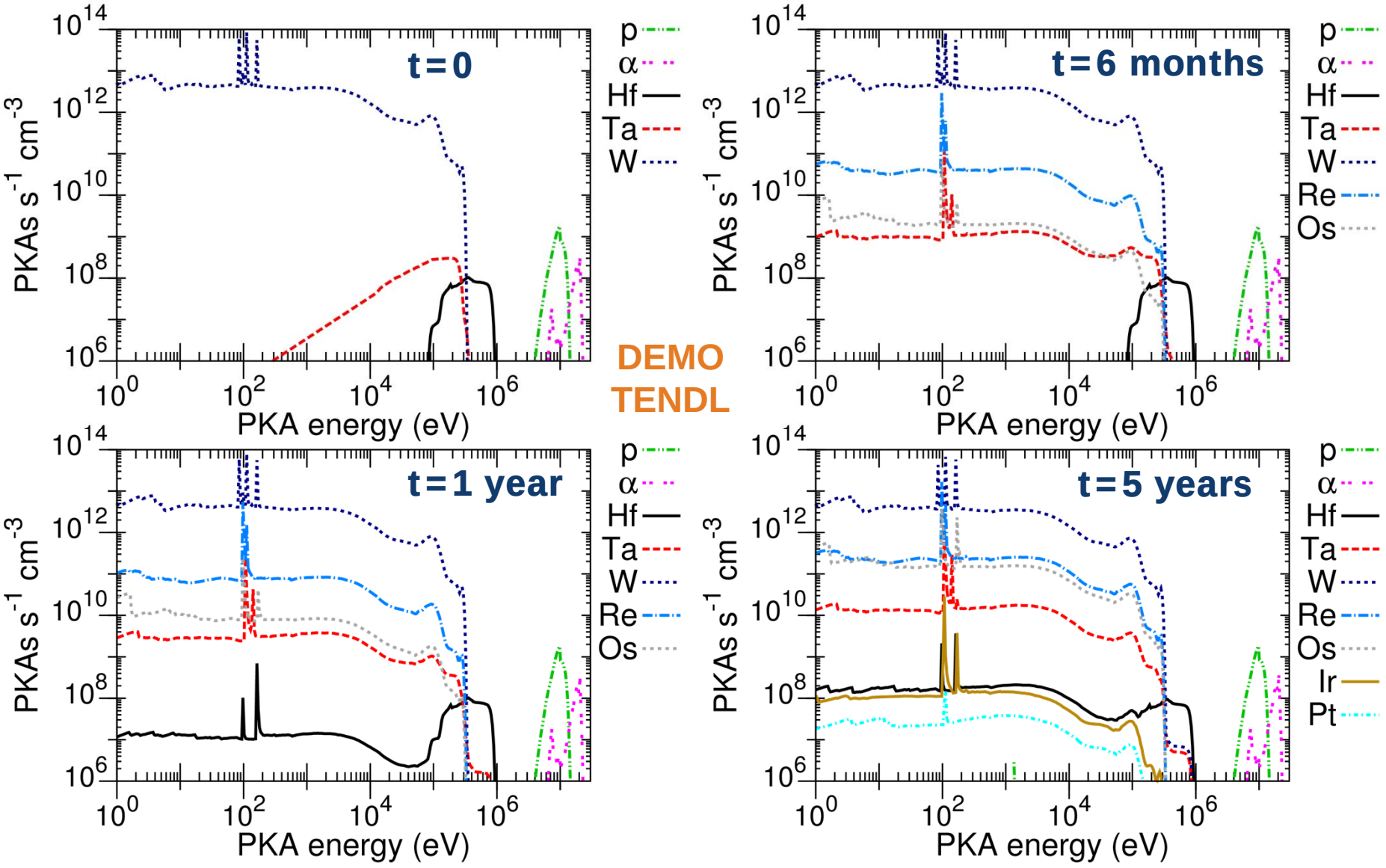






(5) PKA spectra – time evolution

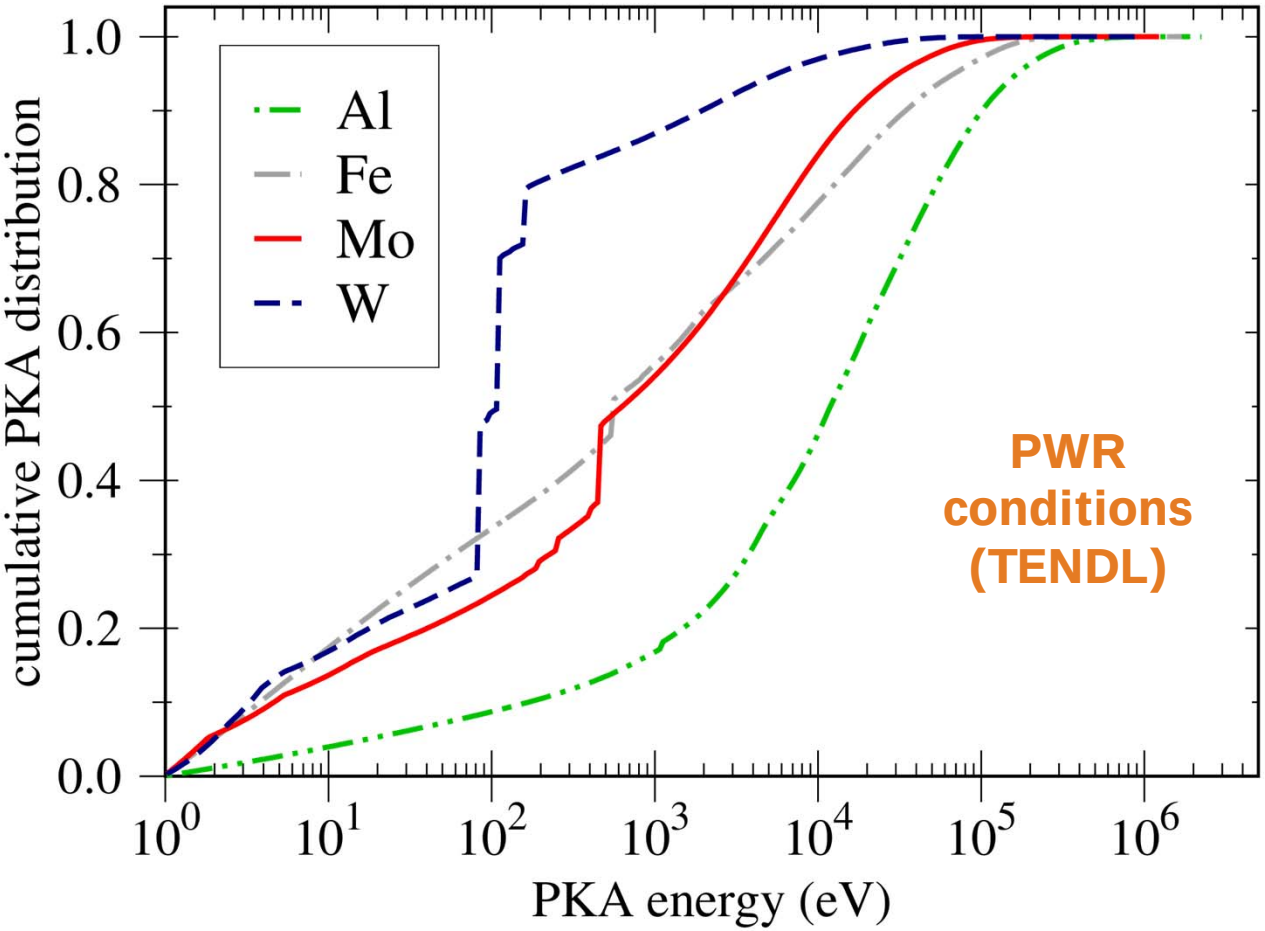
- FISPACT-II & SPECTRA-PKA can show time evolution due to transmutation



- PKAs from collisions with Re, Os, Ta, etc., appear with time

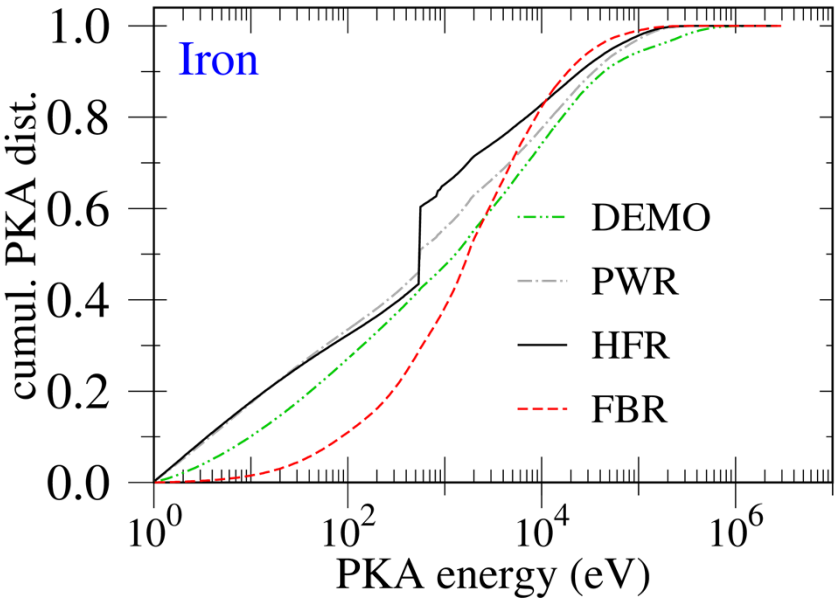
(5) Cumulative PKA distributions (CPDs)

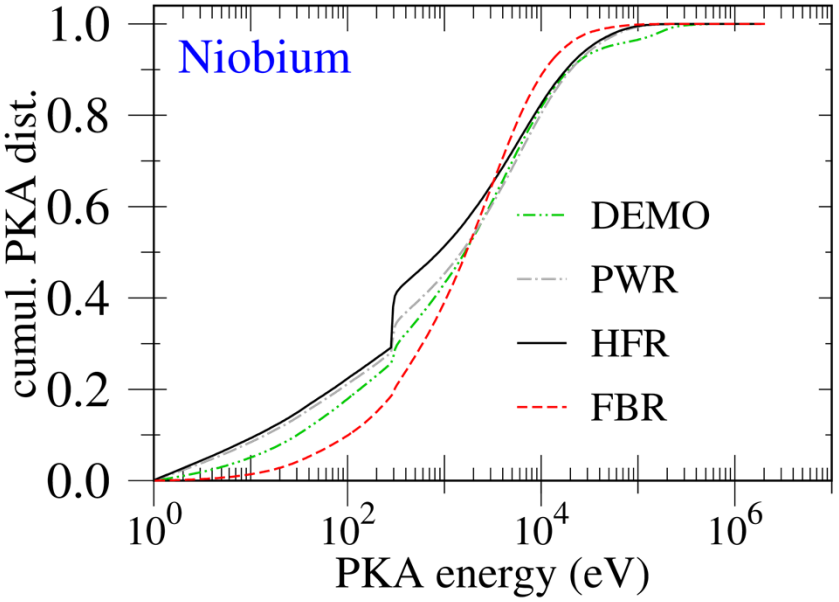
- Summing over all heavy recoils (gases excluded) reveals fundamental differences between materials
- **CPDs can be used as a sampling distribution for damage cascade modelling**

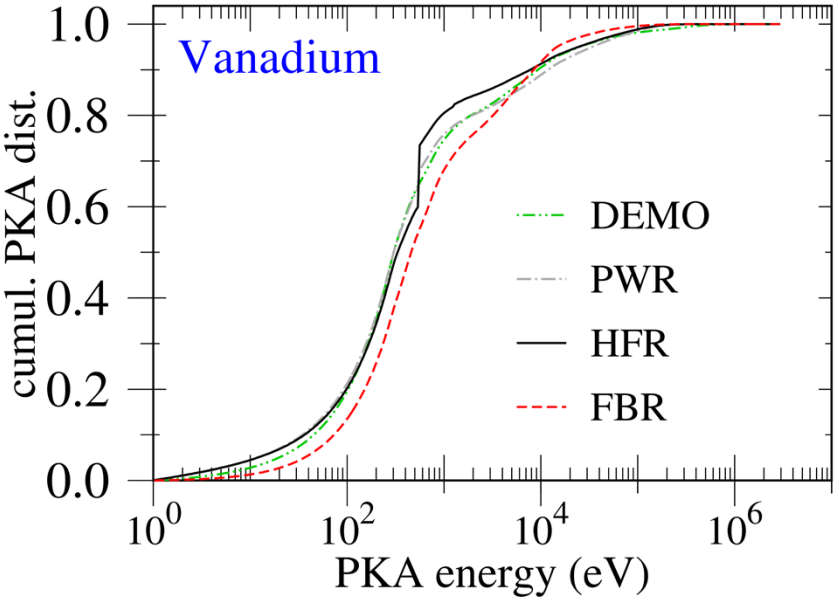


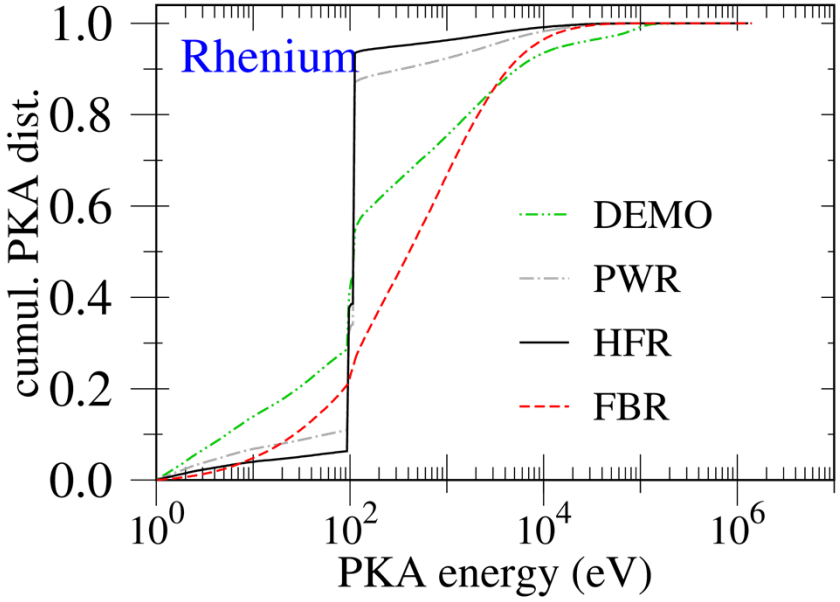
- Distributions of lighter elements shifted to higher energies

(5) CPDs: fusion vs. fission





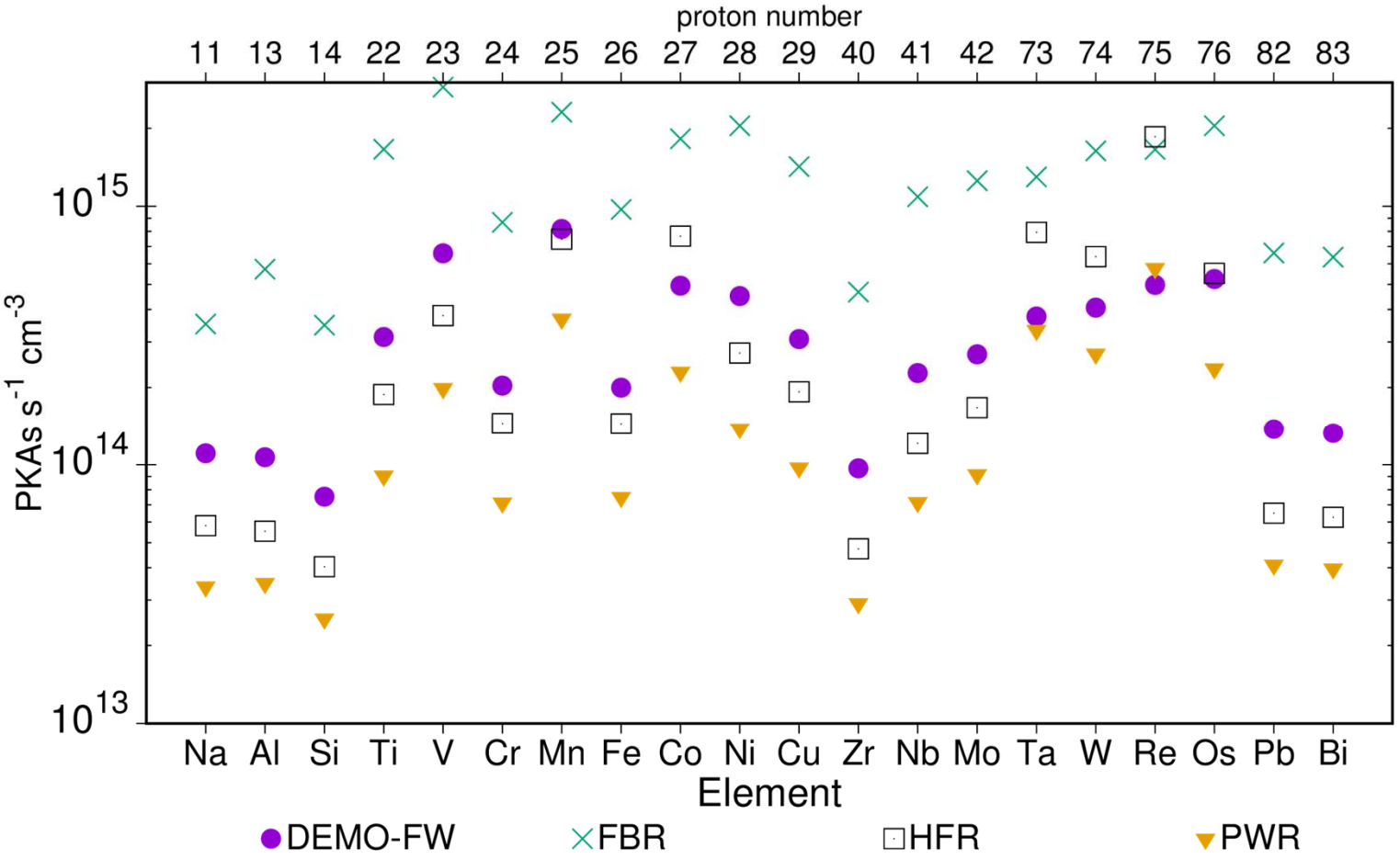




- FBR missing low and high energy parts due to peaked spectrum

(5) Total PKAs: fusion vs. fission

- Total 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
- More problems matching fusion in fission systems

(6) Reaction pathway analysis

- Separate FISPACT-II simulations for neutrons in each of four different energy ranges:
  - thermal or slow neutrons at energies from 0.02 to 0.05 eV (groups 525-545 inclusive from 709 structure)
  - intermediate neutrons from 20 to 40 keV (230-245)
  - fast neutrons at energies typically generated in fission reactors, from 1 to 3 MeV (136-160)
  - 13 to 15 MeV neutrons covering the 14 MeV neutrons generated in Deuterium-Tritium fusion reactions (85-95)
- Pathways requested using `UNCERTAINTY` key word:

`LOOKAHEAD` – look at long-cooling times for extra dominant nuclides

`TOLERANCE 1 5.0E1 1.0E-4` – optimised limits of solver

`UNCERT -1 0.001 0.01 25 2` – search limits & request output

(6) Reaction pathway analysis

- Pathways output for dominant/important radionuclides
  - appearing in either the importance diagrams or activation tables

Tungsten pathways for short-lived nuclides:

Nuclide	$T_{1/2}$	Pathway	0.02–0.05 eV	20–40 keV	1–3 MeV	13–15 MeV
W183m	5.25s	W182(n,γ)W183m	91.2	100.0	7.2	
		W180(n,γ)W181(β^+)Ta181(n,γ)Ta182(n,γ)Ta183(β^-)W183m	5.5			
		W180(n,γ)W181(β^+)Ta181(n,γ)Ta182m(IT)Ta182(n,γ) Ta183(β^-)W183m	3.1			
		W183(n,n$'$)W183m			91.5	1.4
		W184(n,2n)W183m				96.9
W185m	1.67m	W184(n,γ)W185m	71.4	98.2	98.8	
		W183(n,γ)W184(n,γ)W185m	15.7	1.8		
		W182(n,γ)W183(n,γ)W184(n,γ)W185m	12.9			
		W184(n,γ)W185(n,n$'$)W185m			1.0	
		W186(n,2n)W185m				99.8
Re188	16.98h	W186(n,γ)W187(β^-)Re187(n,γ)Re188	94.3	95.3	81.3	
		W186(n,γ)W187(β^-)Re187(n,γ)Re188m(IT)Re188	3.1	4.6	18.6	
W187	23.85h	W186(n,γ)W187	97.0	100.0	100.0	100.0
		W184(n,γ)W185(β^-)Re185(n,γ)Re186(β^+)W186(n,γ)W187	1.9			
Re186	3.75d	W184(n,γ)W185(β^-)Re185(n,γ)Re186	78.7	98.3	93.1	
		W183(n,γ)W184(n,γ)W185(β^-)Re185(n,γ)Re186	12.8			
		W182(n,γ)W183(n,γ)W184(n,γ)W185(β^-)Re185(n,γ)Re186	8.3			
		W184(n,γ)W185m(IT)W185(β^-)Re185(n,γ)Re186			6.2	
		W186(n,γ)W187(β^-)Re187(n,2n)Re186				82.7
		W186(n,2n)W185(β^-)Re185(n,γ)Re186				9.3
		W186(n,2n)W185m(IT)W185(β^-)Re185(n,γ)Re186				6.1

(6) Reaction pathway analysis

Tungsten pathways for long-lived nuclides:

Nuclide	$T_{1/2}$	Pathway	0.02–0.05 eV	20–40 keV	1–3 MeV	13–15 MeV
Ta182	114.71d	W180(n,γ)W181(β^+)Ta181(n,γ)Ta182	63.7	63.7	58.1	
		W180(n,γ)W181(β^+)Ta181(n,γ)Ta182m(IT)Ta182	36.2	36.2	40.3	
		W182(n,p)Ta182				47.3
		W182(n,p)Ta182m(IT)Ta182				38.0
		W182(n,p)Ta182n(IT)Ta182m(IT)Ta182				3.2
		W183(n,2n)W182(n,p)Ta182				2.7
		W183(n,2n)W182(n,p)Ta182m(IT)Ta182				2.2
W181	120.99d	W180(n,γ)W181	100.0	100.0	100.0	
		W182(n,2n)W181				93.8
		W183(n,2n)W182(n,2n)W181				5.3
Pt193	50.00y	no pathways found				
Re186m	2.0 10^5y	W184(n,γ)W185(β^-)Re185(n,γ)Re186m	81.0	98.6	93.6	
		W183(n,γ)W184(n,γ)W185(β^-)Re185(n,γ)Re186m	11.8			
		W182(n,γ)W183(n,γ)W184(n,γ)W185(β^-)Re185(n,γ)Re186m	7.0			
		W184(n,γ)W185m(IT)W185(β^-)Re185(n,γ)Re186m			6.3	
Re187	4.4 10^{10}y	W186(n,γ)W187(β^-)Re187	98.0	100.0	100.0	

- Different production pathways at different energies
- Useful for identifying main production routes for problem radionuclides
  - Possible reduction via isotopic tailoring

(6) Reaction pathway analysis

Tungsten pathways for ^{192}Ir:

Nuclide	$T_{1/2}$	Pathway	0.02–0.05 eV	20–40 keV	1–3 MeV	13–15 MeV
Ir192	73.80d	W186(n,γ)W187(β⁻)Re187(n,γ)Re188(β⁻)Os188(n,γ)Os189(n,γ)Os190(n,γ)Os191m(IT)Os191(β⁻)Ir191m(IT)Ir191(n,γ)Ir192m(IT)Ir192	45.1			
		W186(n,γ)W187(β⁻)Re187(n,γ)Re188(β⁻)Os188(n,γ)Os189(n,γ)Os190(n,γ)Os191m(IT)Os191(β⁻)Ir191m(IT)Ir191(n,γ)Ir192	31.5			
		W186(n,γ)W187(β⁻)Re187(n,γ)Re188(β⁻)Os188(n,γ)Os189(n,γ)Os190(n,γ)Os191(β⁻)Ir191m(IT)Ir191(n,γ)Ir192m(IT)Ir192	5.5			
		W186(n,γ)W187(β⁻)Re187(n,γ)Re188(β⁻)Os188(n,γ)Os189(n,γ)Os190(n,γ)Os191(β⁻)Ir191m(IT)Ir191(n,γ)Ir192	3.8			
		W186(n,γ)W187(β⁻)Re187(n,γ)Re188(β⁻)Os188(n,γ)Os189m(IT)Os189(n,γ)Os190(n,γ)Os191m(IT)Os191(β⁻)Ir191m(IT)Ir191(n,γ)Ir192m(IT)Ir192	3.7			
		W186(n,γ)W187(β⁻)Re187(n,γ)Re188(β⁻)Os188(n,γ)Os189m(IT)Os189(n,γ)Os190(n,γ)Os191m(IT)Os191(β⁻)Ir191m(IT)Ir191(n,γ)Ir192	2.6			
		W186(n,γ)W187(β⁻)Re187(n,γ)Re188m(IT)Re188(β⁻)Os188(n,γ)Os189(n,γ)Os190(n,γ)Os191m(IT)Os191(β⁻)Ir191m(IT)Ir191(n,γ)Ir192m(IT)Ir192	1.5			
		W186(n,γ)W187(β⁻)Re187(n,γ)Re188m(IT)Re188(β⁻)Os188(n,γ)Os189(n,γ)Os190(n,γ)Os191m(IT)Os191(β⁻)Ir191m(IT)Ir191(n,γ)Ir192	1.0			

- The production pathways can be very long
  - Particularly at low neutron energy where chains of capture and beta decays occur

Scoping studies summary

- Automated simulation, processing, and reporting structure provides the flexibility to perform scoping studies
  - for different libraries
  - for different irradiation conditions/environments
- Made possible by the suitability of FISPACT-II for scripting
  - 10s of thousands of calculations can be routinely and automatically run
- Element response database, compiled into a report of tabulated & graphical outputs, provides a useful reference for material selection and design activities
- Handbooks also represent a comprehensive test and validation of FISPACT-II and the nuclear data libraries