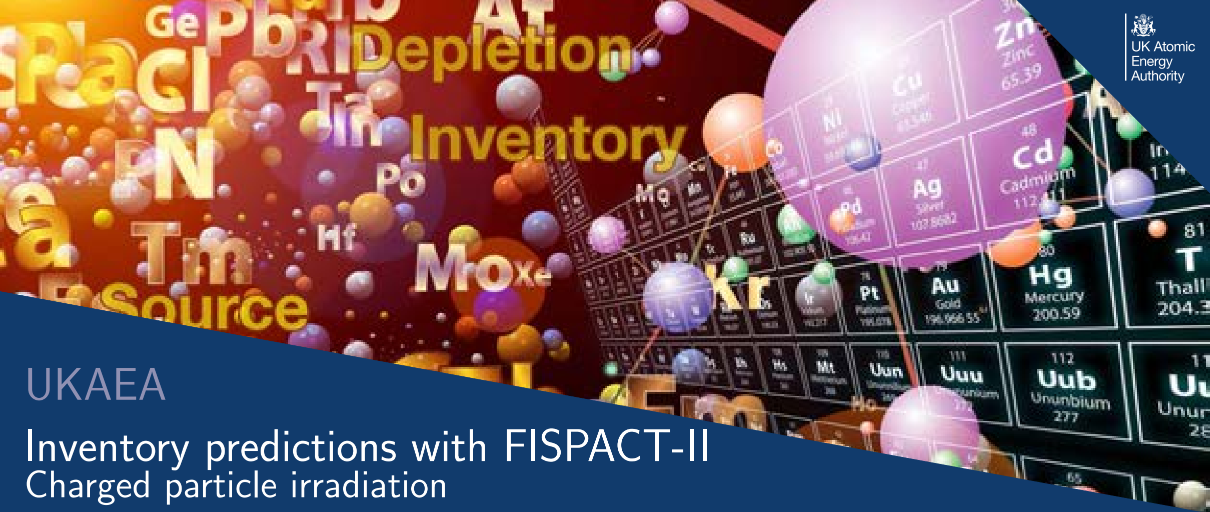

UK Atomic Energy Authority

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Inventory predictions with FISPACT-II
Charged particle irradiation

Mark Gilbert
United Kingdom Atomic Energy Authority

ROYCE TRAINING: ION BEAM IRRADIATION AND CHARACTERISATION - BEST PRACTICE

March 2, 2023

Engineering and Physical Sciences Research Council

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CULHAM CENTRE FOR FUSION ENERGY

This work was funded by the RCUK Energy Programme
[Grant number EP/W006839/1]

Outline

1. Inventory simulations
    - Needs & numerical methodology
    - inputs & outputs
    - neutron examples
2. Charged particle irradiation
    - p/α differences from neutrons
    - simulation methods
    - proton monoenergetic examples

1: Introduction to inventory simulations

What are inventory simulations?

- Inventory simulations are used to predict how the chemical composition of a material will be altered under (neutron/proton/α) irradiation
  - and/or by the decay of radioactive species

- other terms: transmutation, burn-up

Motivation

- vital to have reliable predictions of these time-dependent changes
  - for inclusion in engineering design studies of nuclear systems, including reactors, accelerators, and ion-beams
  - for use to define operational limits & safe working lifetimes of components in fusion/fission devices
  - to evaluate expected masses and costs of waste disposal
  - to support the design of irradiation experiments including predictions of radiological hazards

How to predict inventory change

- via solutions to Inventory rate equations:

$$\frac{dN_i}{dt} = \underbrace{-N_i(\lambda_i + \sigma_i\phi)}_{\text{loss}} + \sum_{j\neq i} \underbrace{N_j(\lambda_{ji} + \sigma_{ji}\phi)}_{\text{creation}}$$

- coupled differential equations
  - one equation for each nuclide i at concentration N_i
  - typically solved numerically & used to evolve composition in time
- σ_{ji} [cm^2]: average reaction rate cross section for $j \rightarrow i$ reaction
  - reactions include (n,γ), (n,α), (n,2n), (p,n), (α,n), etc.
  - obtained by collapsing energy-dependent cross sections (typically from nuclear data libraries) with projectile (n/p/α) energy spectra
  - σ_i is sum over all $i \rightarrow j$ reactions
- λ_i, λ_{ji} decay constants [s^{-1}]
- ϕ total projectile flux [cm^{-2} s^{-1}]

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Methodology details

- assumed that irradiation spectrum (energy profile) is not altered by change in composition in a time-step
- and also that spectrum is the same for all atoms in a material (zero dimensional approximation)

→ equations are linear and coefficients are constant and independent of Ns

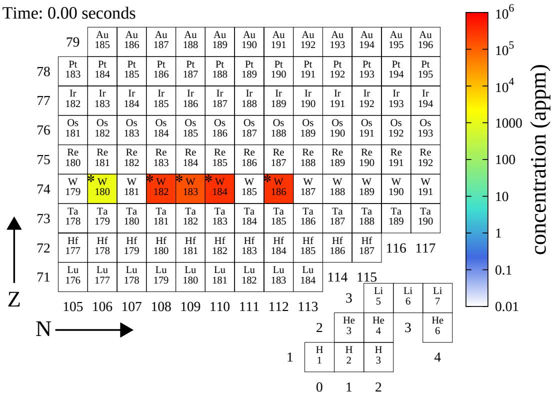
∴ can be expressed in matrix form:

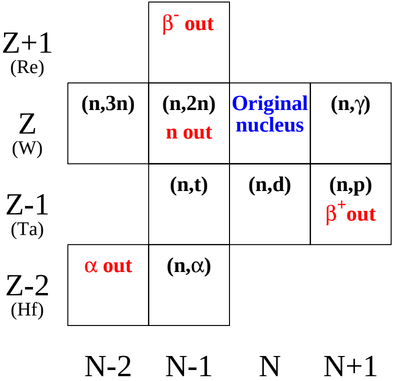
$$\dot{\mathbf{N}} = \mathbf{A}\mathbf{N} = (\boldsymbol{\Lambda} + \phi\boldsymbol{\Sigma})\mathbf{N}$$

- the matrix **A** is sparse ($\sim 3\%$ occupied even when fission is included)
- & stiff due to very large range of decay constants (i.e. small change in solutions have large fluctuations)
- the FISPACT-II inventory code uses the well-established LSODE package for this stiff and sparse system of linear ODEs

Inventory evolution example

- 5-year irradiation of pure tungsten in D-T fusion neutron environment
- nuclide/isotope distribution changes with time





"chart of nuclide visualization": *Nucl. Sci. Eng* **117** (2014) 291-306

appm - atomic parts per million
*nuclide present in input composition
m – concentration dominated by metastable state

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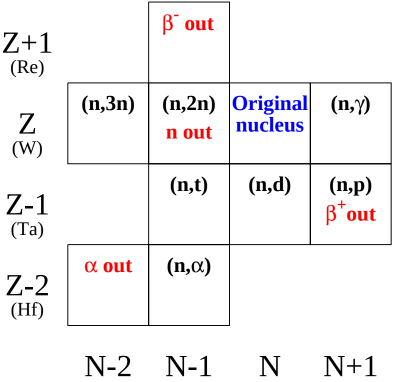

	N-2	N-1	N	N+1
Z+1 (Re)		β^- **out**		
Z (W)	**(n,3n)**	**(n,2n)** **n out**	**Original nucleus**	**(n,γ)**
Z-1 (Ta)		**(n,t)**	**(n,d)**	**(n,p)** β^+**out**
Z-2 (Hf)	α **out**	**(n,α)**		

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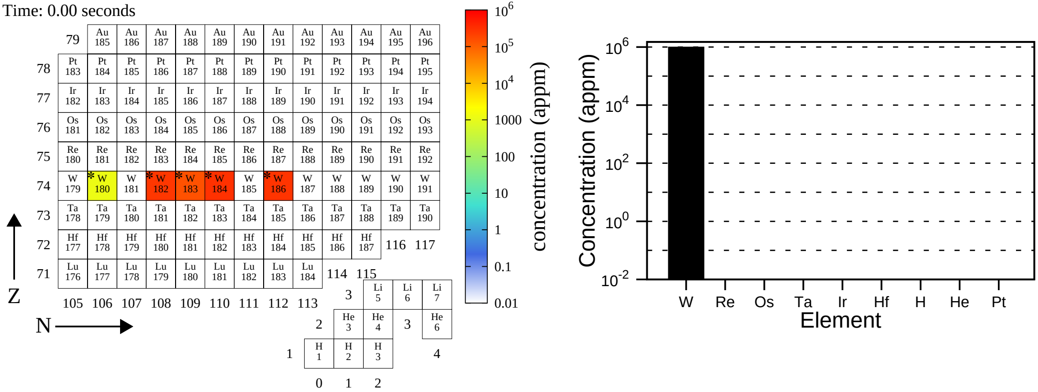

Z \ N	105	106	107	108	109	110	111	112	113	114	115	116	117
79		Au 185	Au 186	Au 187	Au 188	Au 189	Au 190	Au 191	Au 192	Au 193	Au 194	Au 195	Au 196
78	Pt 183	Pt 184	Pt 185	Pt 186	Pt 187	Pt 188	Pt 189	Pt 190	Pt 191	Pt 192	Pt 193	Pt 194	Pt 195
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71	Lu 176	Lu 177	Lu 178	Lu 179	Lu 180	Lu 181	Lu 182	Lu 183	Lu 184				

Z \ N	0	1	2	3	4
3			Li 5	Li 6	Li 7
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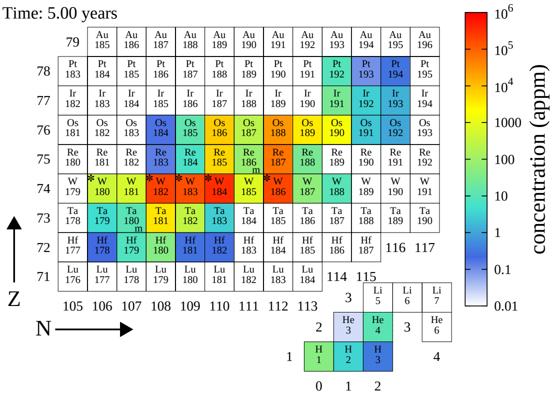

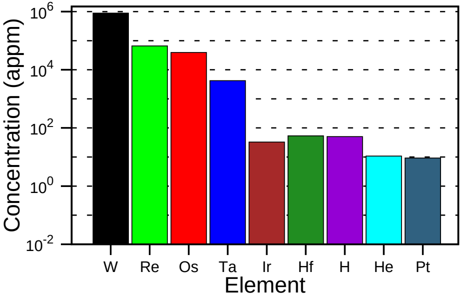

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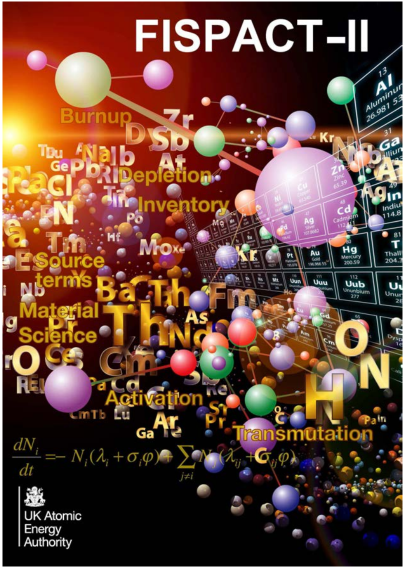
Inventory simulation platform

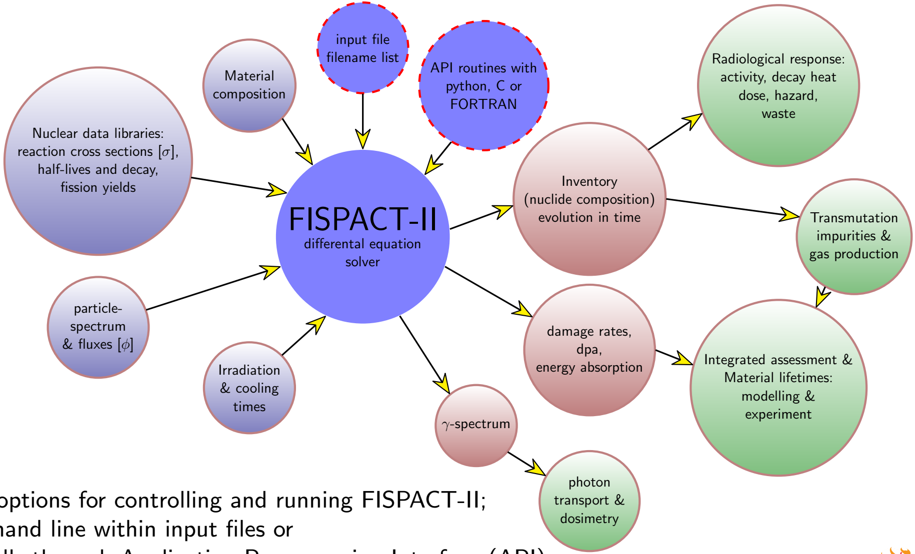


- multiphysics platform for predicting the composition changes under both neutron and charged-particle interactions
  - calculates activation, transmutation, burn-up, dpa, gas production, gamma spectra, etc.
- can use all major nuclear data libraries containing nuclear reaction data, radioactive decay data and fission yield data

  `fispact.ukaea.uk`

  `fispact.ukaea.uk/wiki`
- Available from OECD/NEA-databank `https://www.oecd-nea.org/tools/abstract/detail/nea-1890/`

Inventory calculations: data flow



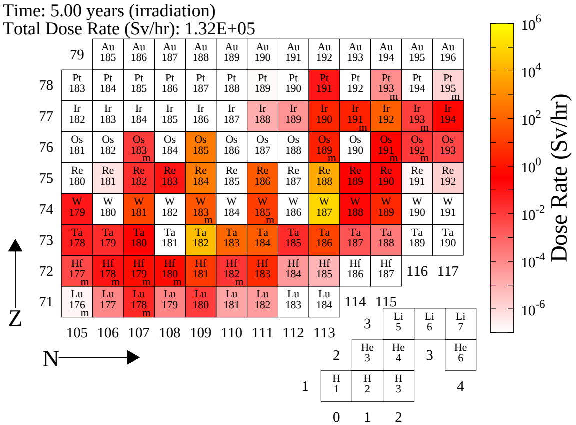
Two options for controlling and running FISPACT-II;
command line within input files or
via calls through Application Programming Interface (API)

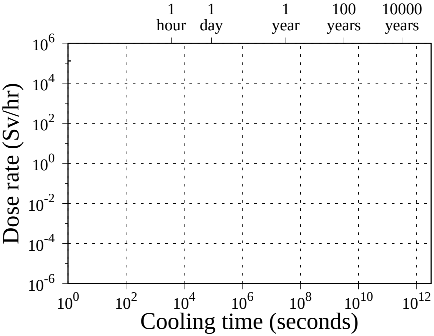
Types of radiological output

- Activity measured in becquerels (Bq) – number of disintegrations (decays) per second – the primary measure
    - can be separated by decay type – α, β, γ
- decay heat, measured in kilowatts (kW)
    - can be separated by decay type - α, β, γ
    - how much heat will be generated by the decay of radioactive species even after irradiation
- γ dose rate, measured in Sieverts (Sv) per hour
    - contact or point dose approximations only in inventory codes
    - J kg^{-1} deposition rate of radiation energy in biological tissue
    - and also ingestion and inhalation hazard conversions
- clearance index
    - IAEA based measure
    - a nuclide can be disposed of as if it were non radioactive when the index is less than 1

Radiological response evolution example

- Starting from contact dose rate after 5-year irradiation of pure W
- nuclide chart shows decay of radionuclides
- sum over all nuclides give total dose output





m – Dose Rate dominated by metastable nuclide(s)

Radiological response evolution example

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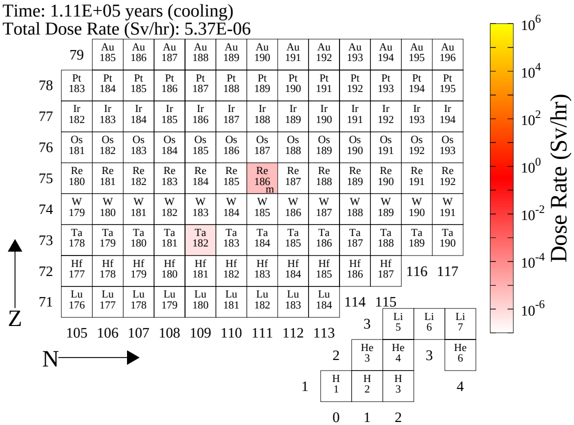
Time: 1.11E+05 years (cooling)
Total Dose Rate (Sv/hr): 5.37E-06

Z \ N	105	106	107	108	109	110	111	112	113	114	115	116	117
79		Au 185	Au 186	Au 187	Au 188	Au 189	Au 190	Au 191	Au 192	Au 193	Au 194	Au 195	Au 196
78	Pt 183	Pt 184	Pt 185	Pt 186	Pt 187	Pt 188	Pt 189	Pt 190	Pt 191	Pt 192	Pt 193	Pt 194	Pt 195
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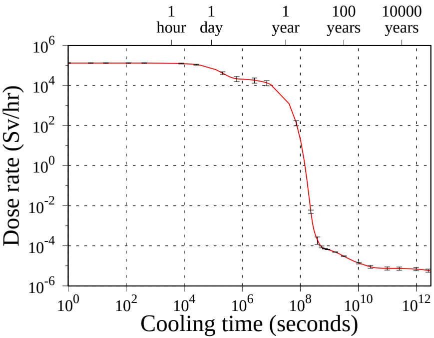
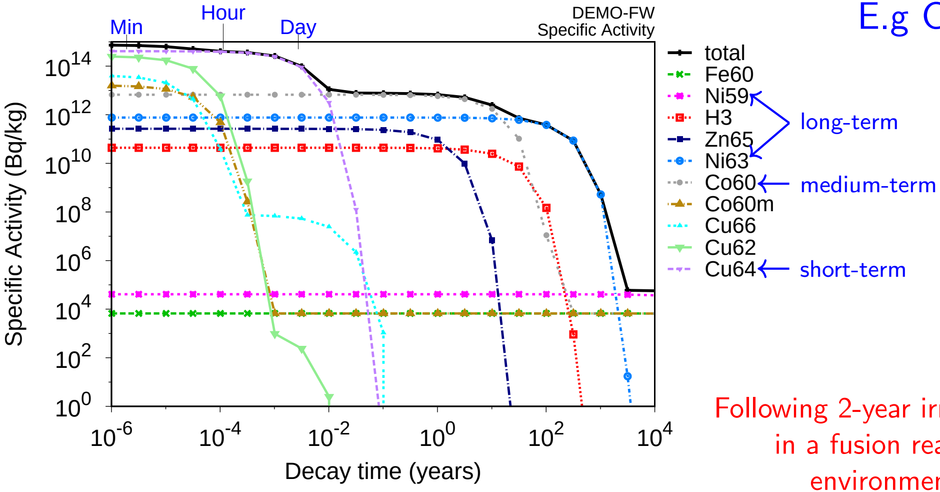


m – Dose Rate dominated by metastable nuclide(s)

Activation response – full nuclide contributions

- Evolution for (dominant) nuclide contributions as a function of time

E.g Copper



long-term

medium-term

short-term

Following 2-year irradiations in a fusion reactor environment

- shows which nuclides are important and when

Nuclear data libraries – recommendation

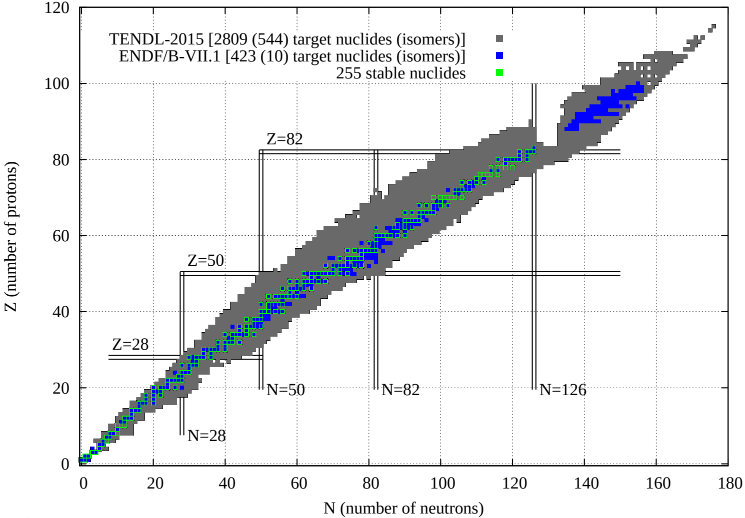
TENDL (latest version 2021[†])

- TALYS-based Evaluated Nuclear Data Libraries
- generated using various physical, theoretical, and semi-empirical models
- fully-automated production with *near* complete coverage of nuclides & reactions
  - avoids under-estimation due to missing data
- contains data more than 2800 target nuclides with half-lives $>$ 1 second
  - includes sub-libraries for neutron, d, t, p, α, ^{3}He, γ exposure
  - need to be combined with a decay library, various available
    - decay2020, available from FISPACT website, is recommended
- processed versions for FISPACT-II are not pointwise – data is stored on a fixed energy grid; neutron one is higher resolution than charged particle ones

[†] A. J. Koning, D. Rochman, *et al.*. Release date: December 30, 2021.
https://tendl.web.psi.ch/tendl_2021/tendl2021.html
FISPACT-II compatible versions available there

TENDL nuclide coverage

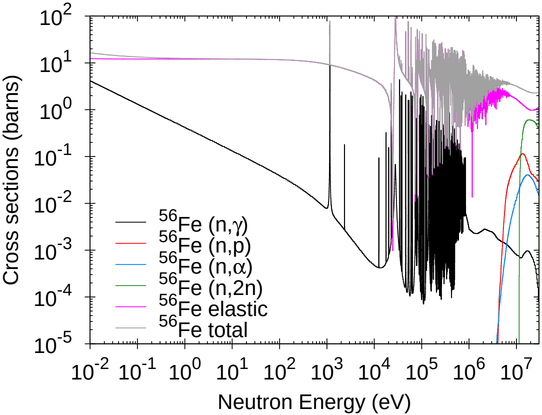
- Target nuclide coverage in TENDL libraries is more complete than elsewhere:



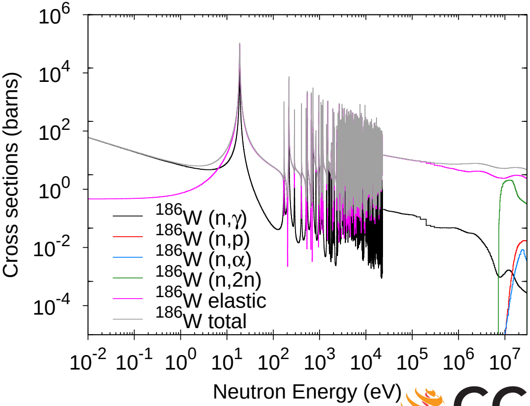
- Many more isomeric states are included as both targets (parents) and daughters of reactions – vital for correct prediction of activity

2. Charged particle irradiation

Typical cross sections σ – neutrons

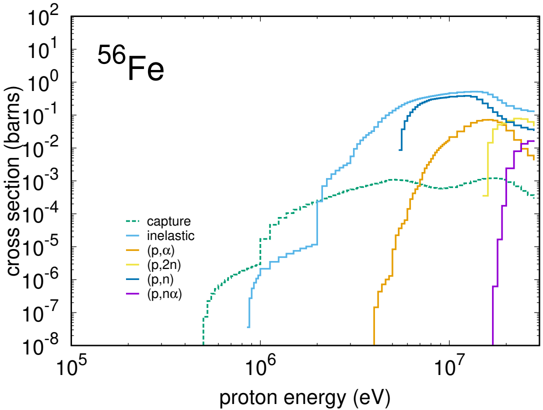


- cross section (xs) ≈ ‘reaction likelihood’
- Many different reactions possible on each nuclide/isotope



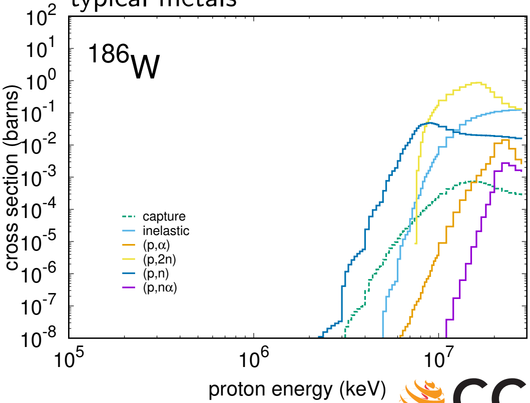
- Most channels are threshold type and are only ‘open’ at high energy
- but neutron capture can happen at all energies

Typical cross sections σ – protons

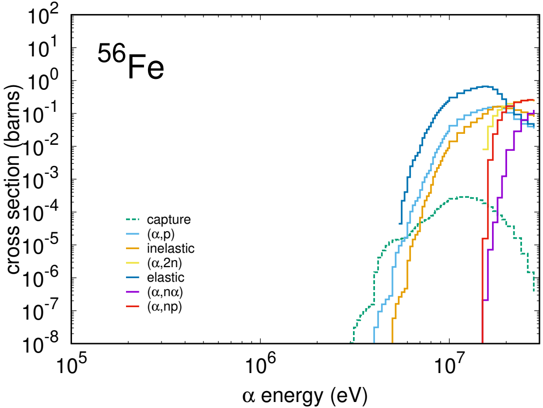


- similar break-up reactions as seen for neutron irradiation also occur

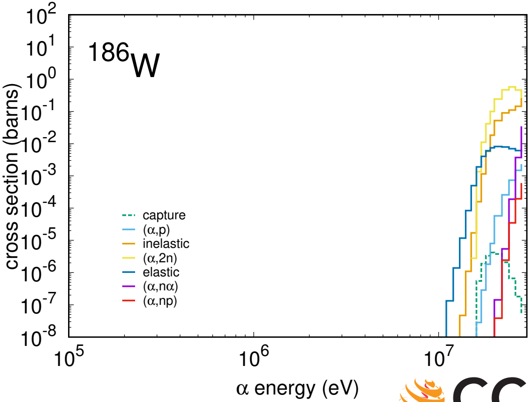
- under proton irradiation, capture has a threshold due to the coulomb barrier and only becomes significant at MeV energies in typical metals



Typical cross sections $\sigma - \alpha$



- similar under α bombardment
- only high energy irradiation will cause transmutation and activation

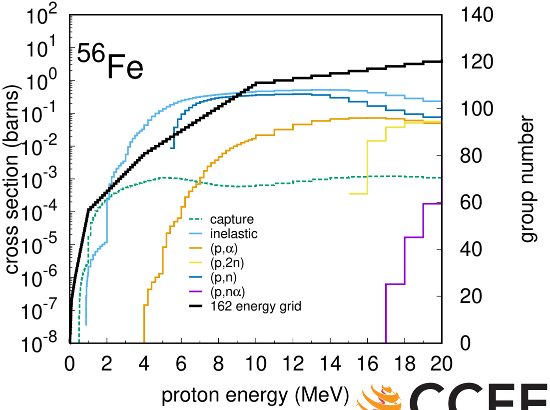


Monoenergetic irradiation comparisons

- scoping of response as a function of beam (irradiation) energy

Methodology

- monoenergetic irradiation beam approximated as particles in one or more of the energy bins used to store the cross section data
- Irradiation conditions:
  Flux of 10^{13} particles $\mathrm{cm}^{-2}\ \mathrm{s}^{-1}$
  6 month irradiation
- Activity calculated at end of irradiation and following 6 months of decay cooling
- identical simulations performed with neutrons, protons, α



Running FISPACT-II

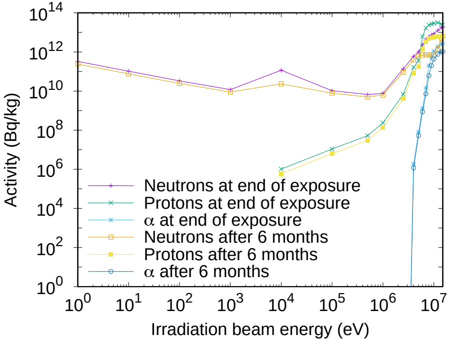
Difference between particle types

- select particle type (`PROJECTILE` keyword or)
- point to the correct library of cross sections (from TENDL)
    - `xs_endf` in 'files'
- everything else the same

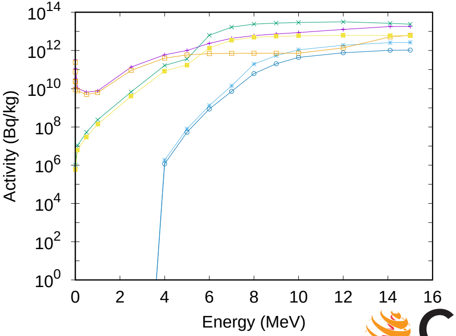
Creating different beam energies

- create a pseudo-monoenergetic spectrum using `GRPCONVERT`
    - arbitrary flux file (`arb_flux`) specifying one energy bin that can be translated to a spectrum with the correct energy grid to merge with reaction data
- see wiki or manual for more details (& API manual for equivalent keys)

monoenergetic beam results: Fe



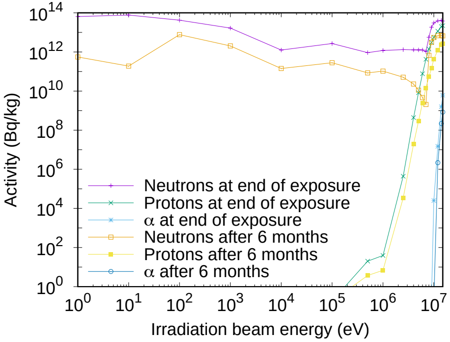
- Proton irradiation at low energy produces much less activation that equivalent energies of neutron irradiation
- however, above ∼5 MeV the p-induced activity can be higher than with neutrons

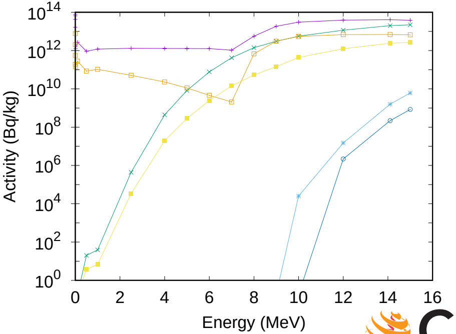


- Similar with α-particle irradiation, although no scenario in this case where α-induced activity is higher than the neutron case (at t=0)

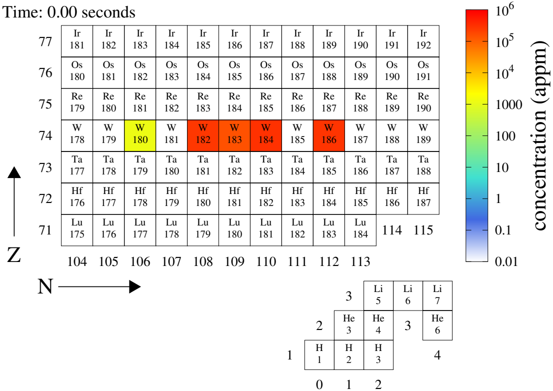
monoenergetic beam results: W

- more extreme difference in some materials
- in W, the high capture cross sections at low neutron energies produces a high activation response





Protons vs neutrons W at 14 MeV



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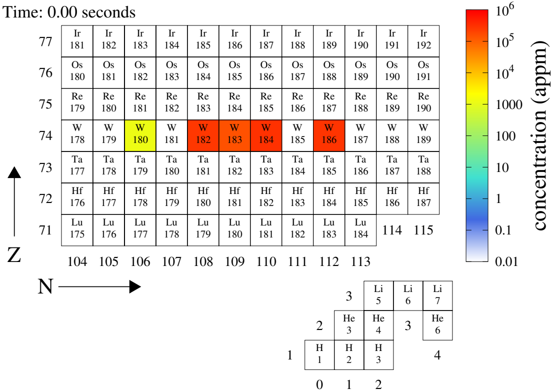
W



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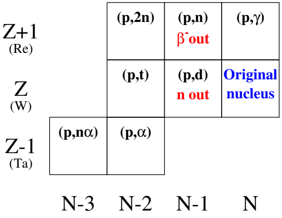
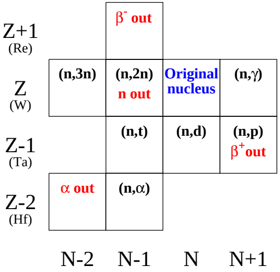


	N-3	N-2	N-1	N
Z+1 (Re)		**(p,2n)**	**(p,n)** **β⁻out**	**(p,γ)**
Z (W)		**(p,t)**	**(p,d)** **n out**	**Original nucleus**
Z-1 (Ta)	**(p,nα)**	**(p,α)**		

Proton

14 MeV beam



	N-2	N-1	N	N+1
Z+1 (Re)		**β⁻ out**		
Z (W)	**(n,3n)**	**(n,2n)** **n out**	**Original nucleus**	**(n,γ)**
Z-1 (Ta)		**(n,t)**	**(n,d)**	**(n,p)** **β⁺out**
Z-2 (Hf)	**α out**	**(n,α)**		

neutron

flux:
10^{14} particles
$\mathrm{cm}^{-2}\ \mathrm{s}^{-1}$

W

	N-3	N-2	N-1	N
Z+1 (Re)		**(p,2n)**	**(p,n)** **β^-out**	**(p,γ)**
Z (W)		**(p,t)**	**(p,d)** **n out**	**Original nucleus**
Z-1 (Ta)	**(p,nα)**	**(p,α)**		

Proton

14 MeV beam

	N-2	N-1	N	N+1
Z+1 (Re)		**β^- out**		
Z (W)	**(n,3n)**	**(n,2n)** **n out**	**Original nucleus**	**(n,γ)**
Z-1 (Ta)		**(n,t)**	**(n,d)**	**(n,p)** **β^+out**
Z-2 (Hf)	**α out**	**(n,α)**		

neutron

flux:
10^{14}particles
cm^{-2} s^{-1}

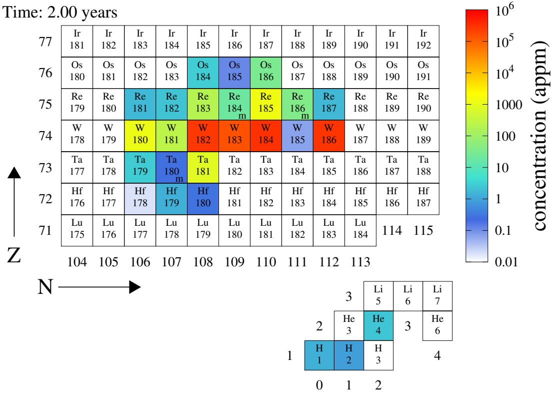
W

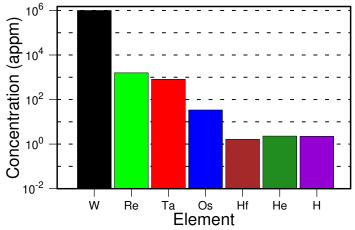
Proton

neutron

14 MeV
beam

flux:
10^{14}particles
$\mathrm{cm}^{-2}\ \mathrm{s}^{-1}$

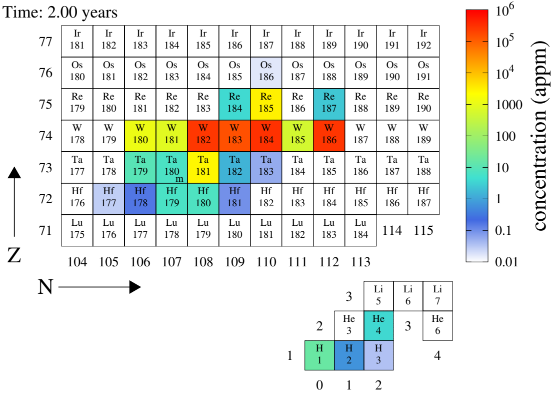


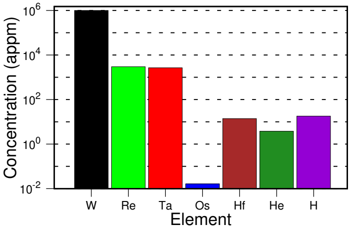


Proton

W

14 MeV beam

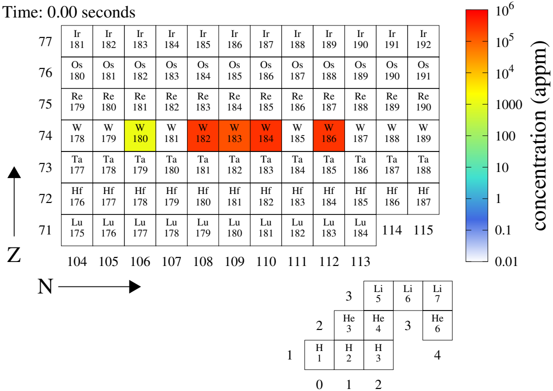




neutron

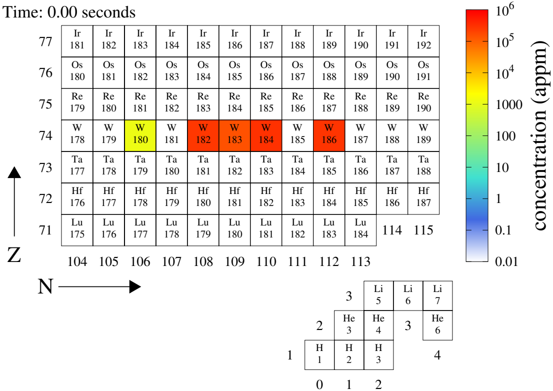
flux: 10^{14} particles $\mathrm{cm}^{-2}\ \mathrm{s}^{-1}$

α vs neutrons
W at 14 MeV



Z \ N	104	105	106	107	108	109	110	111	112	113	114	115
77	Ir 181	Ir 182	Ir 183	Ir 184	Ir 185	Ir 186	Ir 187	Ir 188	Ir 189	Ir 190	Ir 191	Ir 192
76	Os 180	Os 181	Os 182	Os 183	Os 184	Os 185	Os 186	Os 187	Os 188	Os 189	Os 190	Os 191
75	Re 179	Re 180	Re 181	Re 182	Re 183	Re 184	Re 185	Re 186	Re 187	Re 188	Re 189	Re 190
74	W 178	W 179	W 180	W 181	W 182	W 183	W 184	W 185	W 186	W 187	W 188	W 189
73	Ta 177	Ta 178	Ta 179	Ta 180	Ta 181	Ta 182	Ta 183	Ta 184	Ta 185	Ta 186	Ta 187	Ta 188
72	Hf 176	Hf 177	Hf 178	Hf 179	Hf 180	Hf 181	Hf 182	Hf 183	Hf 184	Hf 185	Hf 186	Hf 187
71	Lu 175	Lu 176	Lu 177	Lu 178	Lu 179	Lu 180	Lu 181	Lu 182	Lu 183	Lu 184		

Z \ N	0	1	2	3	4
3			Li 5	Li 6	Li 7
2		He 3	He 4		He 6
1	H 1	H 2	H 3		



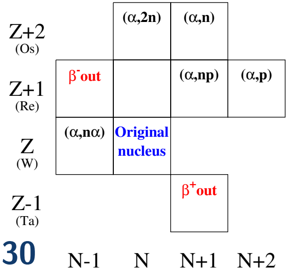
Z \ N	104	105	106	107	108	109	110	111	112	113	114	115
77	Ir 181	Ir 182	Ir 183	Ir 184	Ir 185	Ir 186	Ir 187	Ir 188	Ir 189	Ir 190	Ir 191	Ir 192
76	Os 180	Os 181	Os 182	Os 183	Os 184	Os 185	Os 186	Os 187	Os 188	Os 189	Os 190	Os 191
75	Re 179	Re 180	Re 181	Re 182	Re 183	Re 184	Re 185	Re 186	Re 187	Re 188	Re 189	Re 190
74	W 178	W 179	W 180	W 181	W 182	W 183	W 184	W 185	W 186	W 187	W 188	W 189
73	Ta 177	Ta 178	Ta 179	Ta 180	Ta 181	Ta 182	Ta 183	Ta 184	Ta 185	Ta 186	Ta 187	Ta 188
72	Hf 176	Hf 177	Hf 178	Hf 179	Hf 180	Hf 181	Hf 182	Hf 183	Hf 184	Hf 185	Hf 186	Hf 187
71	Lu 175	Lu 176	Lu 177	Lu 178	Lu 179	Lu 180	Lu 181	Lu 182	Lu 183	Lu 184		

Z \ N	0	1	2	3	4
3			Li 5	Li 6	Li 7
2		He 3	He 4		He 6
1	H 1	H 2	H 3		

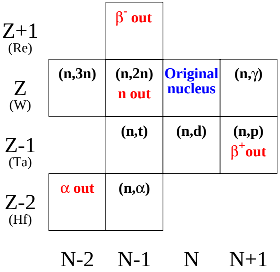
W

α

neutron



	N-1	N	N+1	N+2
Z+2 (Os)		**(α,2n)**	**(α,n)**	
Z+1 (Re)	**β⁻ out**		**(α,np)**	**(α,p)**
Z (W)	**(α,nα)**	**Original nucleus**		
Z-1 (Ta)			**β⁺ out**	



	N-2	N-1	N	N+1
Z+1 (Re)		**β⁻ out**		
Z (W)	**(n,3n)**	**(n,2n)** **n out**	**Original nucleus**	**(n,γ)**
Z-1 (Ta)		**(n,t)**	**(n,d)**	**(n,p)** **β⁺ out**
Z-2 (Hf)	**α out**	**(n,α)**		

14 MeV
beam

flux:
10^{14} particles
$\mathrm{cm}^{-2}\ \mathrm{s}^{-1}$

W

α

	N-1	N	N+1	N+2
Z+2 (Os)		(α,2n)	(α,n)	
Z+1 (Re)	β⁻out		(α,np)	(α,p)
Z (W)	(α,nα)	Original nucleus		
Z-1 (Ta)			β⁺out	

14 MeV beam

neutron

	N-2	N-1	N	N+1
Z+1 (Re)		β⁻ out		
Z (W)	(n,3n)	(n,2n) n out	Original nucleus	(n,γ)
Z-1 (Ta)		(n,t)	(n,d)	(n,p) β⁺out
Z-2 (Hf)	α out	(n,α)		

flux:
10^{14}particles
$\mathrm{cm}^{-2}\ \mathrm{s}^{-1}$

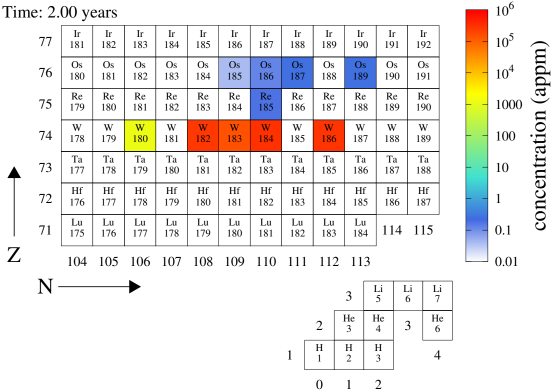
W

α

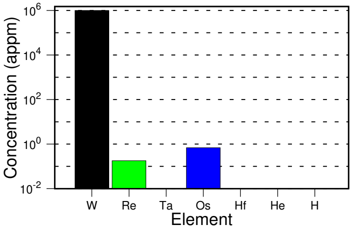
neutron

14 MeV
beam

flux:
10^{14}particles
cm^{-2} s^{-1}

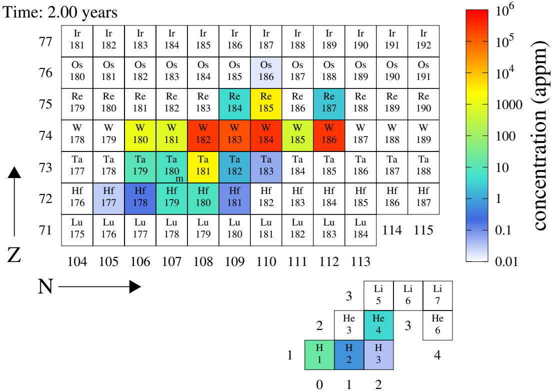


W

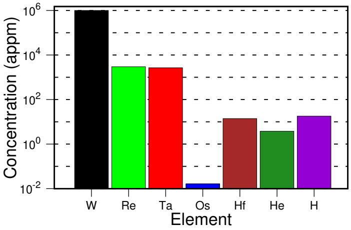


α

14 MeV beam

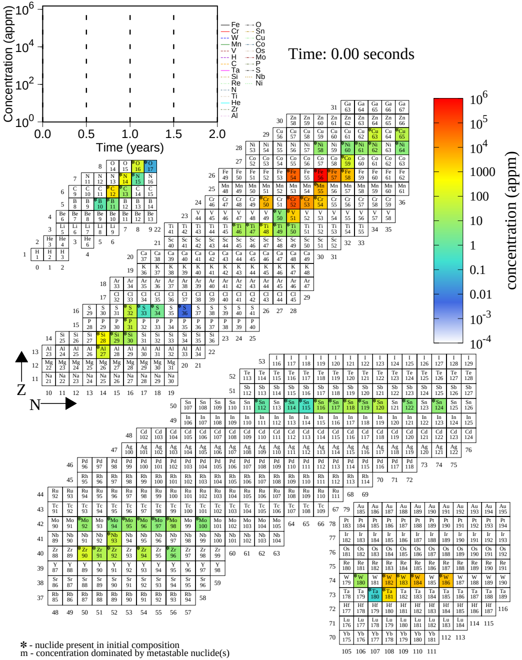


neutron



flux:
10^{14}particles
cm^{-2} s^{-1}

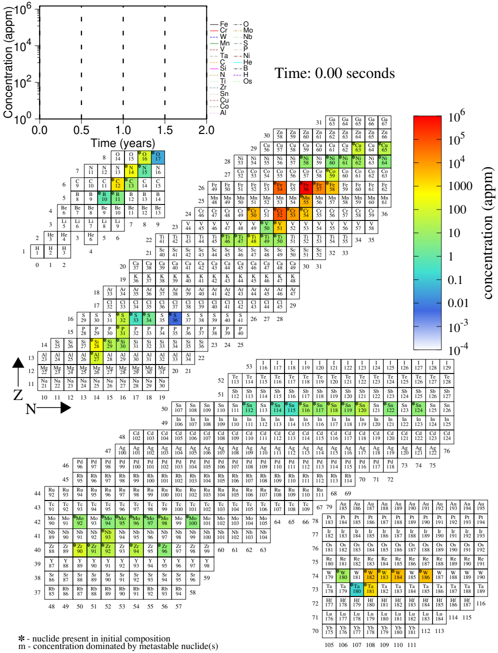
EUROFER at 8 MeV



Fusion FW
←

EUROFER

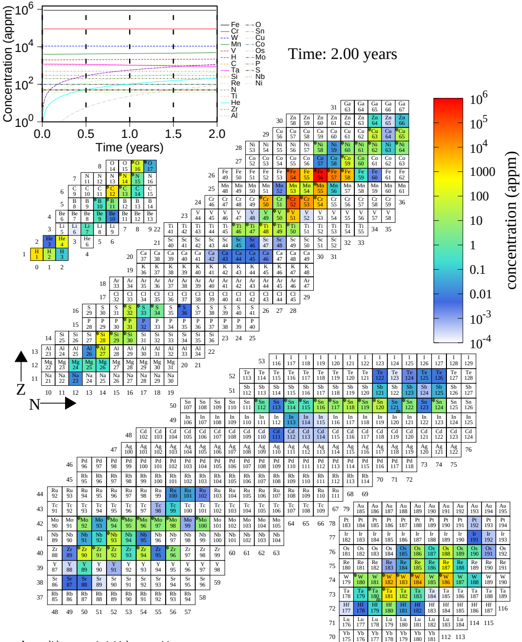
8 MeV Protons
→
10^{14} flux



Fusion
FW
←

EUROFER

8 MeV
Protons
→
10^{14}
flux



* - nuclide present in initial composition
m - concentration dominated by metastable nuclide(s)

Fusion FW

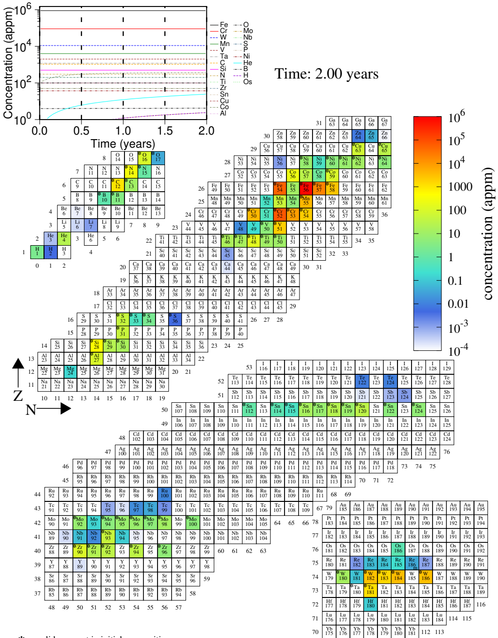
←

EUROFER

8 MeV Protons

→

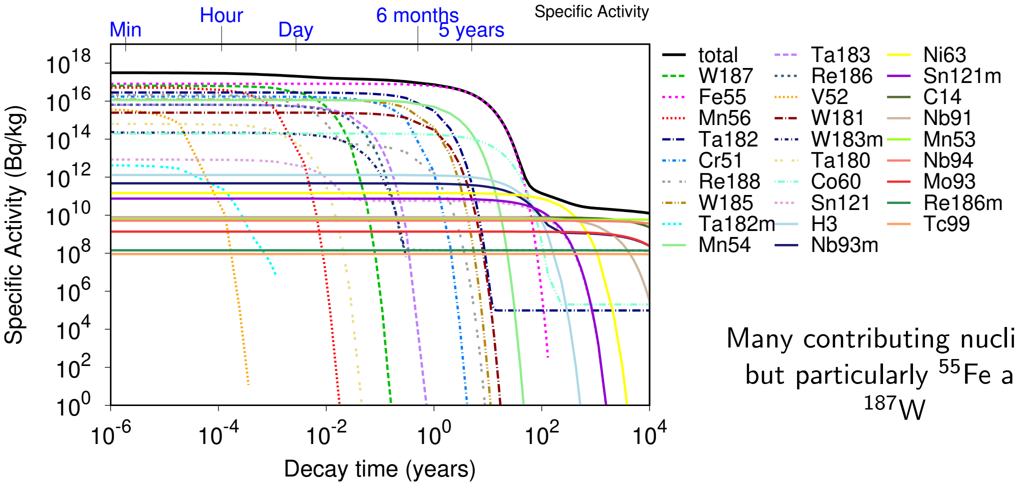
10^{14} flux



* - nuclide present in initial composition
m - concentration dominated by metastable nuclide(s)

Eurofer activation response – nuclide contributions

- **Neutron** fusion first wall (FW):

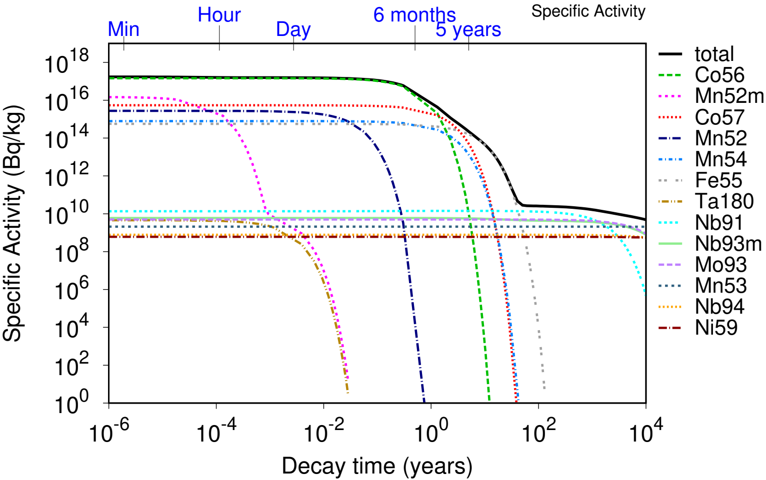


Many contributing nuclides, but particularly ^{55}Fe and ^{187}W

- After 2-year irradiation

Eurofer activation response – nuclide contributions

- **Proton** beam at 8 MeV:



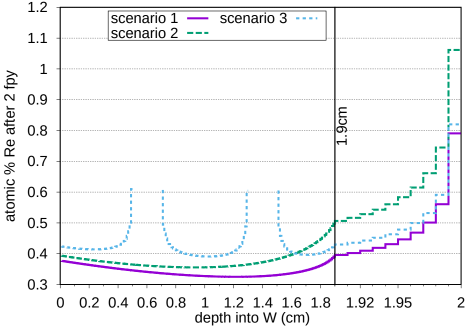
Much fewer nuclides produced (^{56}Co, ^{57}Co, ^{55}Fe are key) but radioactivity is comparable to neutron case initially

- After 2-year irradiation at 10^{14} ions cm^{-2} s^{-1}

Caution

- FISPACT-II is zero dimensional – all atoms see same irradiation environment
- for neutrons, this is often a valid assumption due to long free paths of (fast) neutrons
  - but local variation in thermal flux can alter transmutation rates
- for charged particles, care should be taken to consider variation in energy spectrum with position (depth)
  - validity of monoenergetic assumption should be checked (e.g. with SRIM)

Combined transport and inventory simulations showing the local variation in Re production near to water pipes in W



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- for charged particles, care should be taken to consider variation in energy spectrum with position (depth)
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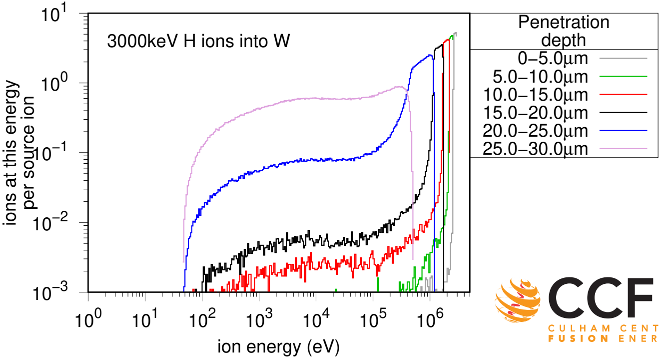
SRIM calculation of 3 MeV protons into W shows that the ion spectrum changes with depth – only monoenergetic in first 10 μm



Discussion

- FISPACT-II inventory simulations are a powerful tool for studying the impact that irradiation has on the chemical composition of materials
- with the latest nuclear data libraries, simulations are now routine for charged particle irradiation, including p, d, t, α
  - can provide nuclide finger-printing for use in planning the handling and transport of activated materials
  - comparing predictions for experimental conditions with simulations of fusion/fission environments can be useful in designing experiments that aim to understand the transmutation-induced impacts that materials will experience under operation
- Further reading:
  - Sublet, Eastwood, Morgan, Gilbert, Fleming, and Arter, "**FISPACT-II: An Advanced Simulation System for Activation, Transmutation and Material Modelling**",
    Nucl. Data Sheets **139** (2017) 77–137
    `http://dx.doi.org/10.1016/j.nds.2017.01.002`