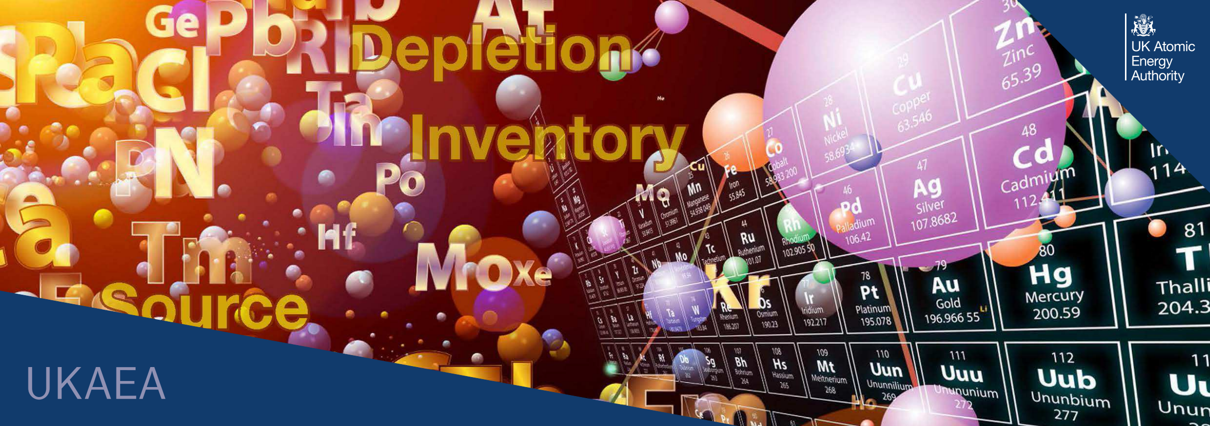

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An advanced inventory simulation platform for nuclear observables

Mark Gilbert
United Kingdom Atomic Energy Authority

FISPACT-II workshop

November 23 - December 3, 2020

This work was funded by the RCUK Energy Programme
[Grant number EP/P012450/1]

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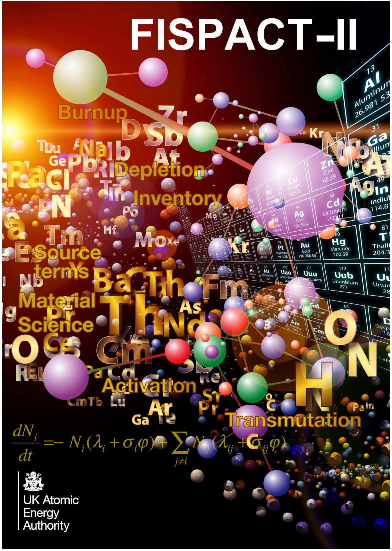
Session 1: Introduction to inventory simulations with FISPACT-II

FISPACT-II



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Nuclear Data Sheets

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FISPACT-II: An Advanced Simulation System for Activation, Transmutation and Material Modelling

J.-Ch. Sublet,[1,*] J. W. Eastwood,[2] J. G. Morgan,[2] M. R. Gilbert,[1] M. Fleming,[1] and W. Arter[1]

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FISPACT-II is a code system and library database for modelling activation-transmutation processes, depletion-burn-up, time dependent inventory and radiation damage source terms caused by nuclear reactions and decays.

The FISPACT-II code, written in object-style Fortran, follows the evolution of material irradiated by neutrons, alphas, gammas, protons, or deuterons, and provides a wide range of derived radiological output quantities to satisfy most needs for nuclear applications. It can be used with any ENDF-compliant group library data for nuclear reactions, particle-induced and spontaneous fission yields, and radioactive decay (including but not limited to TENDL-2015, ENDF/B-VII.1, JEFF-3.2, JENDL-4.0u, CENDL-3.1 processed into fine-group-structure files, GEFY-5.2 and UKDD-16), as well as resolved and unresolved resonance range probability tables for self-shielding corrections and updated radiological hazard indices. The code has many novel features including: extension of the energy range up to 1 GeV; additional neutron physics including self-shielding effects, temperature dependence, thin and thick target yields; pathway analysis; and sensitivity and uncertainty quantification and propagation using full covariance data.

The latest ENDF libraries such as TENDL encompass thousands of target isotopes. Nuclear data libraries for FISPACT-II are prepared from these using processing codes PREPRO, NJOY and CALENDF. These data include resonance parameters, cross sections with covariances, probability tables in the resonance ranges, PKA spectra, kerma, dpa, gas and radionuclide production and energy-dependent fission yields, supplemented with all 27 decay types. All such data for the five most important incident particles are provided in evaluated data tables.

The FISPACT-II simulation software is described in detail in this paper, together with the nuclear data libraries. The FISPACT-II system also includes several utility programs for code-use optimisation, visualisation and production of secondary radiological quantities. Included in the paper are summaries of results from the suite of verification and validation reports available with the code.

CONTENTS

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http://dx.doi.org/10.1016/j.nds.2017.01.002

Sublet, Eastwood, Morgan, Gilbert, Fleming, and Arter
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What are inventory simulations?

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

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Why is this important?

- changes in composition can have a profound influence on how a material behaves
  - change in mechanical properties; embrittlement, loss of strength, etc. (including from gas production)
  - change in thermal properties (conductivity, resistivity)
  - change in magnetic properties (e.g. in coils of fusion tokamaks)
  - increase in radioactivity
    - build-up of radioactive waste
- therefore, it is vital to have reliable predictions of these time-dependent changes
  - so they can be included in engineering design studies of nuclear systems, including reactors (shielding requirements, maintenance schedules, etc.)
  - used to define operational limits & lifetimes of components
  - used to evaluate expected masses and costs of waste disposal
  - & feed into multi-scale (integrated) modelling

How do we do them?

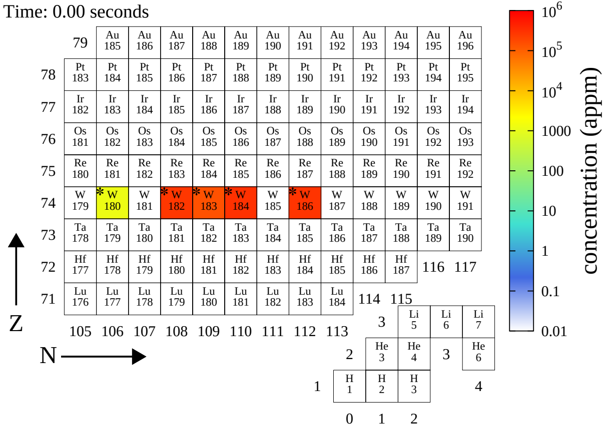
Inventory rate equations

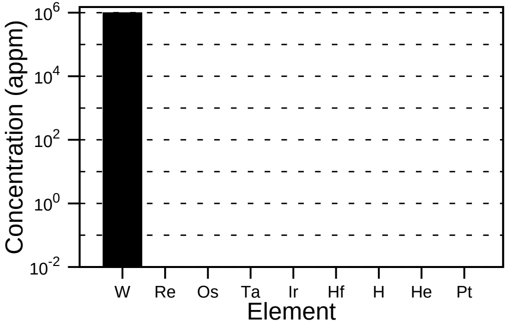
$$\frac{dN_i}{dt} = \underbrace{-N_i(\lambda_i + \sigma_i\phi)}_{\text{loss}} + \sum_{j\neq i} \underbrace{N_j(\lambda_{ji} + \sigma_{ji}\phi)}_{\text{creation}}$$

- coupled differential equations
  - one equation for each nuclide i at concentration N_i
  - solved numerically by FISPACT-II (using Livermore ODE solver, LSODE)
  - & used to update material composition
- σ_{ji}: energy-dependent reaction cross sections for $j \to i$ reactions (e.g. (n,γ), (n,α), (n,2n), etc.) from nuclear libraries collapsed with (normalised) neutron energy spectra from neutron transport; σ_i is sum over all $i \to j$ reactions
- decay constants λ_i, λ_{ji} (from decay library of measurements)
- total fluxes ϕ from neutron transport (neutronics) simulations

What does this look like?

- Pure tungsten





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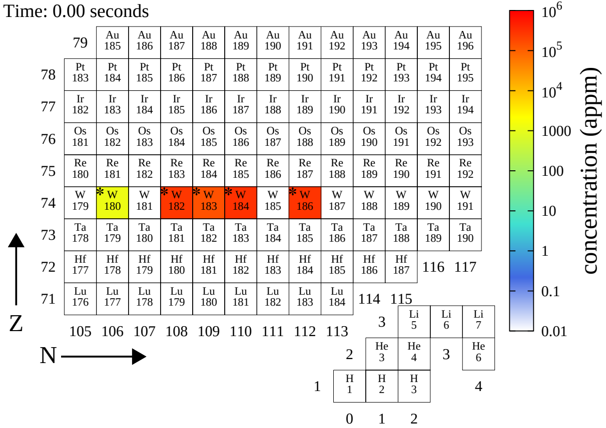
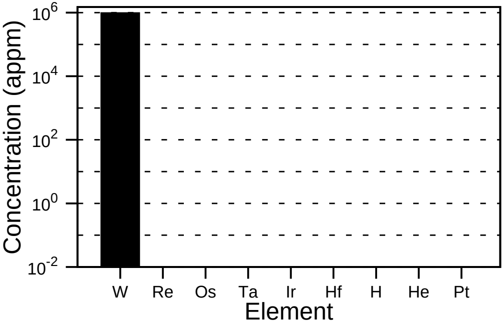
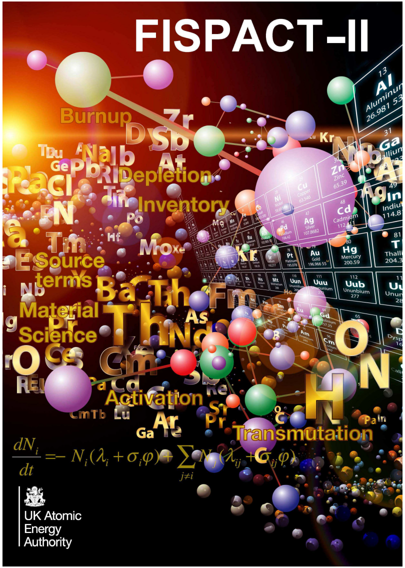


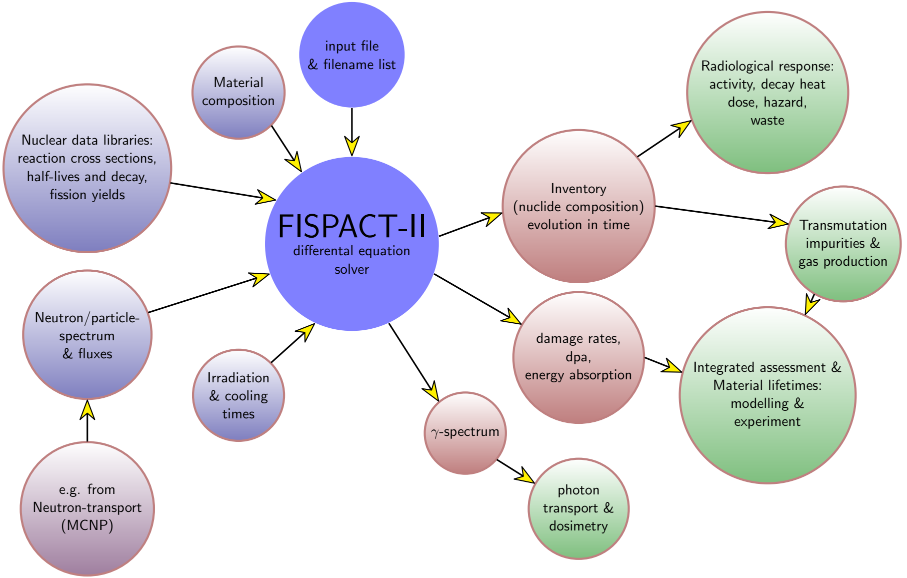


Inventory simulation platform

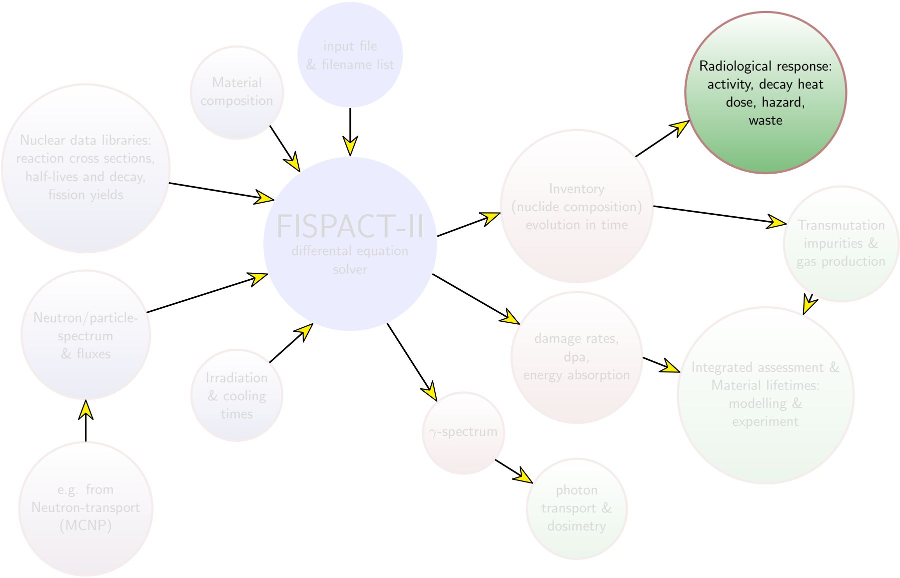


- multiphysics platform
  for predicting the inventory changes in materials under both neutron and charged-particle interactions
  - calculates activation, transmutation, burn-up, dpa, gas production, gamma spectra, etc.
- employs the most up-to-date international nuclear data libraries containing:
  - nuclear reaction data (reaction cross sections)
  - radioactive decay data (half-lives and decay schemes)
  - fission yield data (ratios)

Inventory calculations



Inventory calculations



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 – in FISPACT-II output
- decay heat, measured in kilowatts (kw)
  - can be separated by decay type - α, β, γ
  - how much heat will be generated in a material even when not exposed to irradiation
  - critical to determine if cooling is needed to prevent melting
- γ dose rate, measured in Sieverts (Sv) per hour
  - contact or point dose approximations
  - 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

+ γ-spectra in vector format for dose-rate mapping

Inventory rate equations

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- decay constants λ_i, λ_{ji} (s^{-1})
- `GETDECAY` to read-in from pre-prepared `ARRAYX` file
  - or to create `ARRAYX`

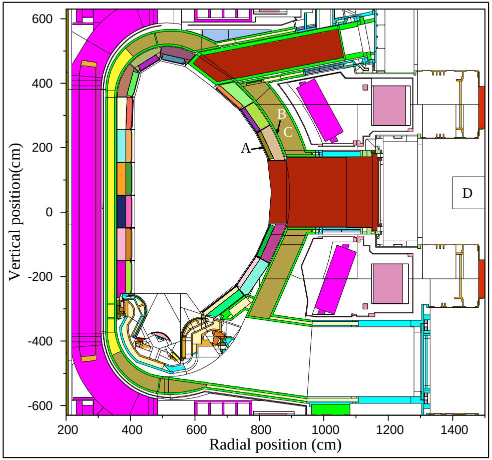
Inventory rate equations

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

- (neutron) fluxes ϕ and energy dependent spectra in neutrons $\mathrm{cm}^{-2}\mathrm{s}^{-1}$
- `GETXS` to collapse (fold) `FLUXES` file with reaction data to produce `COLLAPX` file of σ_i, σ_{ji} values (or read from it)
- `FLUX` to specify total flux ϕ

ϕ & spectra from neutron transport – Monte Carlo simulations

- Geometry of a reactor or other neutron environment is converted into a finite-element model of "cells"
- Then a Monte Carlo simulation (usually with MCNP§) generates and transports neutrons one (history) at-a-time
  - using same nuclear reaction physics data as an inventory simulation
  - decisions (reaction type, recoil direction, etc.) are made using probabilities
  - statistical results are built-up (tallied) in regions of interest



ITER finite-element model

§https://mcnp.lanl.gov/

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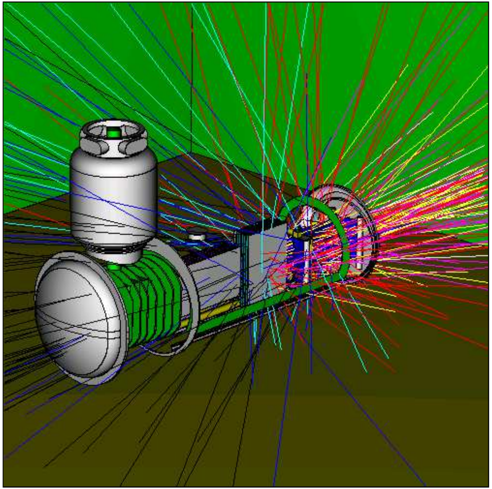
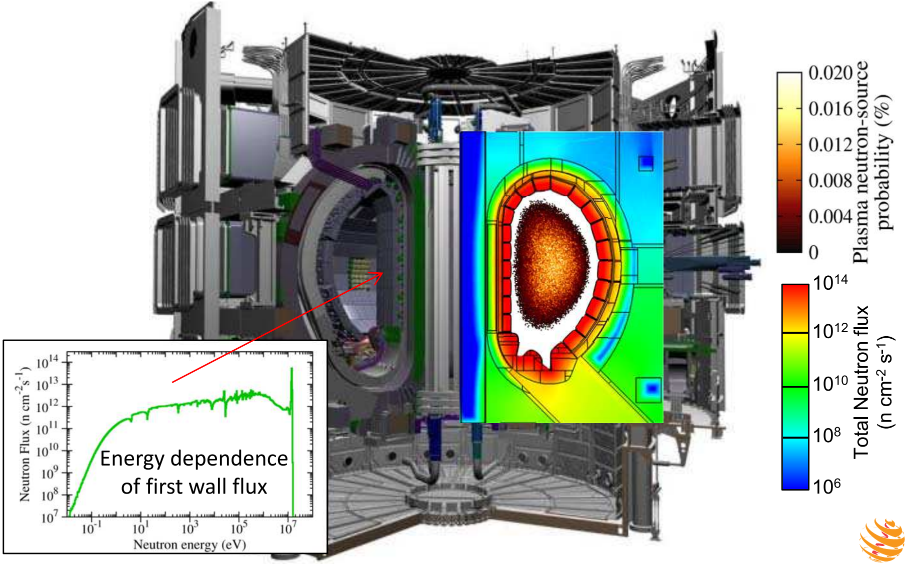


Initial trajectories for a neutron beam

[§] https://mcnp.lanl.gov/

Typical result for a fusion design



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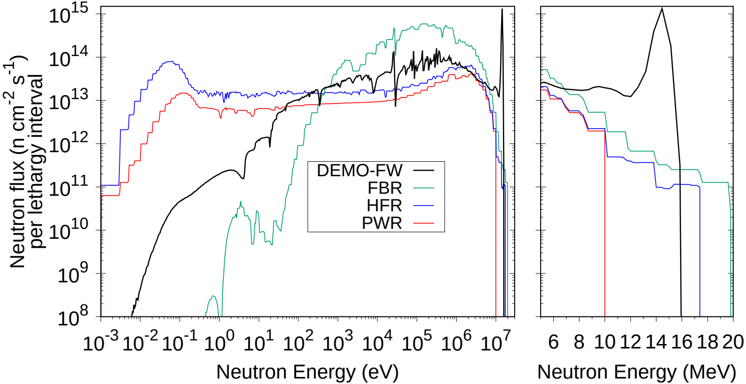
Neutron irradiation fields: fusion vs. fission

- For a fusion DEMOnstration power plant
  & typical fission reactors:



total fluxes ϕ:

($\times 10^{14}$ n cm^{-2} s^{-1})	
DEMO	6
FBR	24
HFR	5
PWR	3

- fusion spectrum in first wall (FW) dominated by 14 MeV peak
- well-moderated (averaged) fission spectra don't have such dominant peaks but can have tails that explore the 14 MeV region of fusion

FBR – superphenix Fast Breeder Reactor
HFR – High Flux Reactor, Petten
PWR – Pressurized Water-cooled Reactor

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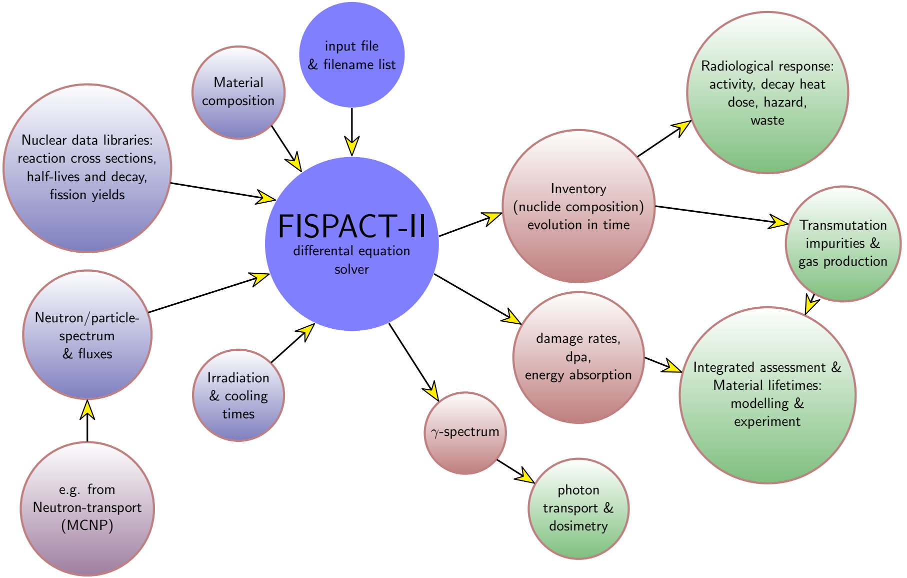
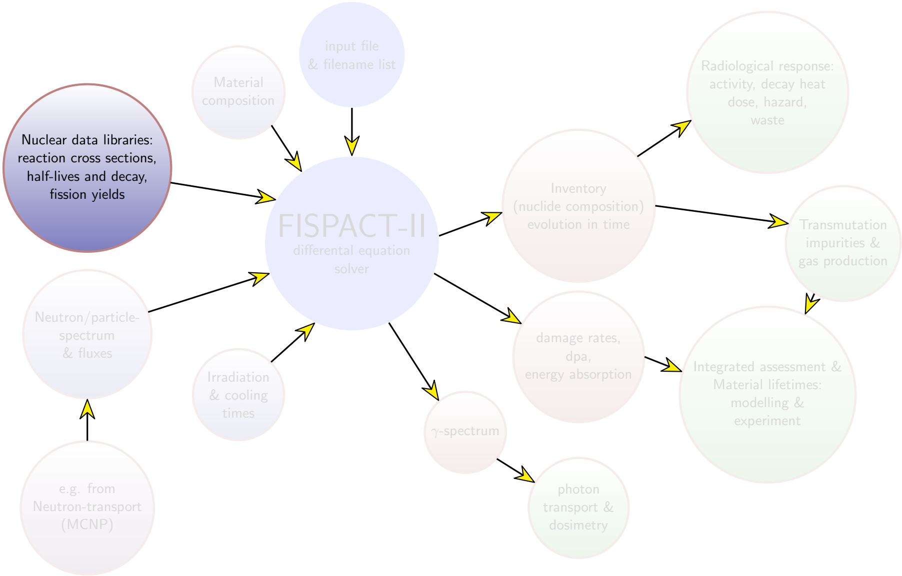
Inventory calculations



Inventory calculations



Nuclear data libraries – recommendation

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TENDL (latest version 2019†)

- TALYS-based Evaluated Nuclear Data Libraries
- generated using various physical, theoretical, and semi-empirical models
- fully-automated production with *near* complete coverage of nuclides & reaction
  - avoids under-estimation due to missing data
- contains data for 2809 target nuclides with half-lives $>$ 1 second in neutron file
  - the FISPACT-II decay files includes data on a further 1000 radionuclides with sub-second half-lives
- processed version for FISPACT-II covers energies up to 1 GeV
  - in a fine, high-resolution 1102 & 709 energy group structures

†A. J. Koning, D. Rochman, *et al.*. Release date: December 13, 2019.
https://tendl.web.psi.ch/tendl_2017/tendl2017.html
FISPACT-II compatible versions available at
https://fispact.ukaea.uk/nuclear-data/downloads/

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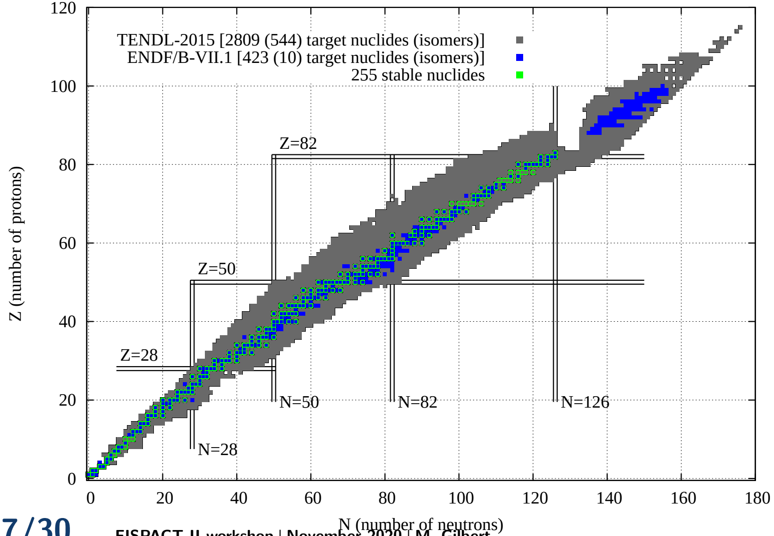
TENDL nuclide coverage

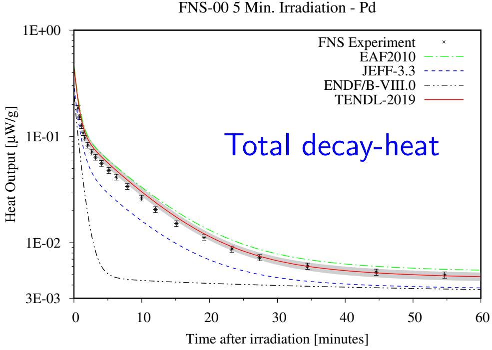
- Target nuclide coverage in TENDL libraries is more complete than elsewhere:

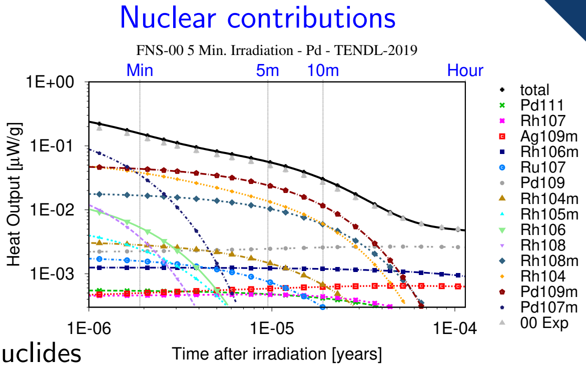


- Many more isomeric states are included as both targets (parents) and daughters of reactions – vital for correct prediction of activity

Why is nuclide coverage important?

- Comparison to 5 minute experimental irradiation of pure palladium





- a complex case with many contributing nuclides
  - particularly metastables such as ^{109m}Pd and ^{107m}Pd
  - a mixture of (n,2n) and (n,p) reactions dominate
  - TENDL-2019 outperforms all others

	TENDL-2019	ENDF/B-VIII.0	EAF2010	JEFF-3.3
mean % diff. from E	12	66	23	32

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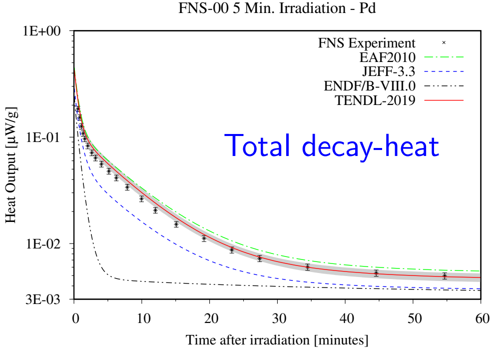
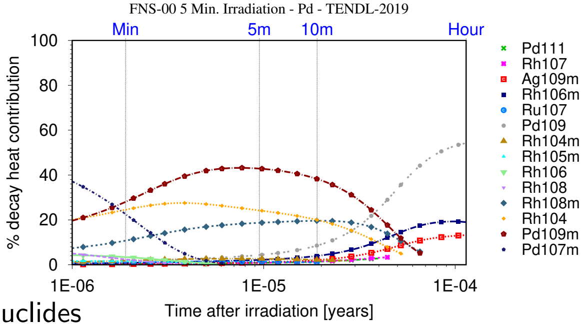


% Nuclear contributions



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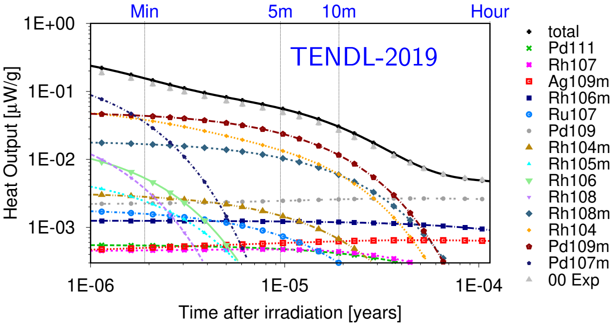
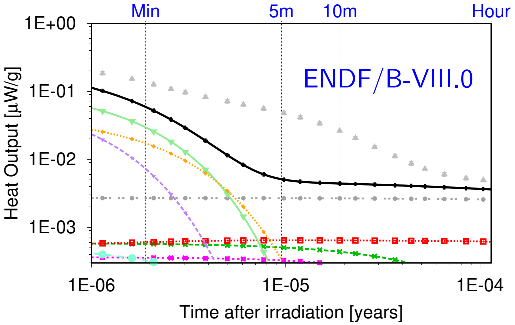
Palladium nuclide comparisons



- ENDF/B-VIII.0 & JEFF-3.3 (not shown) miss the important metastables
- This example is part of the decay-heat benchmark used to validate FISPACT-II – see later lecture



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- neutron reaction cross sections σ
  in barns ($\times 10^{-24}$ cm^2)
- `GETXS` to collapse (fold) data in `xs_endf` ENDF data folder (or in a `crossec` file for legacy EAF data)
  with irradiation spectrum to produce `COLLAPX` file of σ_i, σ_{ji} values (or read from it)
  - these are essentially reaction rates per unit flux of the current irradiation spectrum

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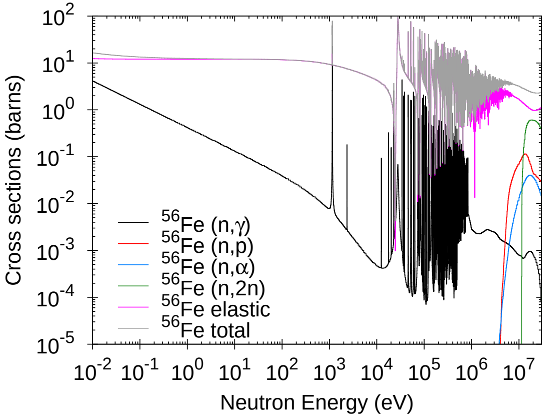
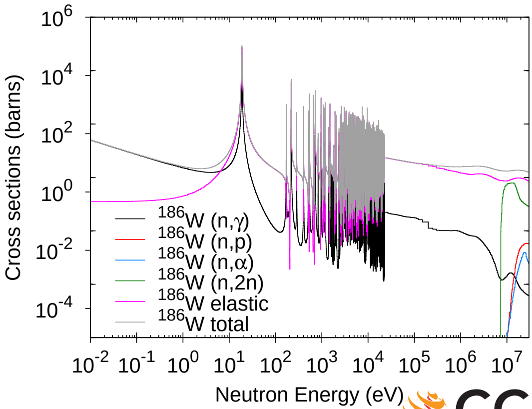
Typical cross sections σ



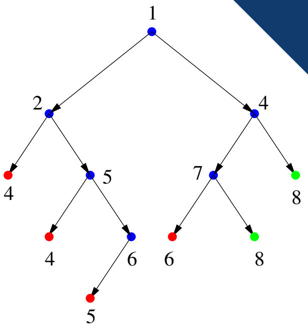
- cross section (xs) $\approx$ 'reaction likelihood'
- Many different reactions possible on each nuclide/isotope



- Some (reaction) channels are only 'open' at high energy (thresholds)

Typical reaction chains (via FISPACT-II tree search algorithm)

- High energy (threshold reactions):
  - ^{56}Fe(n,p)^{56}Mn (3 MeV threshold)
  - ^{186}W(n,2n)^{185}W(β^-)^{185}Re (7.2 MeV)
- Low energy (capture and decay chains):
  - ^{54}Fe(n,γ)^{55}Fe(β^+)^{55}Mn(n,γ)^{56}Mn
  - ^{186}W(n,γ)^{187}W(β^-)^{187}Re
- Gas production:
  - helium: ^{56}Fe(n,α)^{53}Cr (negligible xs below 4 MeV)
  - hydrogen: ^{63}Cu(n,p)^{63}Ni, ^{63}Cu(n,np)^{62}Ni
- Long chains (24-reaction chain)
  - ^{153}Eu(n,γ)^{154}Eu(n,γ)^{155}Eu(n,γ)^{156}Eu(n,γ)^{157}Eu(β^-)
    ^{157}Gd(n,γ)^{158}Gd(n,γ)^{159}Gd(β^-)^{159}Tb(n,γ)^{160}Tb(n,γ)
    ^{161}Tb(β^-)^{161}Dy(n,γ)^{162}Dy(n,γ)^{163}Dy(n,γ)^{164}Dy(n,γ)
    ^{165}Dy(β^-)^{165}Ho(n,γ)^{166}Ho(n,γ)^{167}Ho(β^-)^{167}Er(n,γ)
    ^{168}Er(n,γ)^{169}Er(β^-)^{169}Tm(n,γ)^{170}Tm(n,γ)^{171}Tm



A single-visit tree starting from "nuclide" 1

Inventory evolution example

- Evolution in time of compositions from FISPACT-II output
- nuclide picture shown on a "chart of the nuclides"
- e.g. 5-year irradiation of pure tungsten in DEMO

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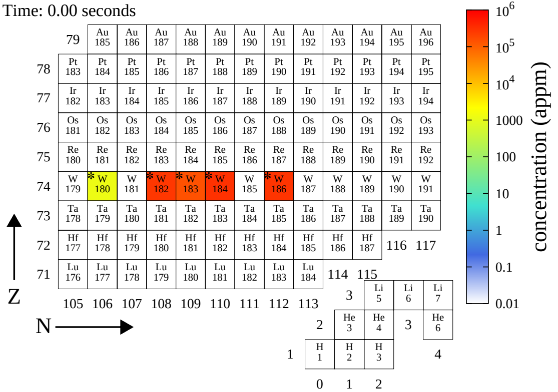

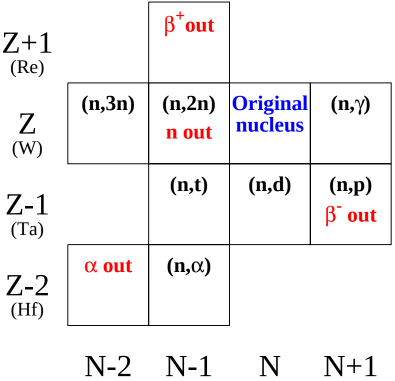

- Large spread of isotopes produced – increasing as a function of time as longer & longer reaction chains are created

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

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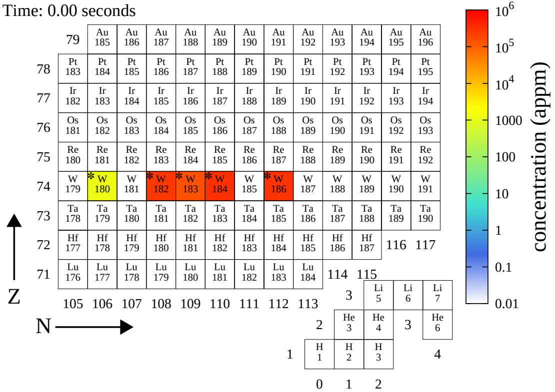

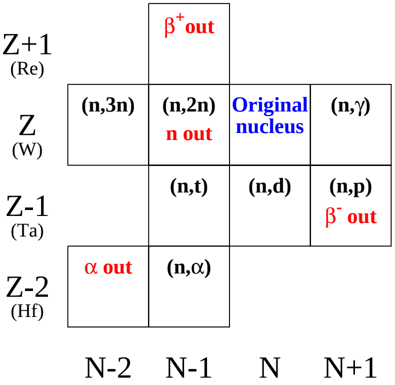

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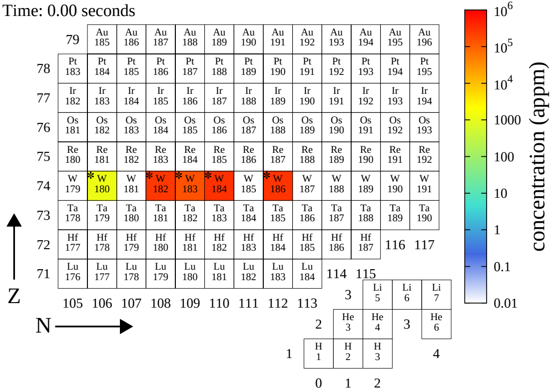

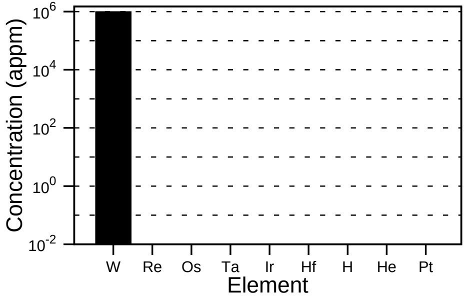

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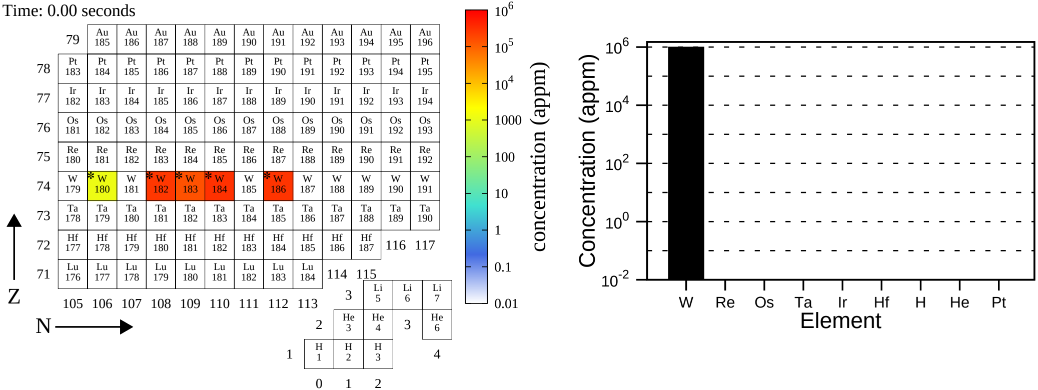

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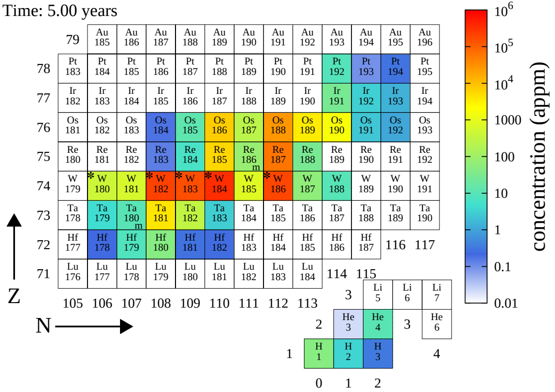
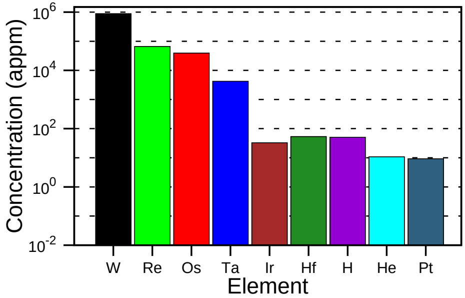
- Evolution in time of compositions from FISPACT-II output
- nuclide picture shown on a "chart of the nuclides"
- e.g. 5-year irradiation of pure tungsten in DEMO

Nucl. Sci. Eng **117** (2014) 291-306





- Large spread of isotopes produced – increasing as a function of time as longer & longer reaction chains are created

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

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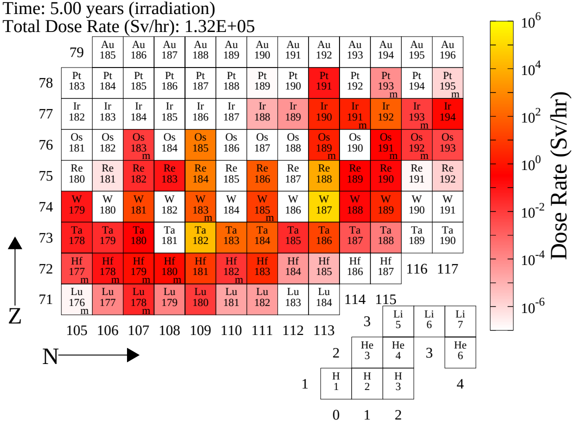
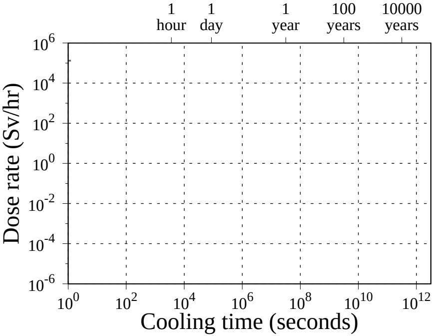
Radiological response evolution example

- e.g. dose rate after 5-year irradiation of pure W in DEMO
- total value for material a standard FISPACT-II output
- nuclide chart shows decay of radionuclides





m – Dose Rate dominated by metastable nuclide(s)

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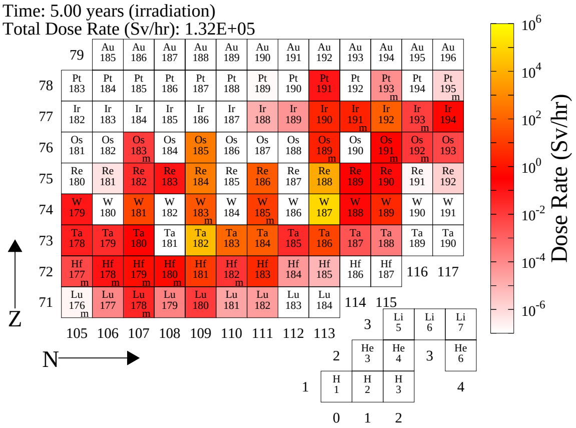

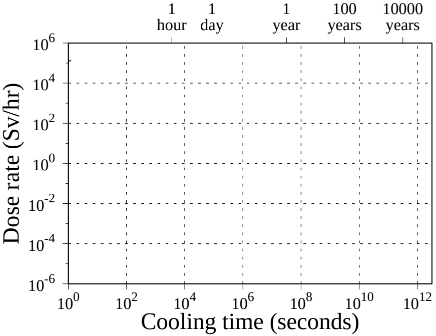

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Radiological response evolution example

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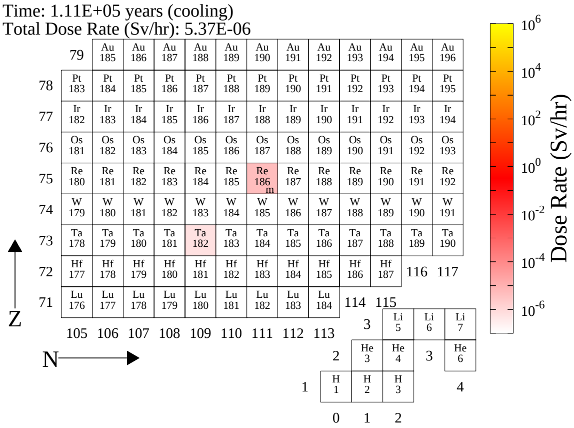
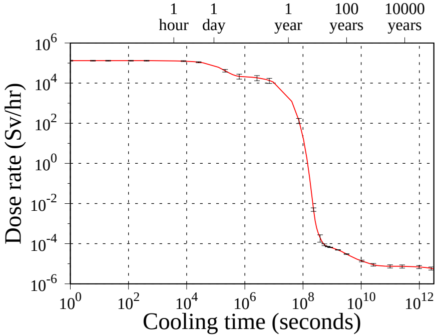
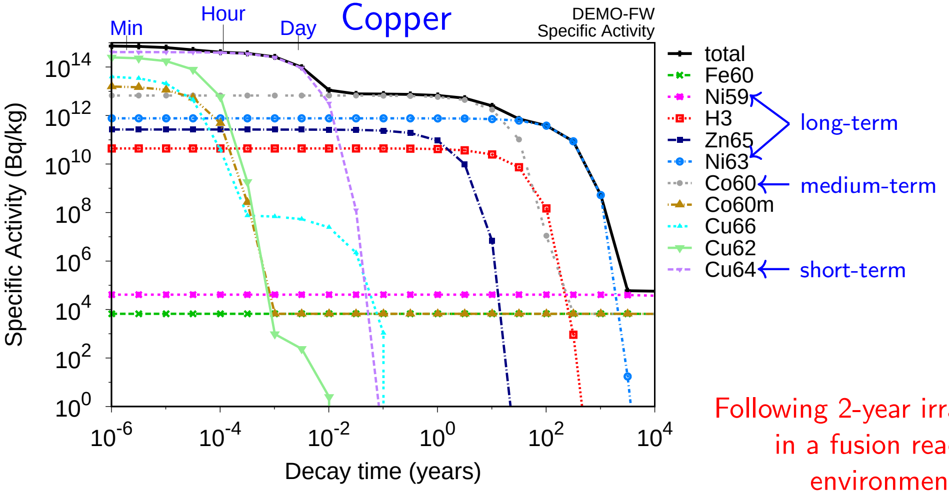




m – Dose Rate dominated by metastable nuclide(s)

Activation response – full nuclide contributions

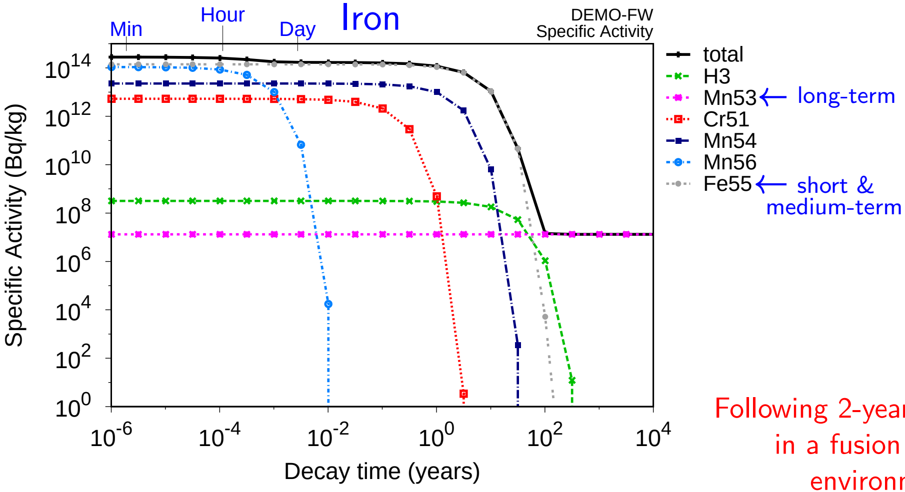
- FISPACT-II automated plotting for (dominant) nuclide contributions as a function of time



Following 2-year irradiations in a fusion reactor environment

Activation response – full nuclide contributions

- FISPACT-II automated plotting for (dominant) nuclide contributions as a function of time



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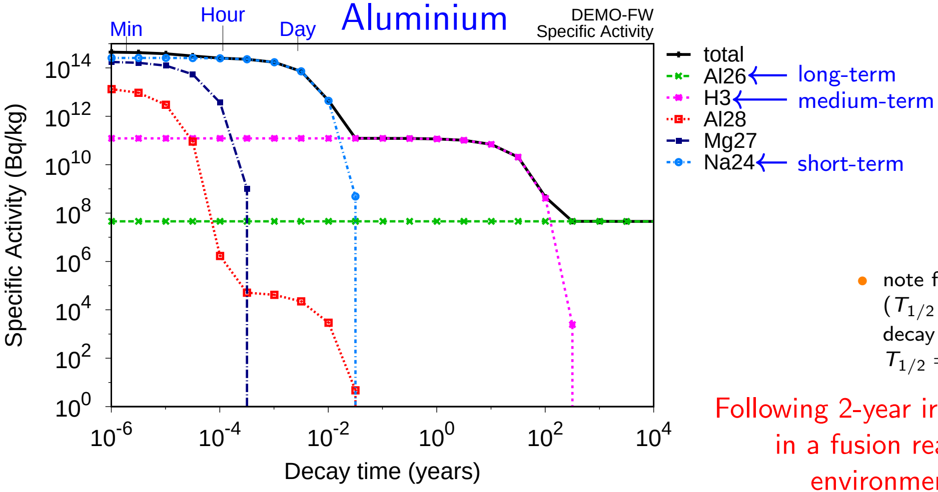

- note feeding of ^{28}Al ($T_{1/2} = 2.3$ min) from β^- decay of ^{28}Mg (not shown, $T_{1/2} = 21$ hr)

Following 2-year irradiations in a fusion reactor environment

Activation response – full nuclide contributions

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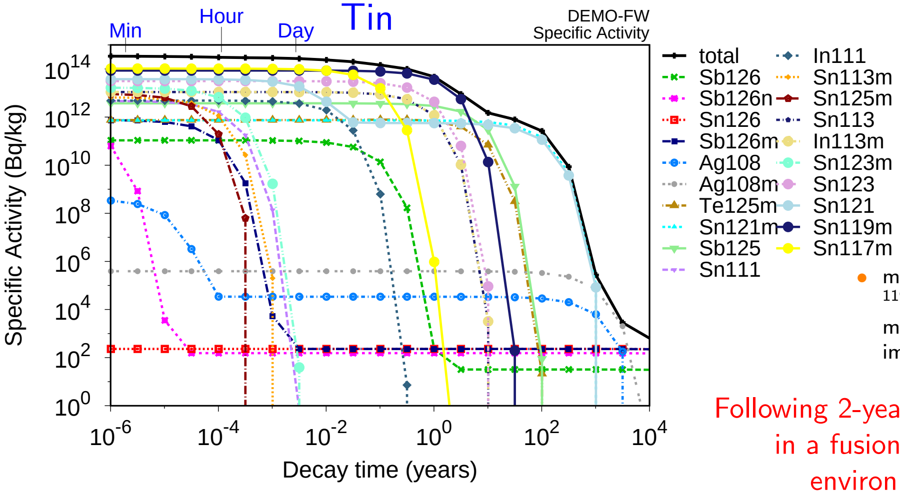
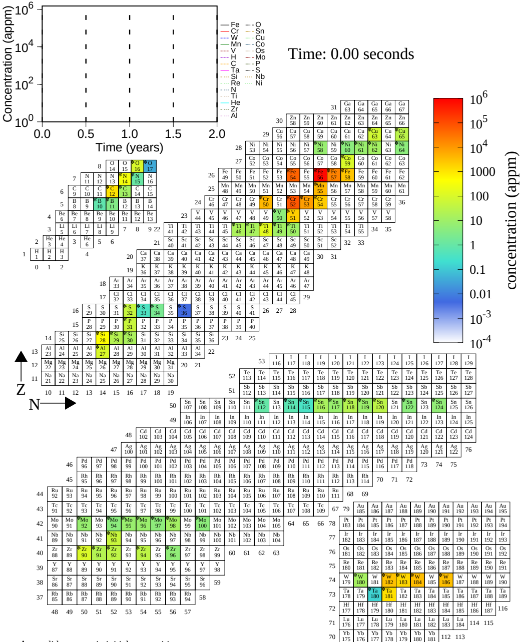


- many nuclides, but can still see ^{119m}Sn dominance in the medium-term & ^{121}Sn, ^{121m}Sn importance at longer times

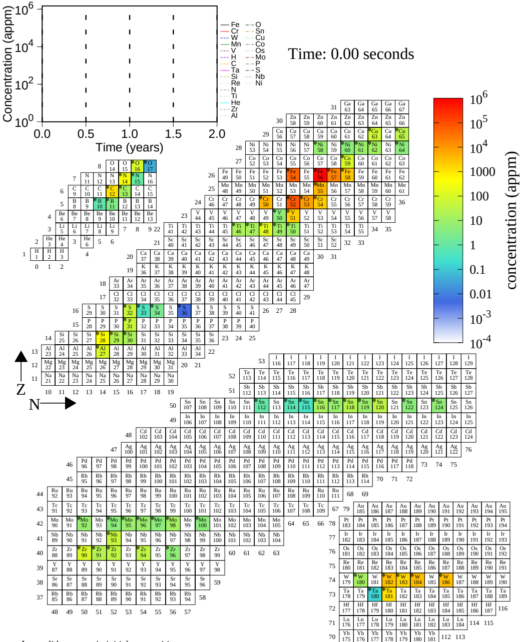
Following 2-year irradiations in a fusion reactor environment

More complex materials:
Eurofer steel



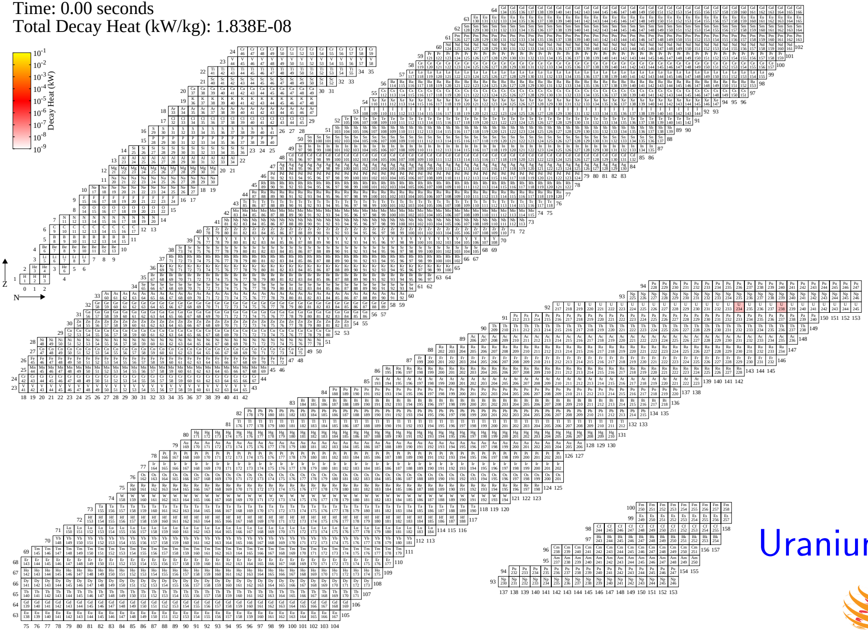
✱ - nuclide present in initial composition
m - concentration dominated by metastable nuclide(s)

More complex materials: Eurofer steel



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

Time: 0.00 seconds
Total Decay Heat (kW/kg): 1.838E-08



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Uranium in PWR

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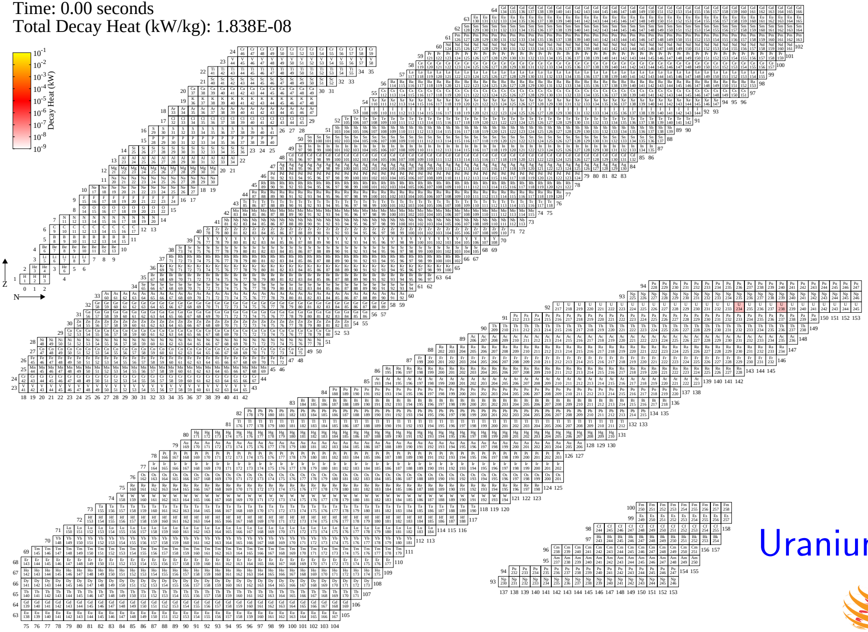
Time: 0.00 seconds

Total Decay Heat (kW/kg): 1.838E-08



Uranium in PWR

Summary

- Inventory simulations are a powerful tool for studying the impact that neutrons (and other irradiating particles) have on the chemical composition of materials
- FISPACT-II is a modern and efficient example, with advanced features and the ability to utilise the latest nuclear data (& to compare between libraries)
- More details about FISPACT-II at http://fispact.ukaea.uk
- Further reading:
  - User-manual, validation reports, material response handbooks, and much more available at http://fispact.ukaea.uk
  - 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

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