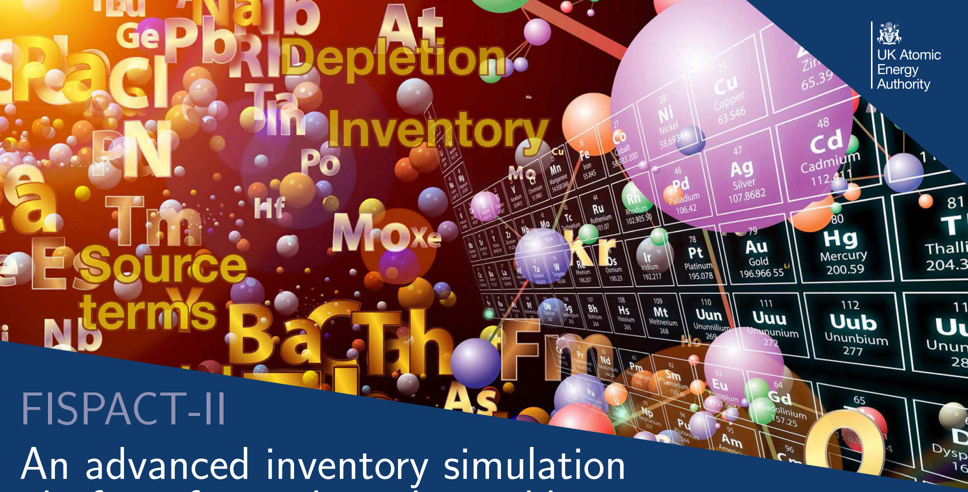

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FISPACT-II

An advanced inventory simulation platform for nuclear observables

Mark Gilbert
United Kingdom Atomic Energy Authority

FISPACT-II workshop

June 13-15, 2018, OECD/NEA, Paris

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

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Overview

- Session 1
  - Introduction to inventory simulations with FISPACT-II
- Session 2
  - Running FISPACT-II: Getting Started
- Session 3
  - FISPACT-II: Uncertainties, Pathways, and all things nice
  - Self-shielding case study: tungsten in a fusion device
- Session 4
  - Running FISPACT-II: Advanced Usage
- Session 5
  - FISPACT-II applications: material activation, damage and waste
- Session 6
  - CAD-based Radiation transport: DAGMC Toolkit

Session 1:
Introduction to inventory simulations with FISPACT-II

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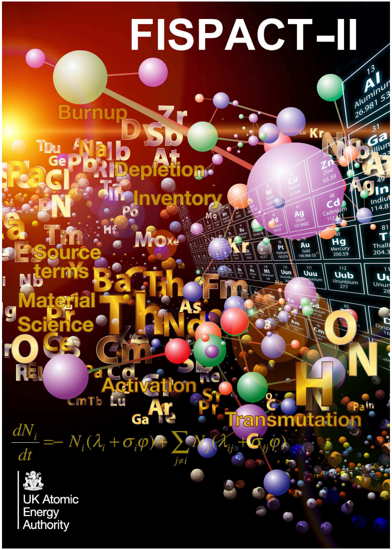

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Nuclear Data Sheets 139 (2017) 77–137

Nuclear Data Sheets

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

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[2] *Culham Electromagnetics Ltd, Culham Science Centre, Abingdon OX14 3DB, UK*

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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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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

Why is this important?

- changes in composition can have a profound influence on how a material behaves
  - change in mechanical properties; embrittlement, loss in 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 reactor components (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) and used to update material composition
- σ_{ji}: energy-dependent reaction cross sections for $j \rightarrow i$ 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 $i \rightarrow j$ reactions
- decay constants λ_i, λ_{ji} (from decay library of measurements)
- total fluxes ϕ from neutron transport (neutronics) simulations

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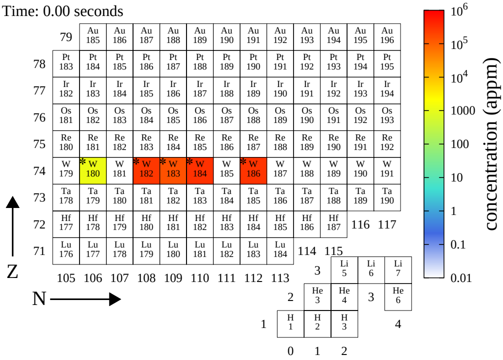
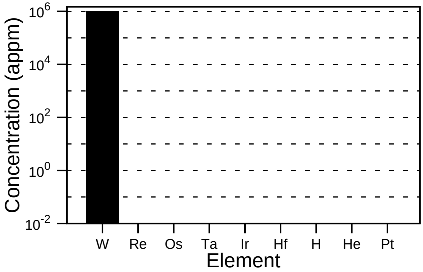
What does this look like?

- Pure tungsten





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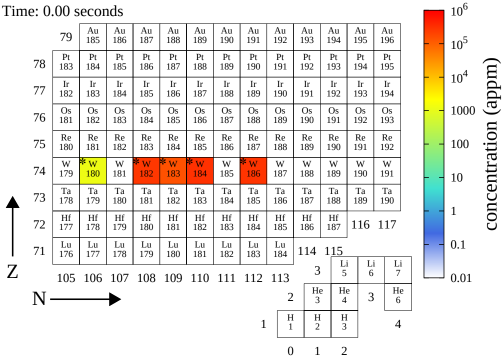
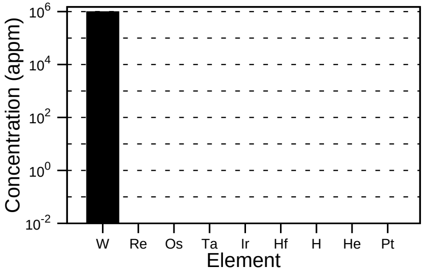
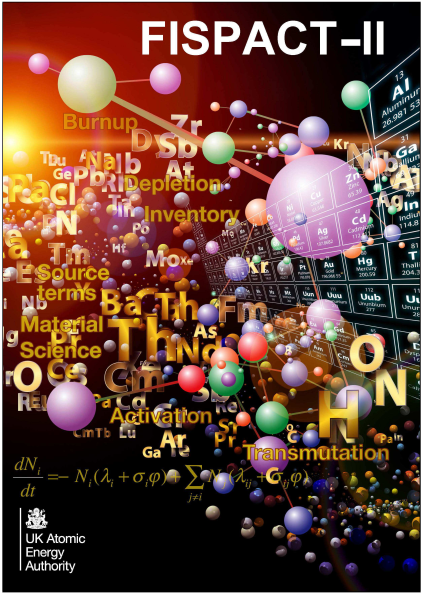


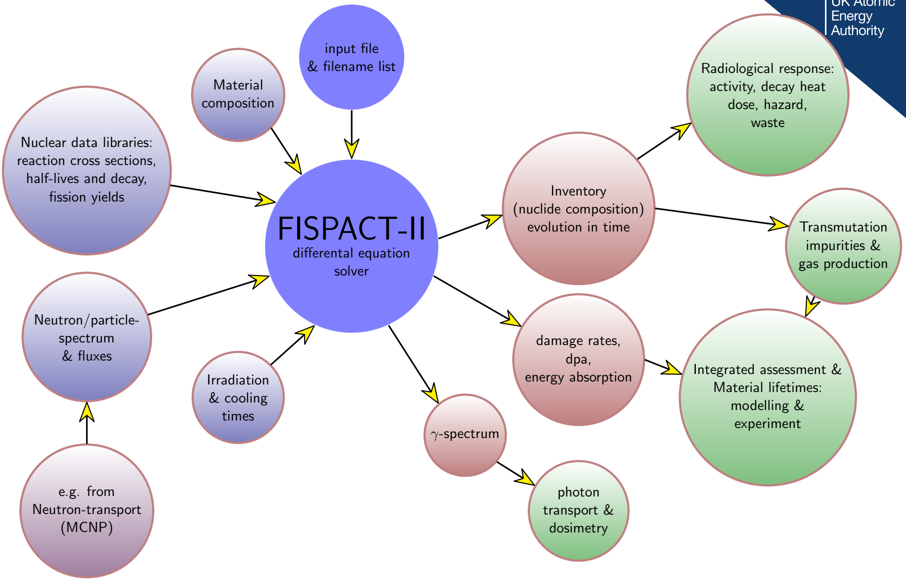


Inventory simulation platform



- multiphysics platform for predicting the inventory changes in materials under both neutron and charged-particle interactions
  - calculates activation, transmutation, burn-up, dpa, PKAs, gas production, 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



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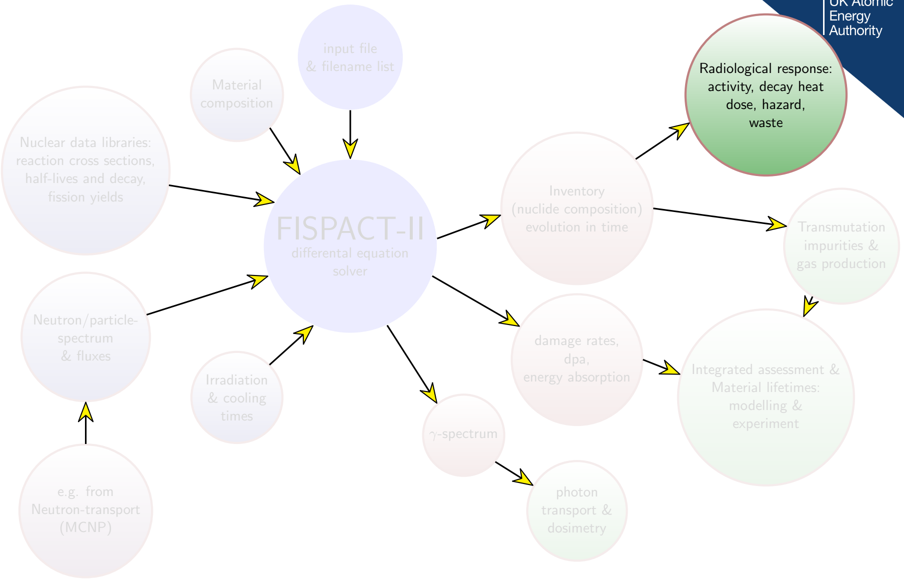

Types of radiological output

- 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 whether cooling is needed to prevent melting
- (contact) γ dose rate, measured in sieverts (Sv) per hour
  - J kg^{-1} deposition rate of radiation energy in biological tissue
  - there are also ingestion and inhalation hazard versions
- clearance index
  - IAEA based measure
  - a nuclide can be disposed of as if it were non radioactive when the index is less than 1

Inventory rate equations

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

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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

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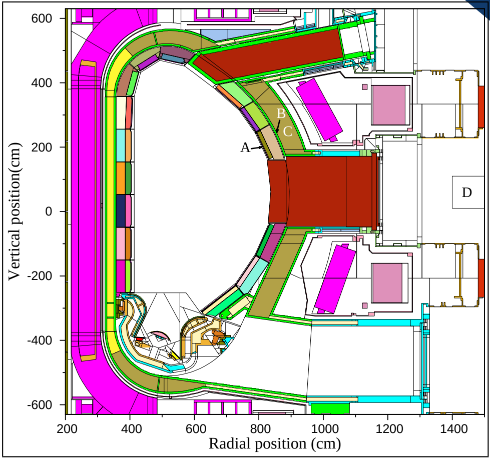
- Geometry of a reactor or other neutron environment is converted into a finite-element model of "cells"
- Then a Monte Carlo simulation (usually with MCNP§) generates and transports neutrons one (history) at-a-time
  - using same nuclear reaction physics data as an inventory simulation
  - decisions (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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ϕ & spectra from neutron transport – Monte Carlo simulations

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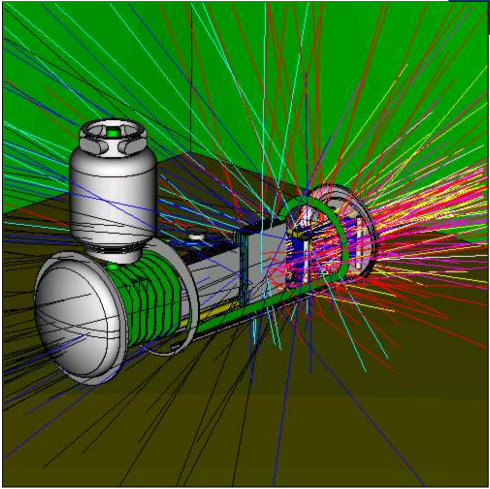
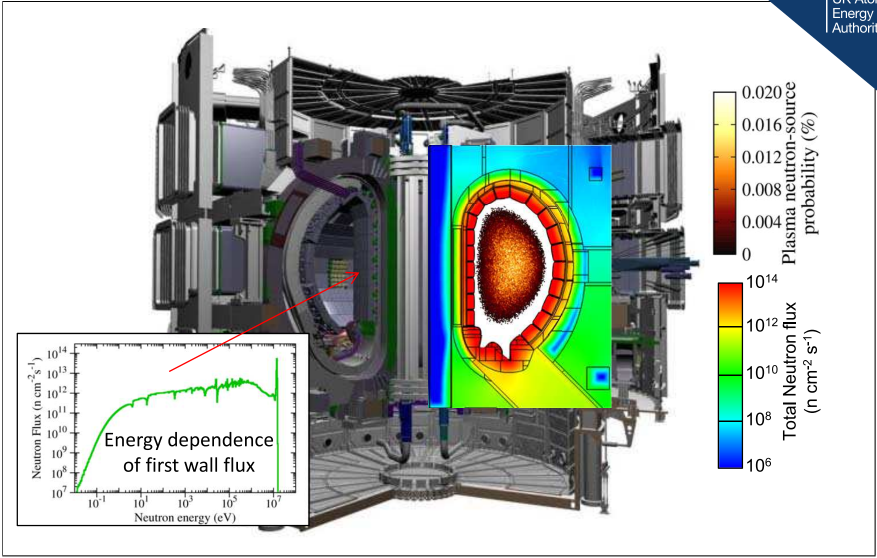


Initial trajectories for a neutron beam test set-up

[§] https://mcnp.lanl.gov/

Typical result for a fusion design



Neutron irradiation fields: fusion vs. fission

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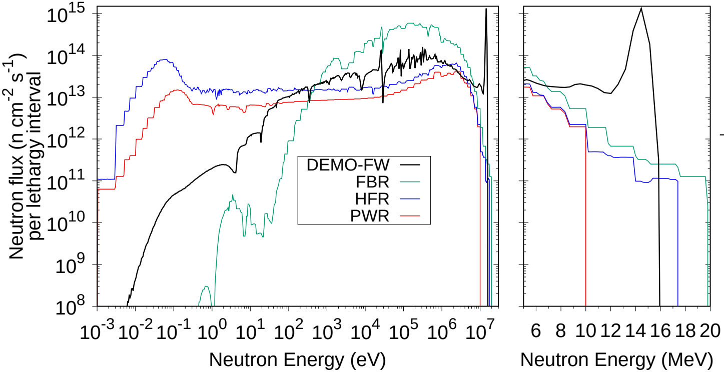
- For a fusion DEMOnstration power plant & typical fission reactors:



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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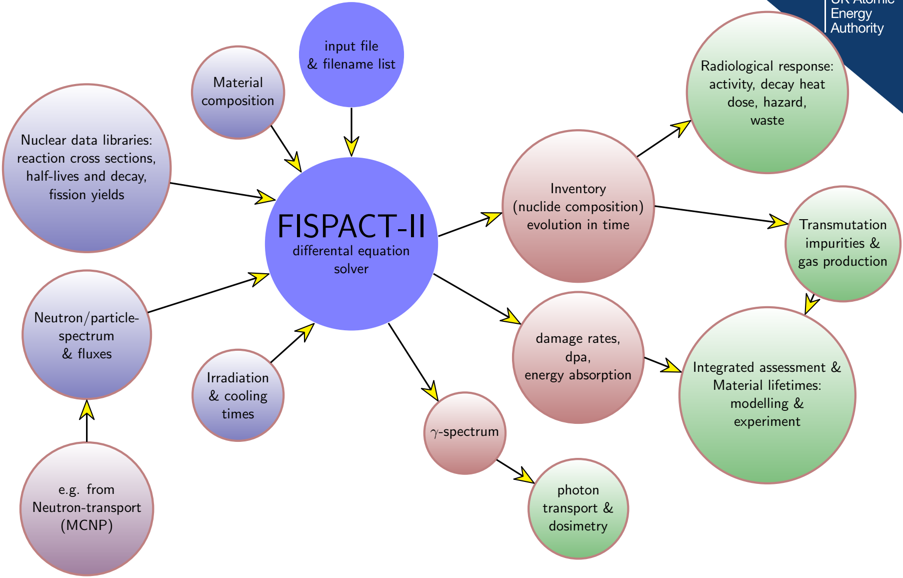
Inventory calculations



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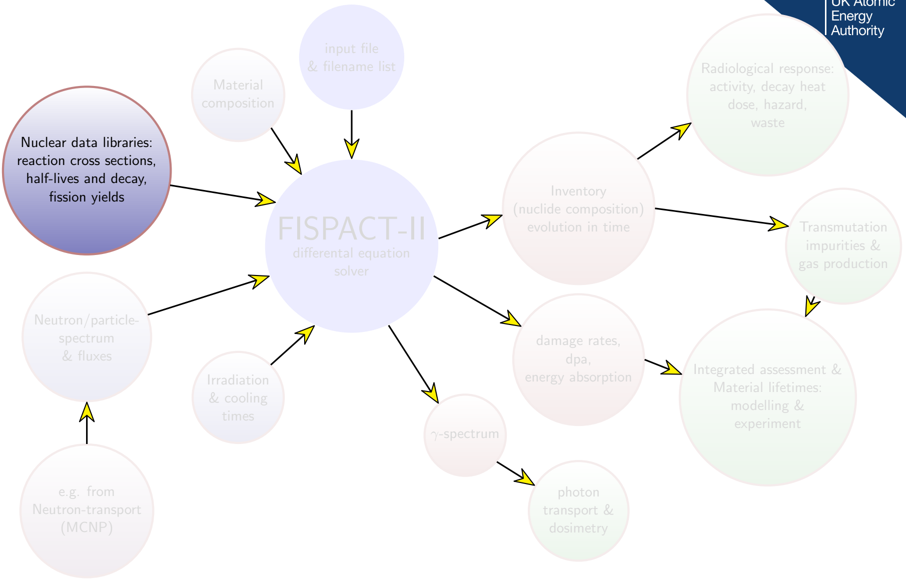

Nuclear data libraries – recommendation

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TENDL (latest version 2017†)

- TALYS-based Evaluated Nuclear Data Libraries
- generated using various physical, theoretical, and semi-empirical models
- fully-automated production with complete coverage of nuclide & reaction set
  - avoids under-estimation due to missing data
- contains data for 2809 target nuclides with half-lives > 1 second
  - 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 709 energy group structure

†A. J. Koning, D. Rochman, *et al.*
Release date: December 30, 2017.
https://tendl.web.psi.ch/tendl_2017/tendl2017.html

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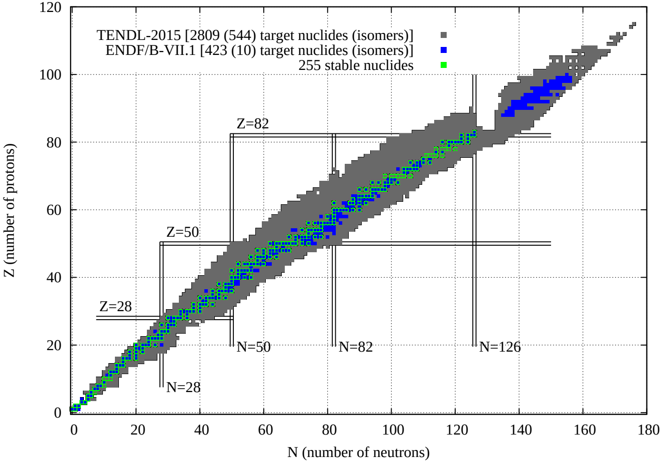
TENDL nuclide coverage

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

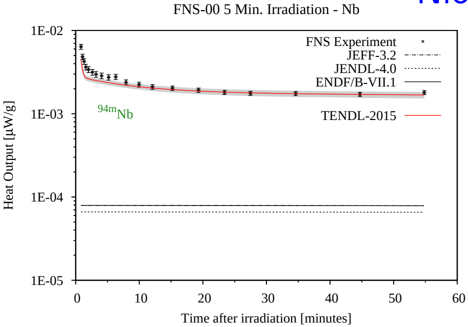


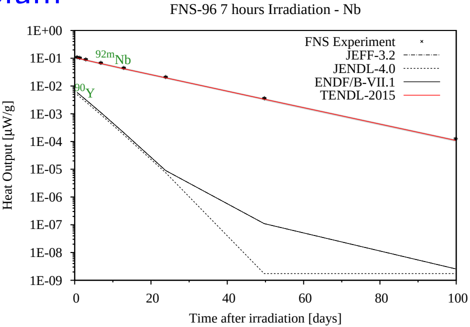
- Many more isomeric states are included as both targets (parents) and daughters of reactions – vital for correct prediction of activity

Why is nuclide coverage important?

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

Niobium





- Only TENDL has open reaction channels to the necessary isomeric states
- ^{94m}Nb ($T_{1/2} = 6.3$ minutes) at short decay times, ^{92m}Nb (10 days) at longer times

TENDL & FISPACT-II validation

- suite of automated validation exercises performed for TENDL
  - 5 reports (with supplements)
    - comprising nearly 2500 pages

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CCFE-R(15)25
January 2015
Jean-Christophe Sublet
Mark R. Gilbert
Decay heat validation, FISPACT-II & TENDL-2014, JEFF-3.2, ENDF/B-VII.1 and JENDL-4.0 nuclear data libraries

CCFE
CCFE-R(15)27
March 2015
Michael Fleming
Jean-Christophe Sublet
Jiri Kopecky
Integro-Differential Verification and Validation, FISPACT-II & TENDL-2014 nuclear data libraries

CCFE
CCFE-R(15)28
June 2015
Michael Fleming
Jean-Christophe Sublet
Validation of FISPACT-II Decay Heat and Inventory Predictions for Fission Events

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UKAEA-R(15)29
August 2015
Jean-Christophe Sublet
Michael Fleming
Maxwellian-Averaged Neutron-Induced Cross Sections for kT=1 keV to 100 keV, KADoNiS, TENDL-2014, ENDF/B-VII.1 and JENDL-4.0u nuclear data libraries

UK Atomic Energy Authority
UKAEA-R(15)30
October 2015
Michael Fleming
Jean-Christophe Sublet
Jiri Kopecky
Dimitri Rochman
Arjan Koning
Probing experimental & systematic trends of the neutron-induced TENDL-2014 nuclear data library

- decay heat validation against fusion experiments
- integral & differential xs validation
- fission & astrophysics benchmarks
- systematic trends
- 2015 CCFE and UKAEA reports 25,27–30
- currently being updated for TENDL-2017 (see `fispact.ukaea.uk`)

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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)

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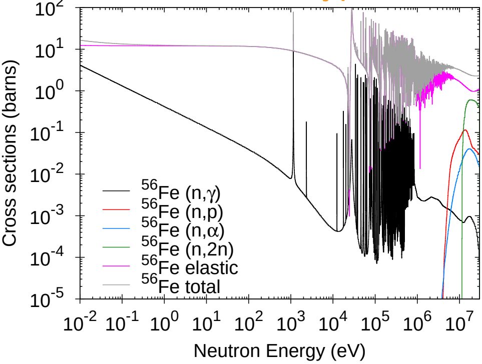
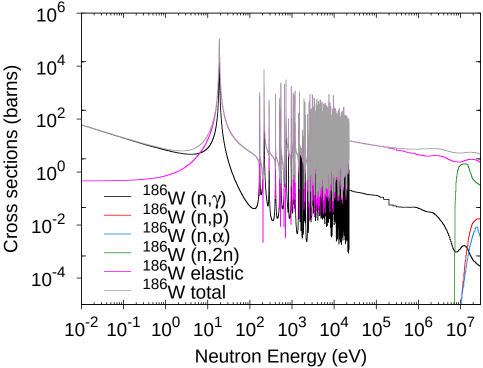
Typical cross sections σ



- 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)

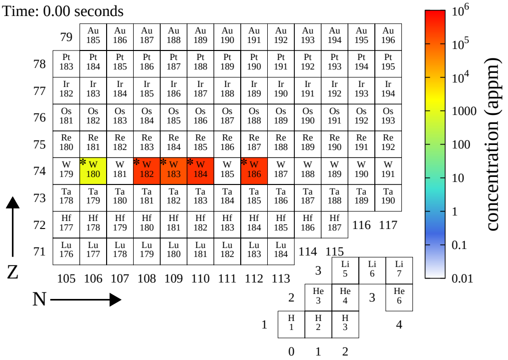
- High energy (threshold reactions):
  - ^{56}Fe(n,p)^{56}Mn (3 MeV threshold)
  - ^{186}W(n,2n)^{185}W(β^-)^{185}Re (7.2 MeV)
- Low energy (capture and decay chains):
  - ^{54}Fe(n,γ)^{55}Fe(β^+)^{55}Mn(n,γ)^{56}Mn
  - ^{186}W(n,γ)^{187}W(β^-)^{187}Re
- Gas production:
  - helium: ^{56}Fe(n,α)^{53}Cr (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)

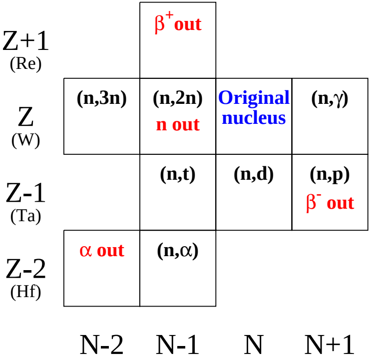
    ^{165}Dy(β^-)^{165}Ho(n,γ)^{166}Ho(n,γ)^{167}Ho(β^-)^{167}Er(n,γ)

    ^{168}Er(n,γ)^{169}Er(β^-)^{169}Tm(n,γ)^{170}Tm(n,γ)^{171}Tm

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





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

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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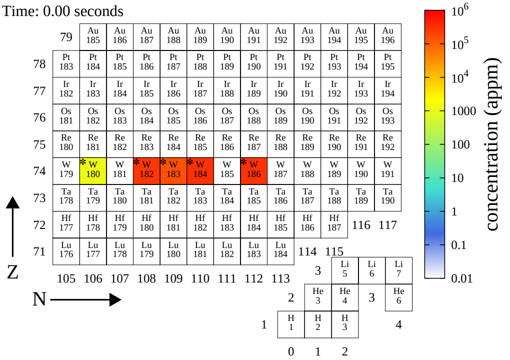

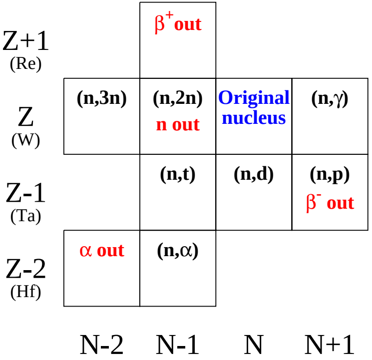

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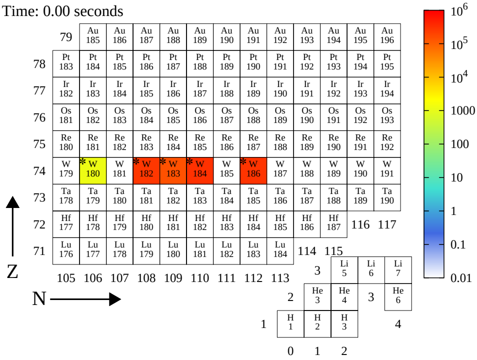

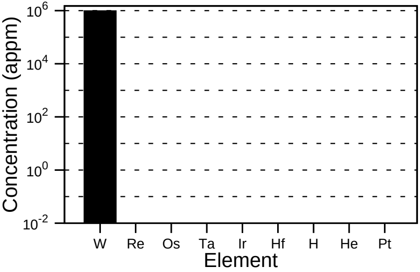

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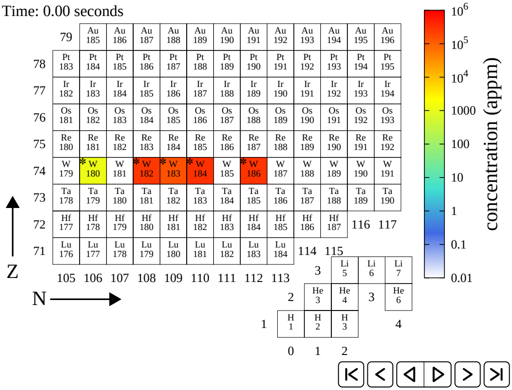

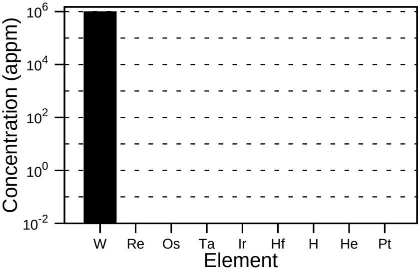

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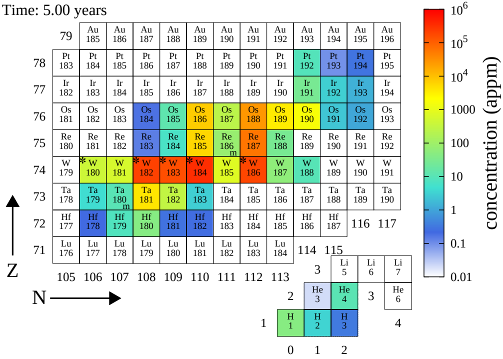

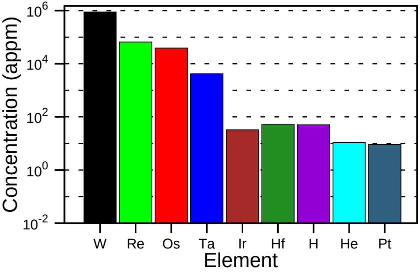

- Large spread of isotopes produced – increasing as a function of time as longer & longer reaction chains are created

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

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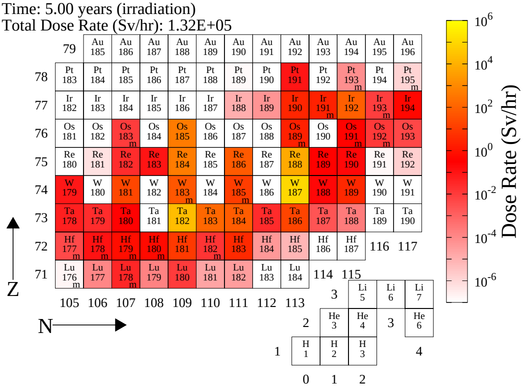
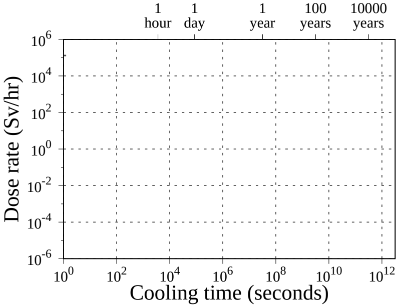
Radiological response evolution example

- 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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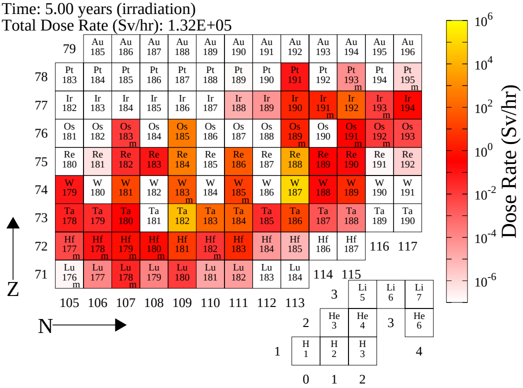

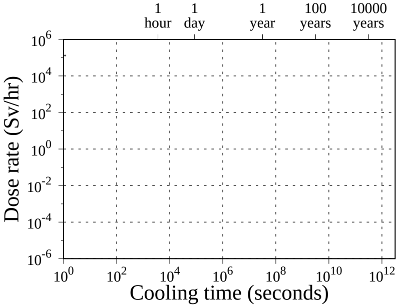

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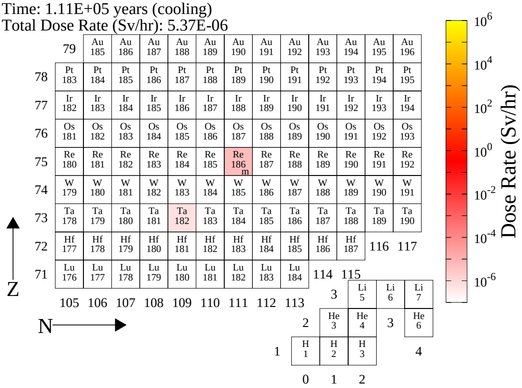
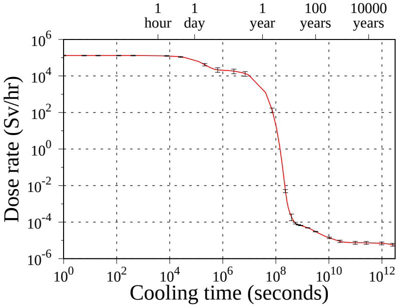
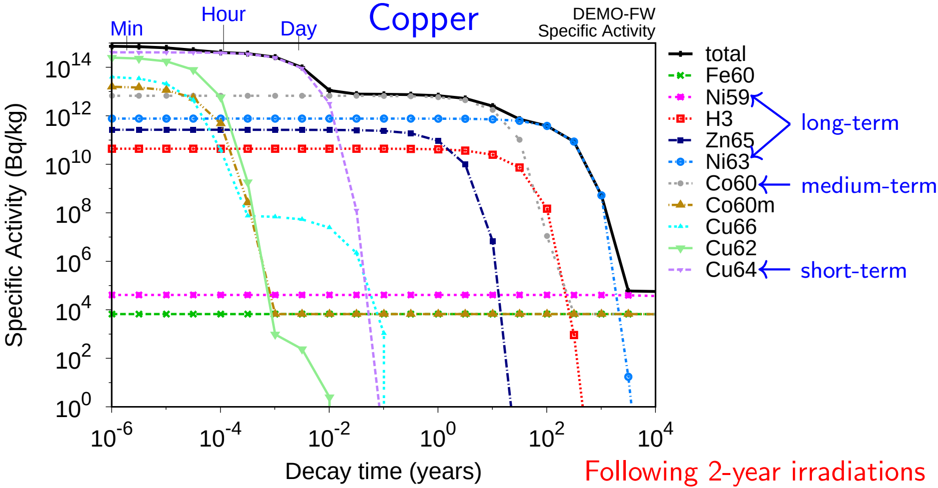




m – Dose Rate dominated by metastable nuclide(s)

Activation response – full nuclide contributions

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



Following 2-year irradiations

Activation response – full nuclide contributions

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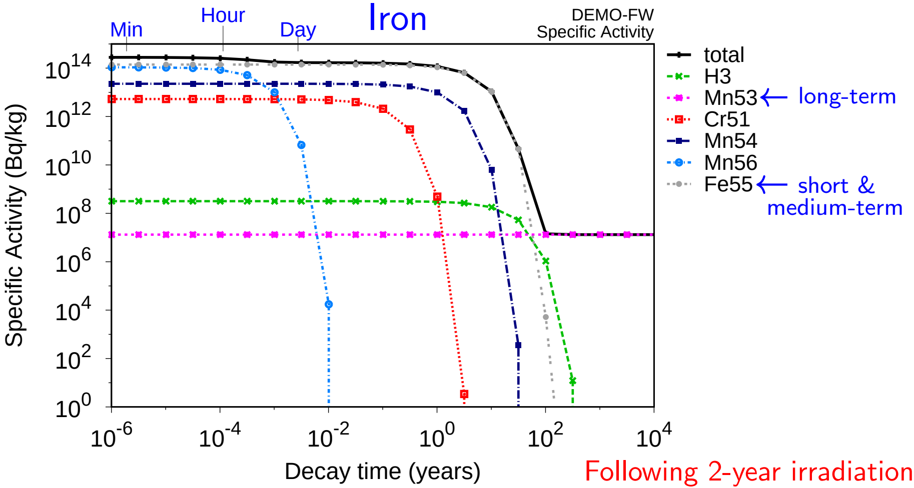

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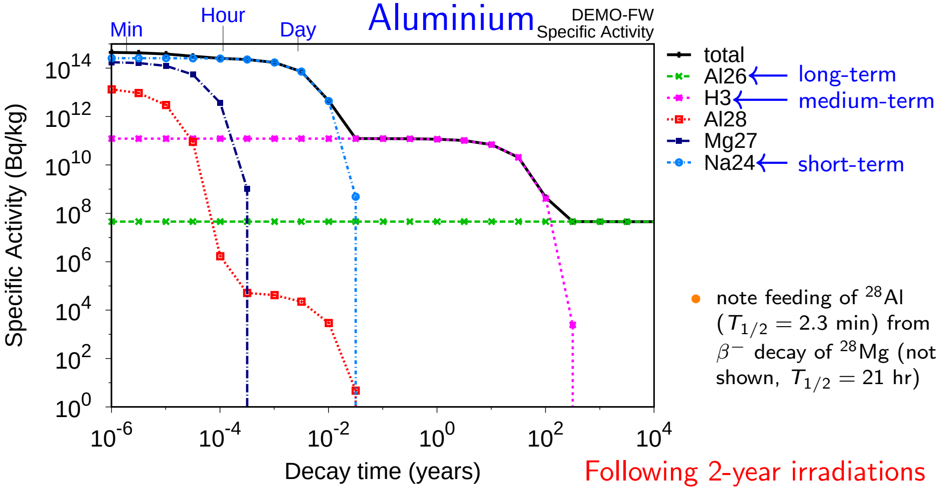

- note feeding of ^{28}Al ($T_{1/2} = 2.3$ min) from β^- decay of ^{28}Mg (not shown, $T_{1/2} = 21$ hr)

Following 2-year irradiations

Activation response – full nuclide contributions

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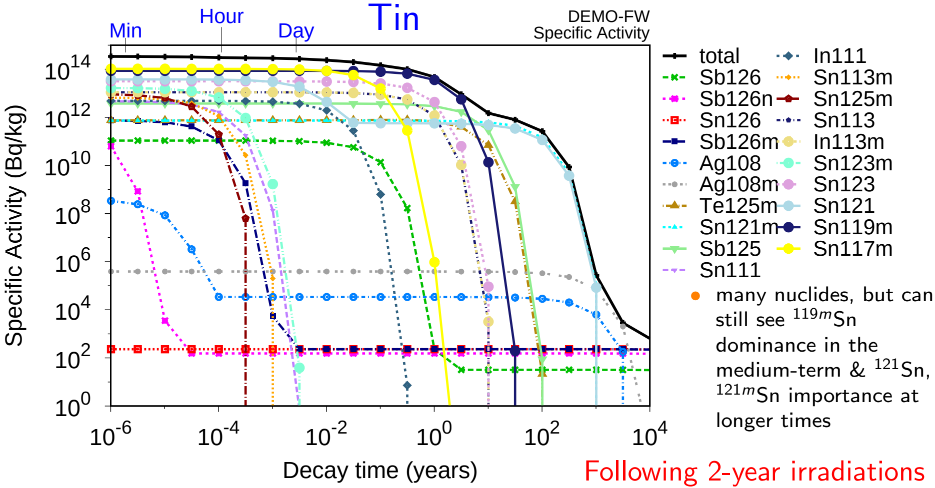
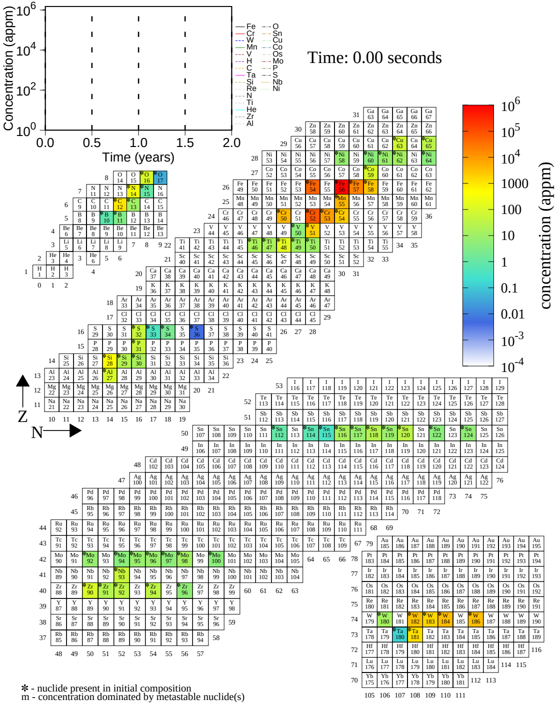


- many nuclides, but can still see ^{119m}Sn dominance in the medium-term & ^{121}Sn, ^{121m}Sn importance at longer times

Following 2-year irradiations

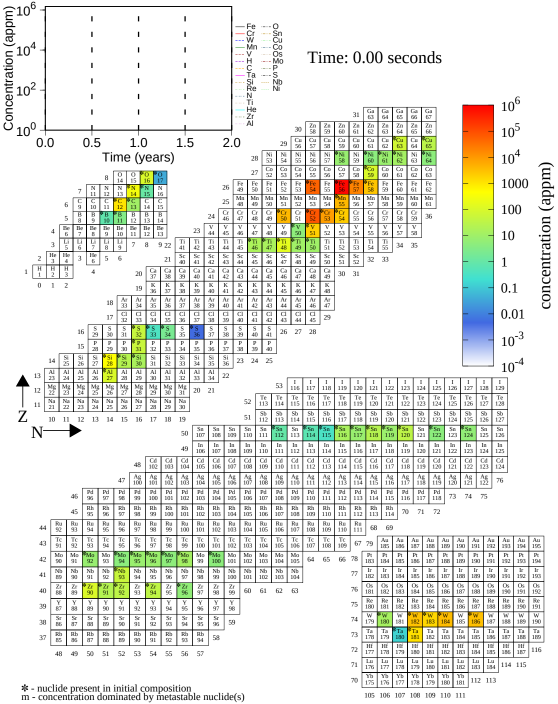
More complex materials: Eurofer steel



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

UK Atomic Energy Authority

More complex materials: Eurofer steel



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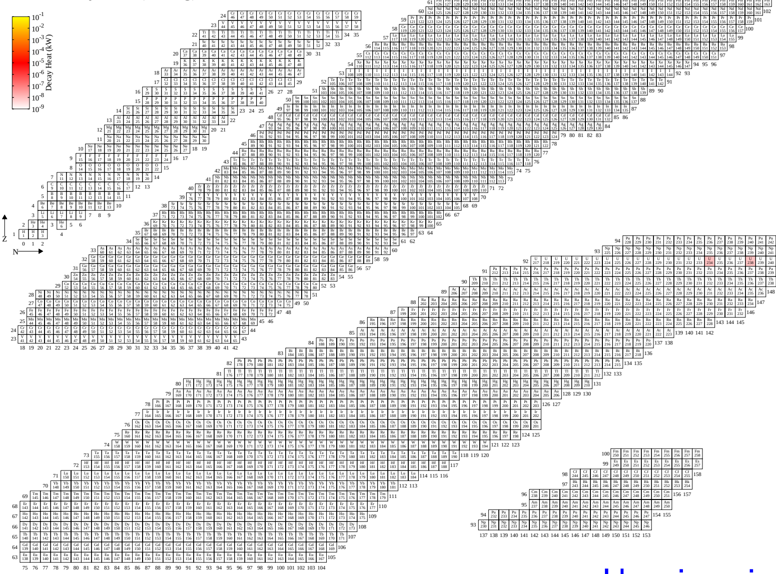
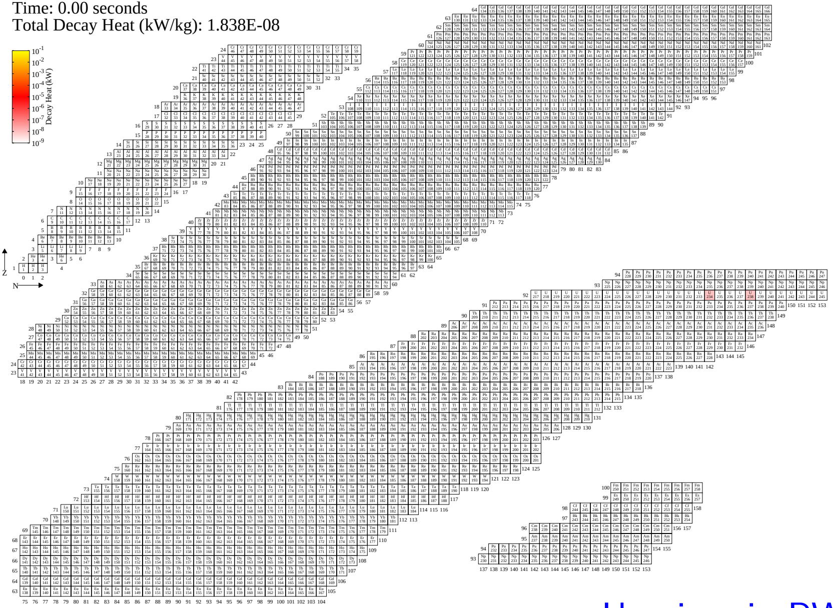
Time: 0.00 seconds

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



Uranium in PWR

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 world-leading example, with, in particular advanced features and the ability to utilise the latest nuclear data
- 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) 77137 http://dx.doi.org/10.1016/j.nds.2017.01.002