F4Epurity: A tool for rapidly assessing the change in dose rate resulting from deviations in material impurity content

Alex Valentine[1], Tim Eade[1], Marco Fabbri[2], Matteo di Giacomo[3], Davide Laghi[2], Raul Pampin[2]

[1]UK Atomic Energy Authority, Culham Campus, Abingdon, OX14 3DB, [2]Fusion for Energy, Josep Pla 2, Barcelona 08019, Spain, [3]ATG Science & Engineering SL, Plaza de Ernest Lluch y Martín 5, Barcelona 08019, Spain

Fusion Neutronics Meeting 2025, Madrid, Spain

Contents

UK Atomic Energy Authority

Introduction and motivation

Impurity requirements at ITER

UK Atomic Energy Authority

- The shutdown dose rate resulting from the activation of components depends directly on the chemical composition of materials, not only alloying elements but also, and in many cases more significantly, their impurity content.
- ITER has specific project requirements related to the impurities in chemical compositions that must be adhered to.
- As ITER construction progresses, deviations and non-conformities are arising in relation to these requirements.
  - COTS & standard parts made of uncertified batches
  - Unavailability of testing

ITER Deviation Requests related to material impurities

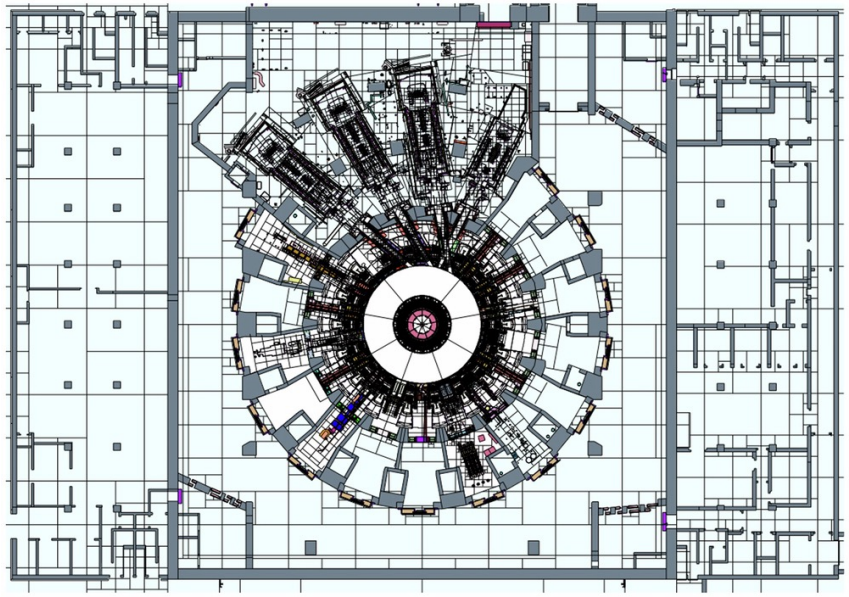
2016	2017	2018	2019	2020	2021	2022
3	3	10	10	5	12	45

Impurity requirements at ITER

UK Atomic Energy Authority

- Assessing the impact of each of these deviations by rigorous Monte-Carlo calculation is not practical.
- **Risk is that safety demonstration does not keep up with the ITER baseline.**
- Generally engineering judgement or prior experience needed/ approximation based on minimal activation calculation.
- Rationalisation needed also in the context of ongoing nuclear rebaselining at ITER.

Develop a tool capable of providing a rapid assessment of the local impact of a given impurity deviation on the shutdown dose rate



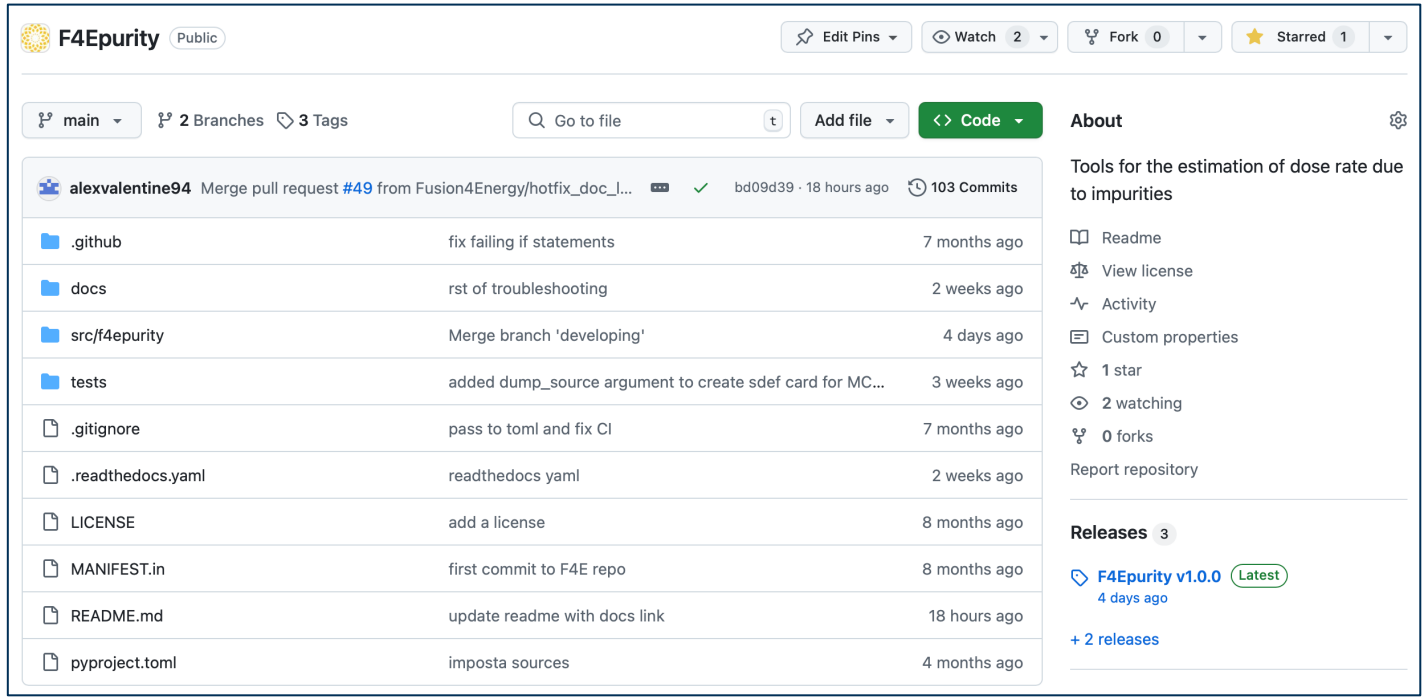
Juarez et al., **ITER full model in MCNP for radiation safety demonstration,** *Nature Communications* **volume 15**, Article number: 8563 (2024)

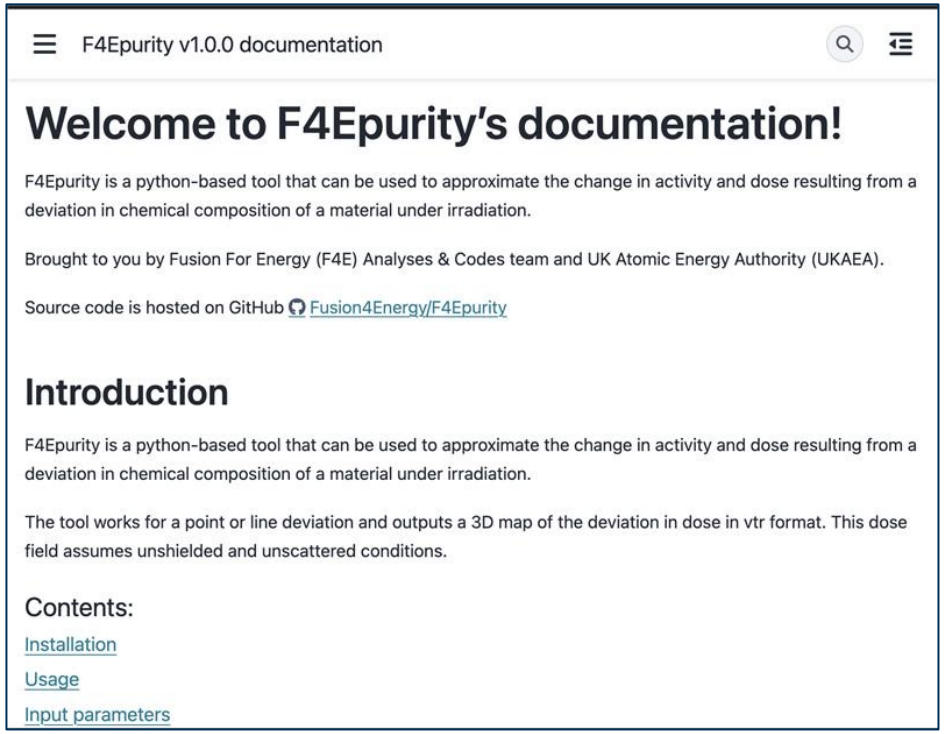
For further details, please see M.Fabbri/R.Pampin talk from day 1

F4Epurity

UK Atomic Energy Authority

- Originally developed by UKAEA under F4E framework contract *OMF-0882-02-01*. Further developed by F4E and UKAEA in a joint collaboration.
- Tool is **open source** and maintained on GitHub: *https://github.com/Fusion4Energy/F4Epurity* with documentation hosted here: *https://f4epurity.readthedocs.io/en/stable/.* CI testing pipeline.
- Written in Python as a command line tool.



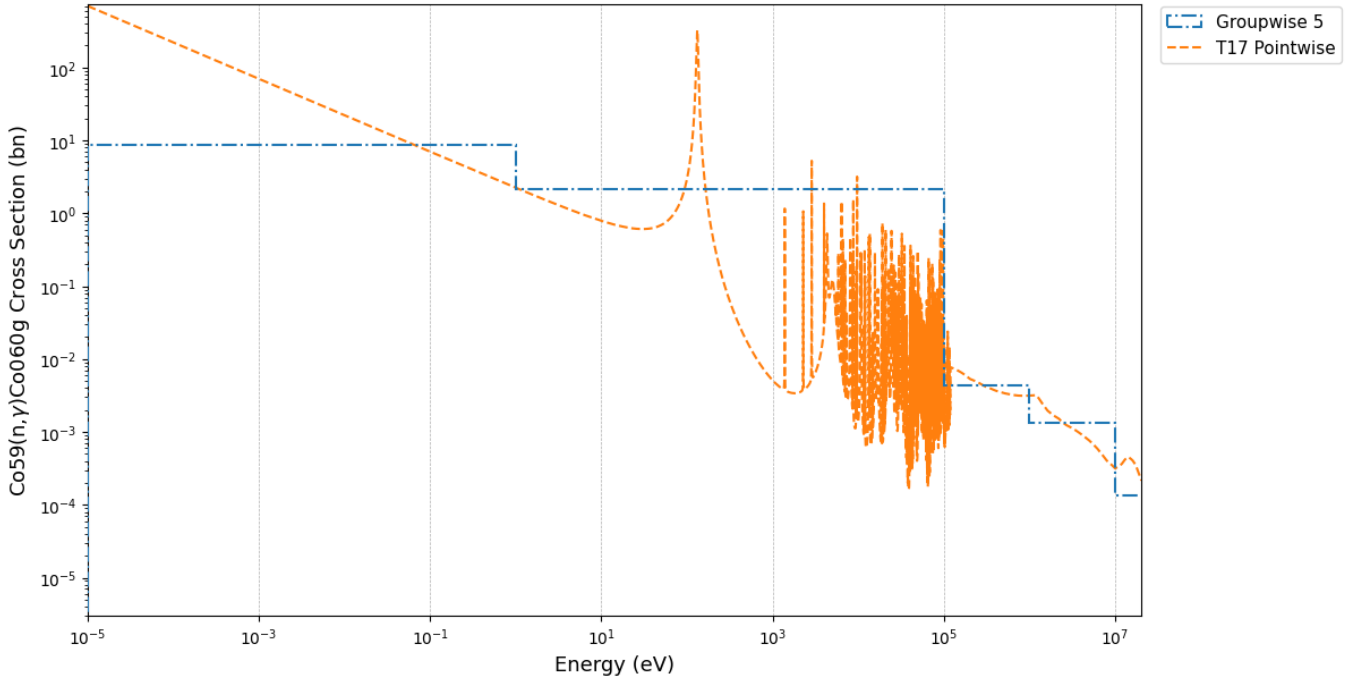


UK Atomic Energy Authority

Theory and implementation

Reaction Rate calculation

- Reaction rate is calculated using an effective cross section. Outside the bioshield, the radiation maps for ITER are available in 5 energy groups*.
- 5 group cross sections produced for important elements using the pointwise TENDL 2017 data. Includes metastable pathways.



$$\Delta RR(x,y,z) = \Delta N.\sigma_{eff}(x,y,z).\phi_{total}(x,y,z)$$

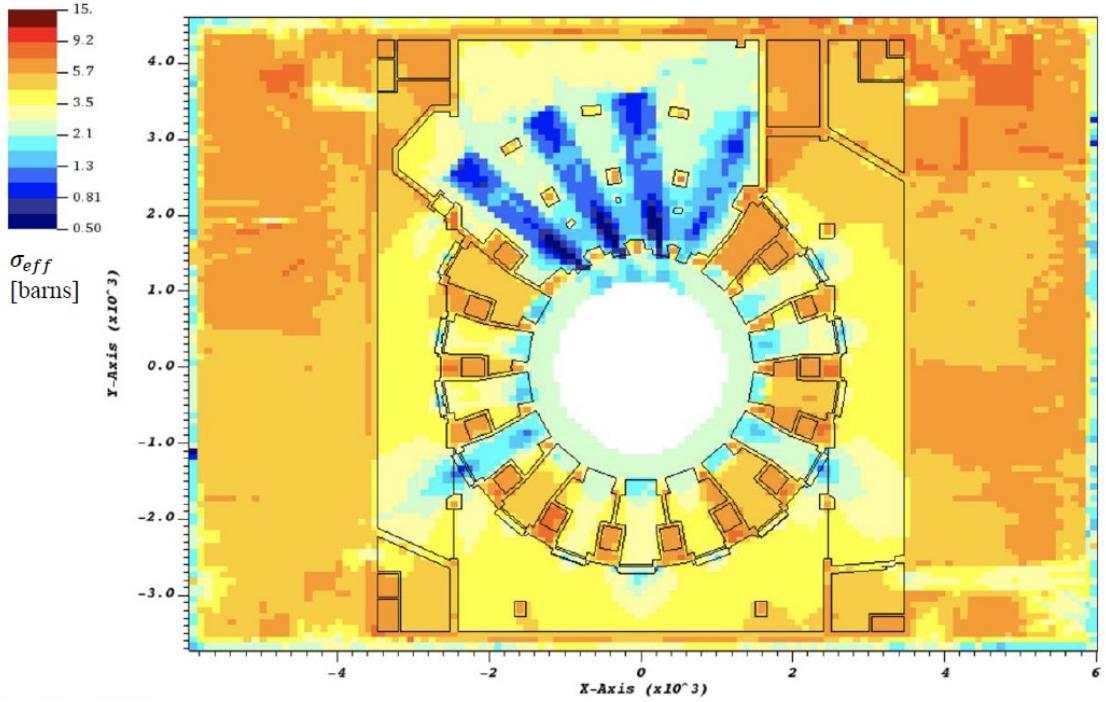
$$\sigma_{eff} = \frac{1}{\phi_{total}} \sum_{e} \sigma_e \phi_e$$

$$\sigma_g = \frac{\int_{e_{min}}^{e_{max}} \sigma(E)\chi(E)dE}{\int_{e_{min}}^{e_{max}} \chi(E)dE}$$

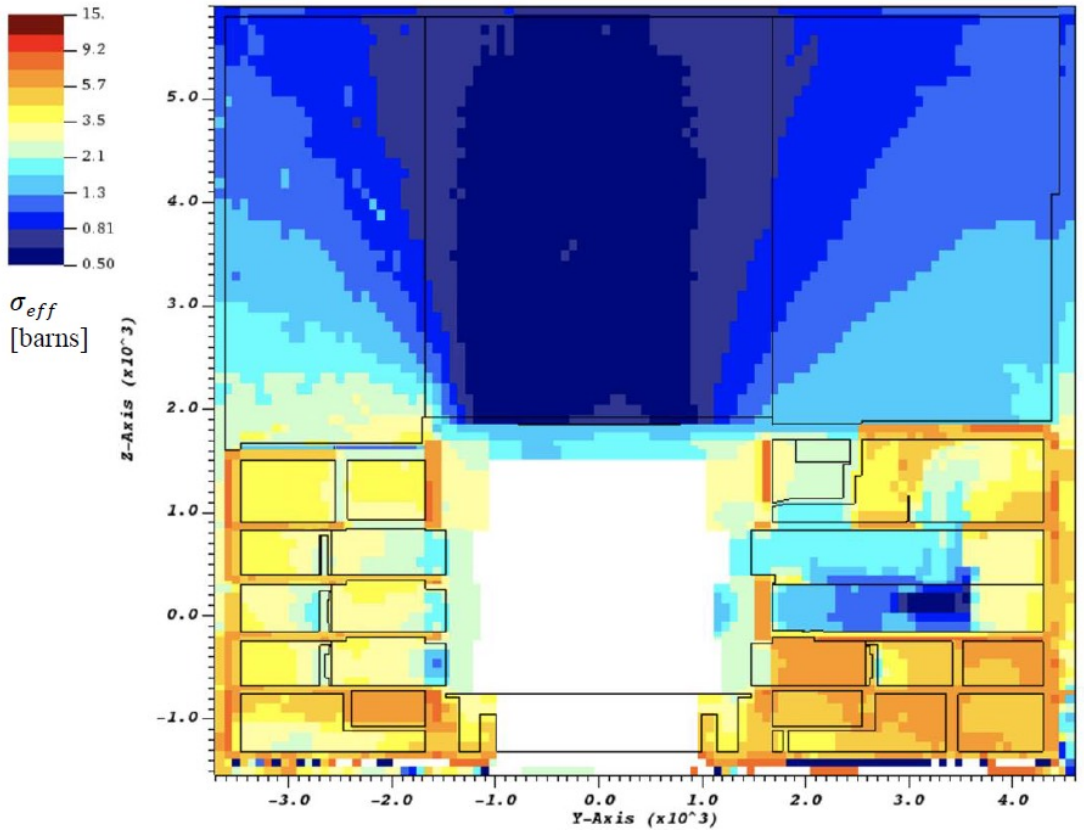
* Note that provided the xs is available to the code, any group format can be used.

Effective cross section maps

- 3D maps of the collapsed cross section are output in VTR format.
- Cross sections prepared for cobalt, niobium and tantalum as the dominant drivers of SDDR.
- Effective cross section plots output for all reaction pathways for the specified element.



Co59(n,g) Co60



Co59(n,g) Co60

```
f4epurity-xs --element Co --input_flux ./flux_spectrum.vtr
```

Activity and dose calculation

- The activity is calculated from the reaction rate with an ‘activation function’.
- **All reaction channels are accounted for including to metastable states and decay chains are evaluated to a stable daughter product to determine the activity at the decay time of interest**.

$$\Delta A(x,y,z) = \Delta RR\ (x,y,z).F_a(t)$$

$$\frac{dN_i}{dt} = -N_i(\lambda_{ii} + \sigma_{ii}\phi) + \sum_{j\neq 1} N_j(\lambda_{ij} + \sigma_{ij}\phi)$$

$$\Delta A_n(x,y,z,t) = N_n(t)\lambda_n$$

$$\Delta D_n(x,y,z,t) = \Delta \mathrm{A}_n(\mathrm{x,y,z,t}).F_d(x,y,z)$$

- The dose is determined used pre-computed conversion factor available for all nuclides. These are provided for each nuclide in units of:

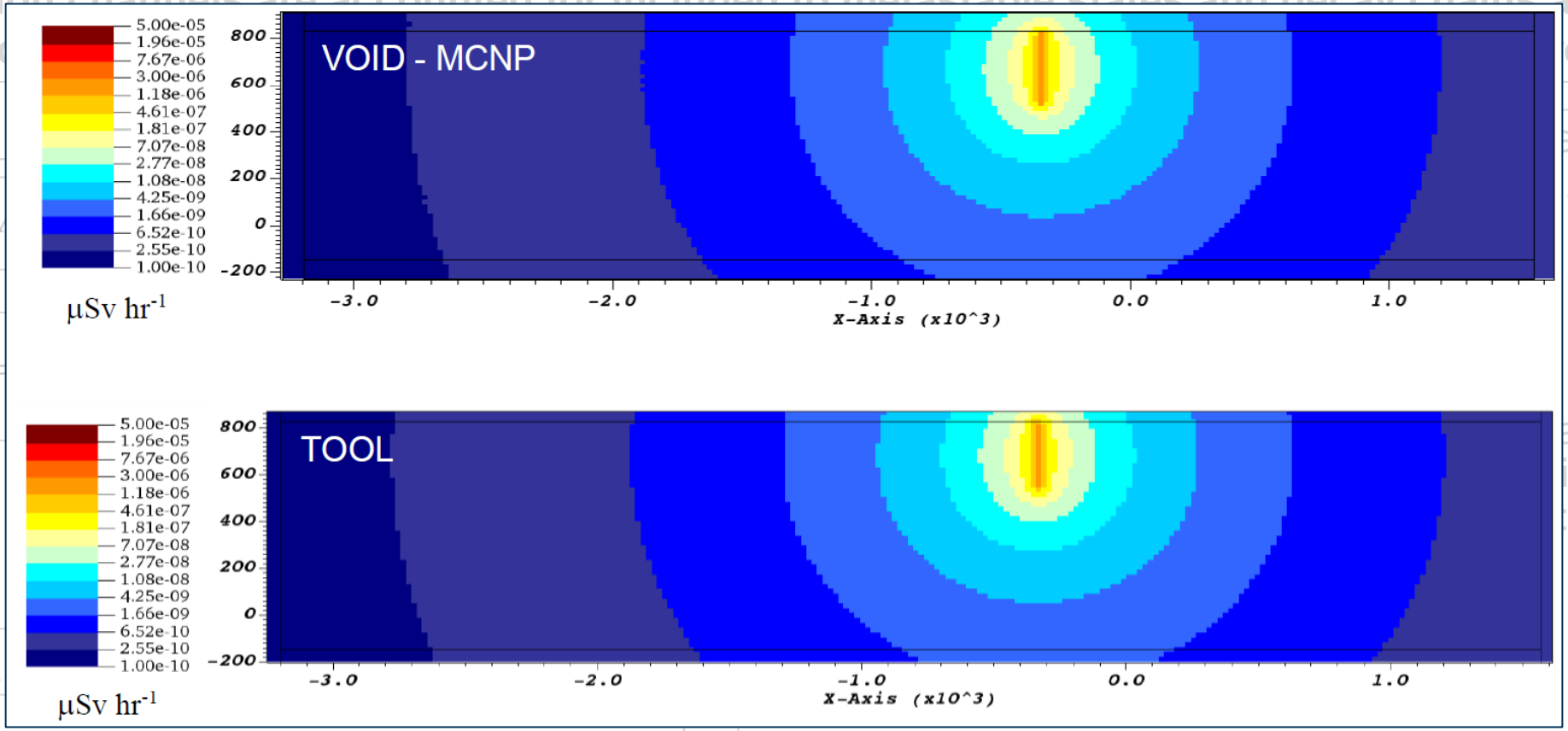
$$\frac{Sv\ cm^2}{Bq\ h}$$

- The dose at some distance is then calculated analytically. For a point source, this is a simple $1/r^2$ relation. For a line source this is given by:

$$D = \frac{D_L\theta}{x}$$

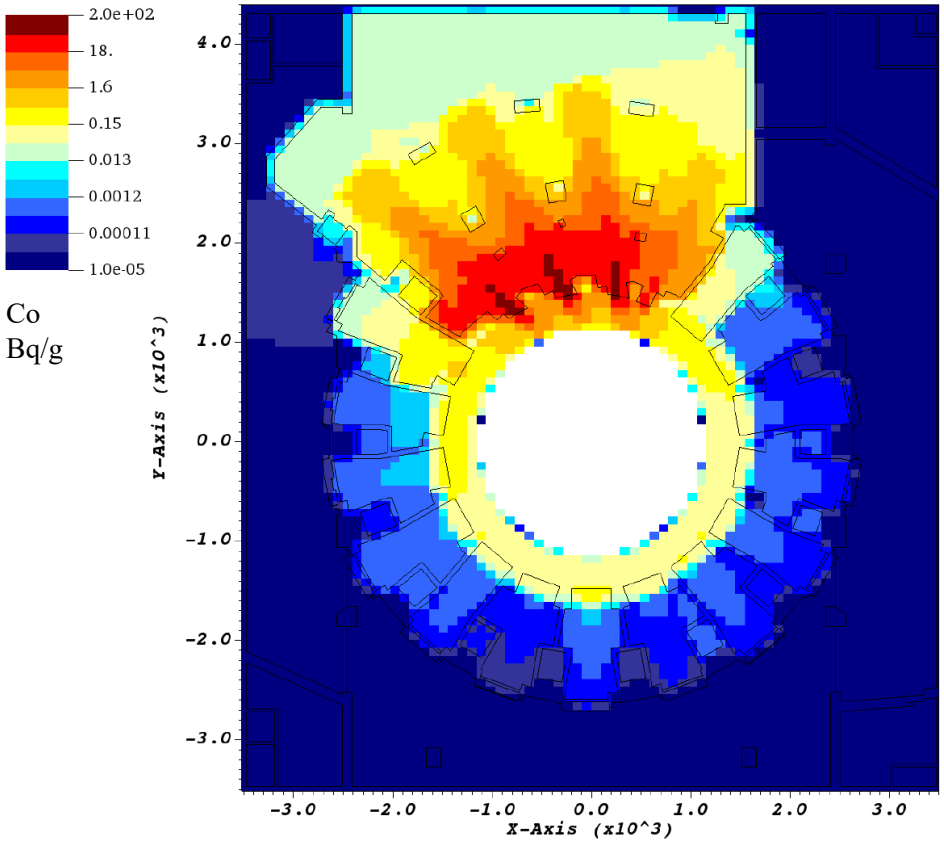
Activity and dose calculation

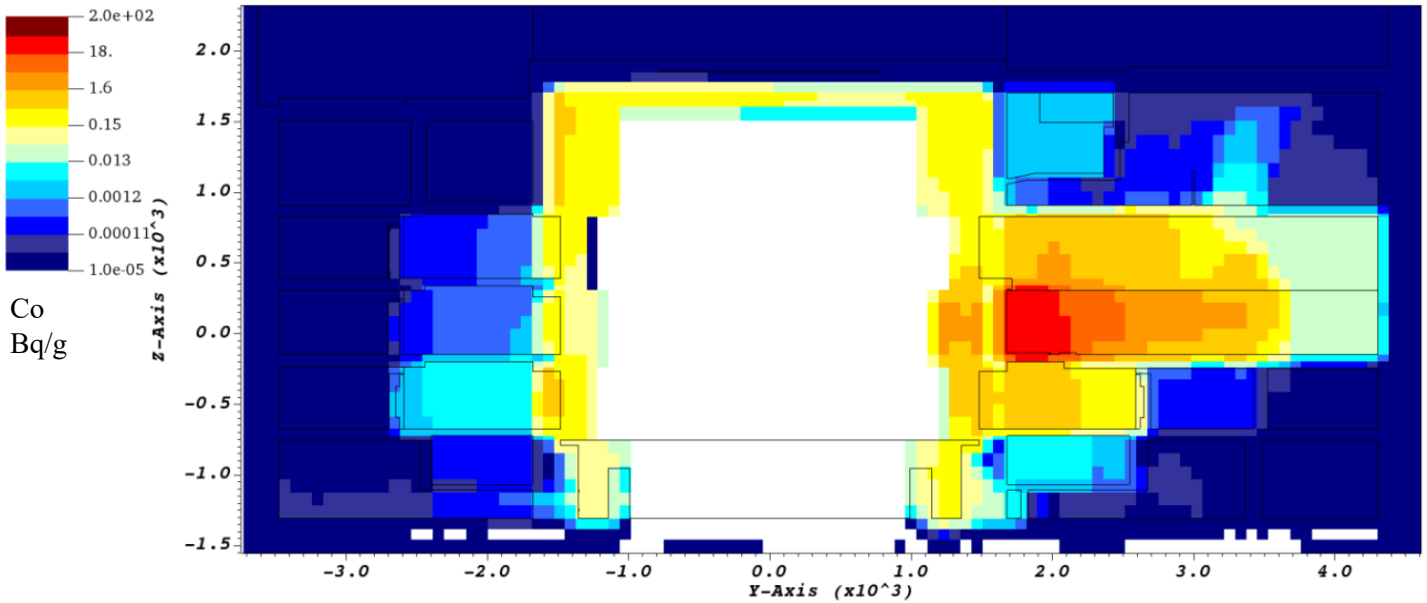
- The activity is calculated from the reaction rate with an ‘activation function’.
- All reaction channels are accounted for included to metastable states and decay chains are evaluated



Activity maps

- 3D maps of the computed activity are output in VTR format.
- Requires input of the irradiation scenario and the decay time of interest to output the activity.

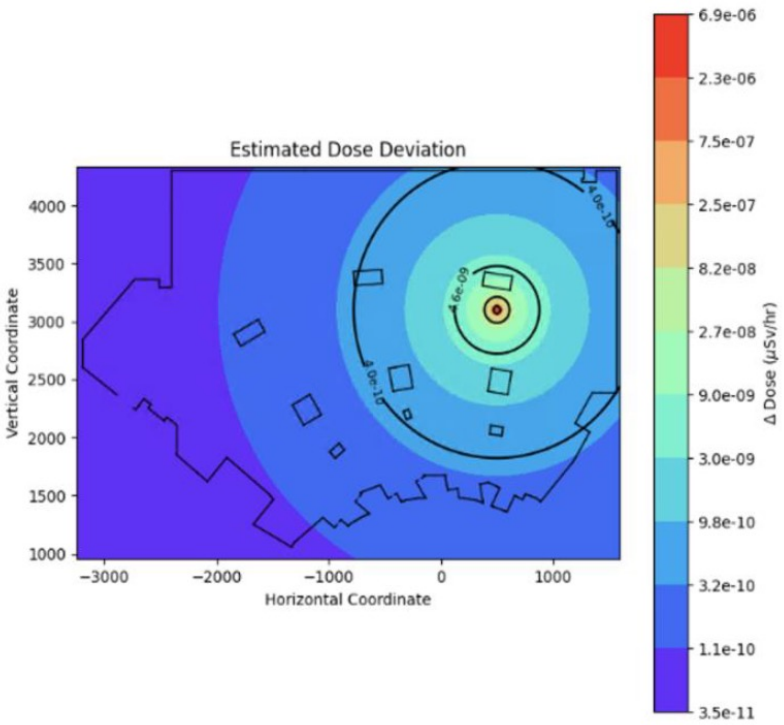


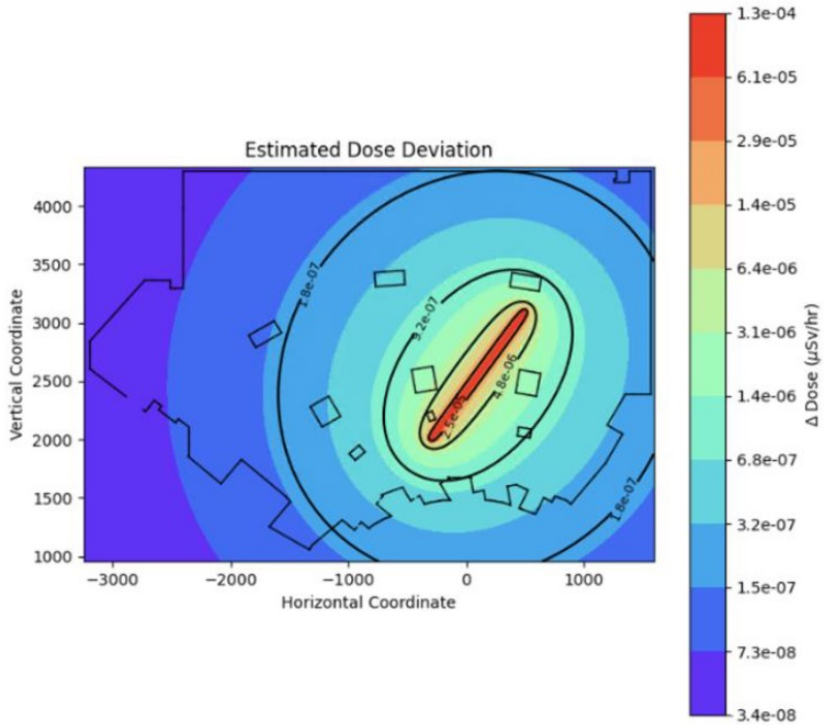



```
f4epurity-activity --element Co --delta_impurity 0.05 --input_flux
./flux_spectrum.vtr --irrad_scenario SA2 --decay_time 1e6
```

Deviation in dose rate

- The maps for the deviation in dose are output in VTR format or viewed using in-built plotter.
- Currently supported source geometries are **point** or **line**.
- Multiple source terms accepted e.g. deviation in multiple TCWS valves. Individual and summed dose maps are output.
- As the number of input arguments is large, they can be defined in a separate *json* or *yaml file.*





Example yaml file for a line source

```
element: Co
delta_impurity: 0.05
input_flux: radmap_path
irrad_scenario: SA2
x1: [-835]
y1: [1994]
z1: [1230]
x2: [100]
y2: [2019]
z2: [1230]
decay_time: 1e6
```

```
f4epurity --cfg config.yaml --sources_csv source.csv
```

Additional capabilities and future work

UK Atomic Energy Authority

- Output tabulated dose rates can be extracted at workstation locations (provided as coordinates).
- Estimate the impact of shielding on the dose rate for a given source term using buildup factors and attenuation coefficients.
- The major limitation of the default maps output by the tool is the assumption of unshielded and unscattered conditions.
  - An MCNP SDEF can be written by the tool using the activities output from F4Epurity.
  - We have explored the use of an adjoint flux calculation to map contributions to locations of interest.

```
C F4EPurity source definition
sdef PAR=2 POS=d1 ERG FPOS d2
SI1 L  0.0 0.0 0.0
SP1 1.000
DS2 S  3
SI3 L
       1.17e+00 1.17e+00 1.33e+00 1.33e+00
SP3
       4.96e-04 4.96e-04 5.02e-04 5.02e-04
FC4 Dose [muSv/hr]
FMESH4:P  GEOM=XYZ
       ORIGIN -550.0 -550.0 -550.0
       IMESH 550   IINTS  21.
       JMESH 550   JINTS  21.
       KMESH 550   KINTS  21.
C       emesh 14
C       eints 5
FM4 3.579192E-06 $ muSv/hr
DE4
       0.01 0.015 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.10 0.15 0.20 0.3 0.4 0.5 0.6 0.8 1.0 2.0 4.0 6.0 8.0 10.0
DF4
       0.0485 0.1254 0.2050 0.2999 0.3381 0.3572 0.3780 0.4066 0.4399 0.5172 0.7523 1.0041 1.5083 1.9958
       2.4657 2.9082 3.7269 4.4834 7.4896 12.0153 15.9873 19.9191 23.7600
```

Complete list of capabilities of the tool is given in the documentation: https://f4epurity.readthedocs.io/en/stable/

UK Atomic Energy Authority

Validation

Comparison to FISPACT-II

UK Atomic Energy Authority

- Number of nuclides calculated compared to FISPACT by irradiating 1kg of Co and Nb for DT1 and comparing at 10^6 seconds.

		Impurity Deviation Tool (Number of Nuclides)			FISPACT (Number of Nuclides)		
Irradiation Time	Relative Flux	Co59	Co60m	Co60	Co59	Co60m	Co60
730.5 days	1.70e-06	1.02E+25	1.70E+08	3.99E+13	1.02E+25	1.70E+08	3.99E+13
730.5 days	1.17e-04	1.02E+25	1.17E+10	2.78E+15	1.02E+25	1.17E+10	2.78E+15
730.5 days	3.88e-04	1.02E+25	3.88E+10	1.12E+16	1.02E+25	3.88E+10	1.12E+16
730.5 days	9.96e-04	1.02E+25	9.96E+10	3.19E+16	1.02E+25	9.95E+10	3.19E+16
730.5 days	1.59e-03	1.02E+25	1.59E+11	6.17E+16	1.02E+25	1.58E+11	6.10E+16
600 s	5.01e-01	1.02E+25	2.44E+13	6.18E+16	1.02E+25	2.43E+13	6.11E+16
1e6 s	0	1.02E+25	0.00E+00	6.16E+16	1.02E+25	0.00E+00	6.09E+16

- Comparison performed against code equivalent time correction factors and those used in D1SUNED.
- Agreement is found to be very good (within 1%).

Isotope	D1S Time correction factor	Tool derived time correction factors using D1S irradiation schedule
Co60	3.686E-02	3.685E-02
Nb94	1.853E-05	1.853E-05
Nb92m	8.514E-02	8.511E-02

Summary

- A novel open source tool, F4Epurity, has been developed to rapidly assess the change in dose rate resulting from deviations in material impurity content.
- The estimation provided can be determined in minutes vs rigorous 3D Monte-Carlo calculation (days).
- The code has been designed to be flexible for application not only to ITER.
- The tool will be useful in managing the growing number of non-conformances at ITER and as part of rationalisation for ITER impurity requirement throughout the tokamak complex.

UK Atomic Energy Authority

Thank you for listening

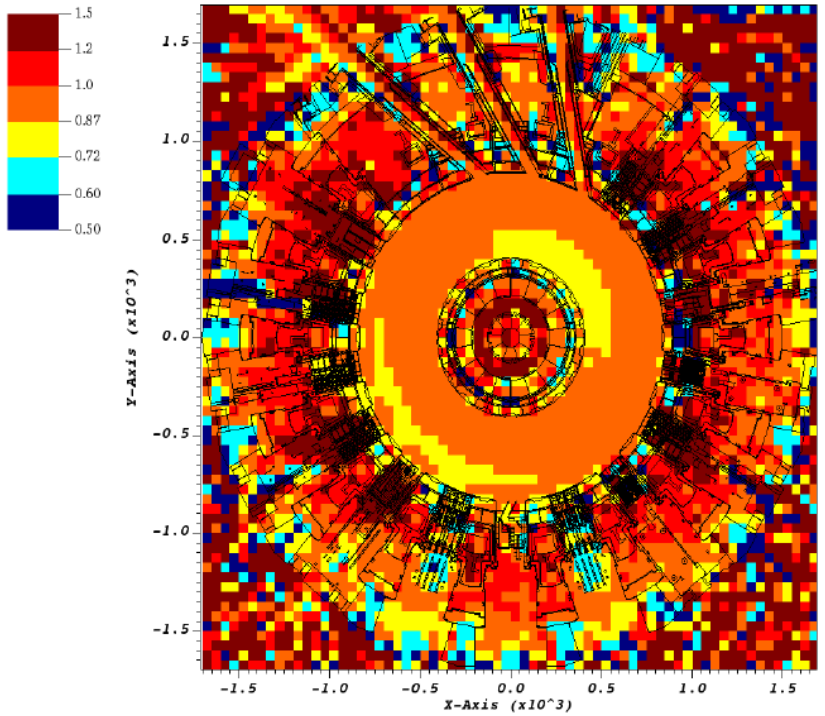
Alex.Valentine@ukaea.uk

175 group vs 5 group

- Compare 5-group data we are using outside the bioshield to a finer 175-group which is available within the bioshield. The tool result using the two different group structures was compared. The results are ~37% different for this location, with 5-group overpredicting.
- Differences related to the calculated effective cross section between the two group structures.
- **Compare the global maps of the effective cross section.**

	5-g	175-g	% diff
Tool, Atoms Co60	7.16E+16	5.2289E+16	**37%**

Effective xs	5-g	175-g
Co59 (n,g) Co60	1.36	1.12
Co59 (n,g) Co60m	2.26	1.41



5-g/175-g effective cross section for Co59(n,g)Co60

Comparison to FISPACT

- A point was selected from the in-bioshield 175g radiation maps (900,900,0) and a FISPACT calculation performed irradiating 1kg of Cobalt for SA2 scenario with EAF2010 data. Tool run using the same *xs* data and selecting the same coordinate point and scenario.
  - Verified that the correct flux was being extracted from the *vtr* by the tool.
  - The effective cross section (collapse of flux & xs) were shown to be identical for the two reaction channels in cobalt (extract_xs in FISPACT can be used to output this).
  - Compared the number of atoms at 12 days after shutdown of Co60 and the Co60 activity. Tabulated below – the results are within 1%.
- **Also checked at multiple locations and agreement shown to be within 1%**

	Tool	FISPACT II
Atoms	5.2289E+16	5.2481E+16
Activity (Bq/kg)	2.1699E+08	2.1869E+08

Assumption of no-scattering

- An MCNP calculation was ran with a Co-60 line source (one of the cryolines) just containing the outer walls of the NB cell (ITER concrete). The results for the dose using the reference DE/DF cards (ICRP-74) were compared between the concrete and void cases. Below plots the ratio of **scattered/unscattered**. The behaviour is as expected that the impact is greater at further distances from the source.