Co-dependent energy and angular spectra of CX atoms in EIRENE, and their impact on W sources in JET

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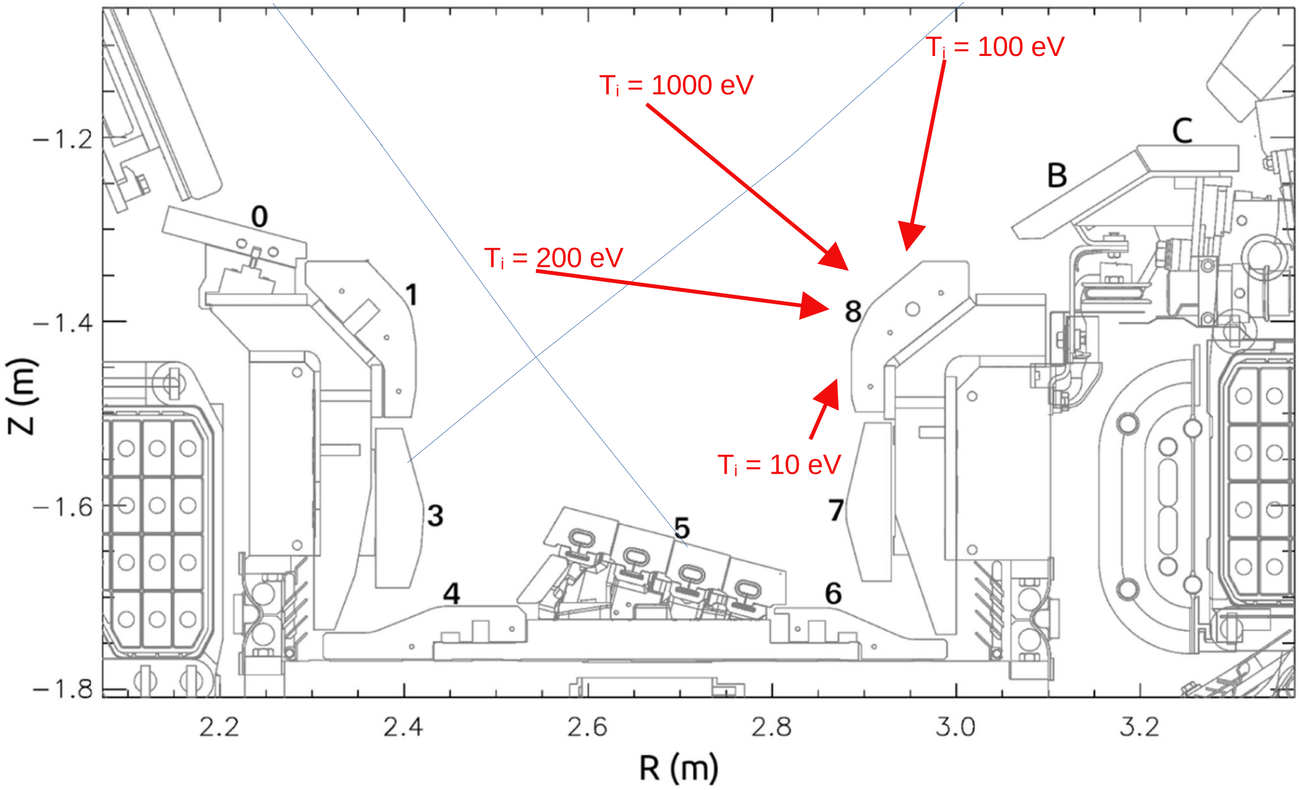
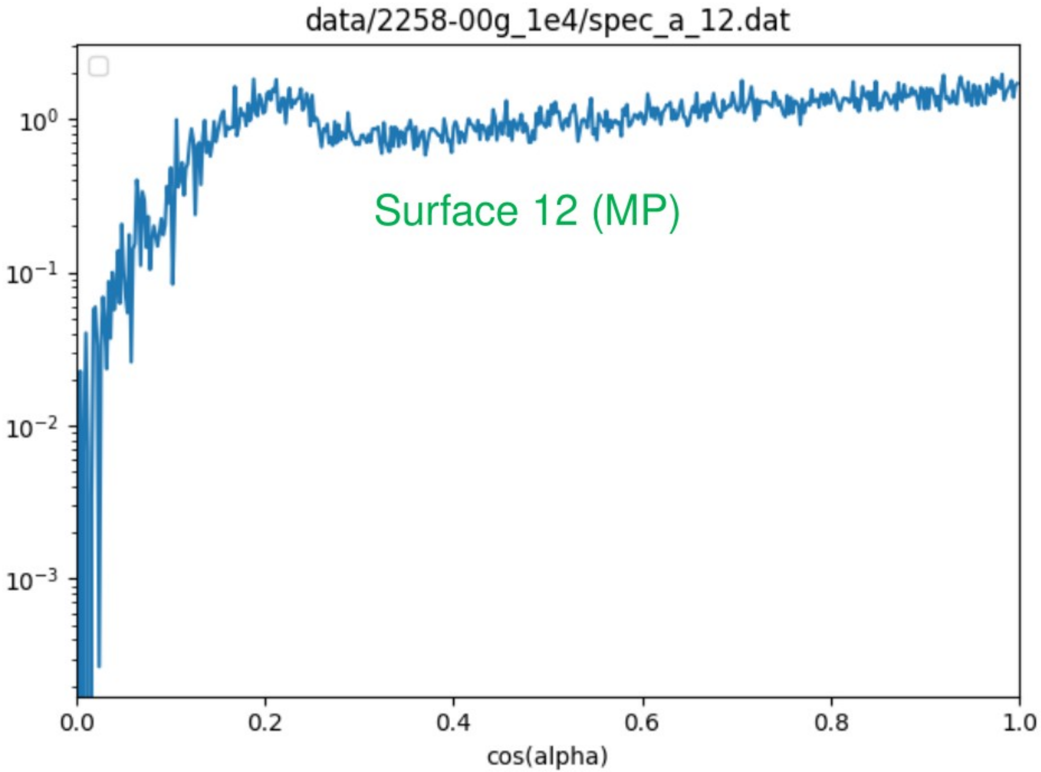
The impact angle distribution of CX atoms is correlated with impact energy



Previously, angular distributions in EIRENE were tallied independently of energy

- EIRENE has been used to study the CXN angular spectrum in JET, ITER, DEMO, ...
- In this work, we implement and study the co-dependence of the energy and angular spectra
- Problem: Sampling the 2D energy-angle distribution with high resolution is computationally expensive
- Solution: Functional expansion tallies [1,2]



S. Wiesen et al. “Detailed charge exchange neutral distribution modelling for the ITER main wall”, 28 Nov 2023

[1] D. Griesheimer PhD thesis, 2005
[2] Z. Wang et al., Nucl. Eng. Tech 2021

Functional expansion tallies avoid the compromise between MC noise and resolution

- Approach:

  1) Define 15 energy bins with logarithmic binning

  2) Compute the Legendre polynomial expansion of the impact angle cosines for each energy bin
     - 10th degree used here, 7th degree should be good enough for most purposes

  3) Store the polynomial coefficients in eirene.out

  4) Reconstruct the energy-resolved angular spectra in post-processing:

$$f(\theta) = \sum_{n=0}^{\text{ISPLDEG}} a_n \cdot \pi sin(\theta) \cdot L_n(2cos(\theta) - 1)$$

  → MC noise greatly reduced w.r.t. histogram binning

- **Implemented, tested, and available in the 'develop' branch**

Source: Wikipedia

n	$P_n(x)$
0	1
1	x
2	$\frac{1}{2}(3x^2-1)$
3	$\frac{1}{2}(5x^3-3x)$
4	$\frac{1}{8}(35x^4-30x^2+3)$
5	$\frac{1}{8}(63x^5-70x^3+15x)$
6	$\frac{1}{16}(231x^6-315x^4+105x^2-5)$
7	$\frac{1}{16}(429x^7-693x^5+315x^3-35x)$
8	$\frac{1}{128}(6435x^8-12012x^6+6930x^4-1260x^2+35)$
9	$\frac{1}{128}(12155x^9-25740x^7+18018x^5-4620x^3+315x)$
10	$\frac{1}{256}(46189x^{10}-109395x^8+90090x^6-30030x^4+3465x^2-63)$

Functional expansion tallies avoid the compromise between MC noise and resolution

- How to use: eirene.input:

```
*** 10. DATA FOR ADDITIONAL TALLIES
     0     0     0     0     0    27
*** 10A.
*** 10B.
*** 10C.
*** 10D.
*** 10E.
** 10F. Spectra, energy resolved
* energy spectrum of D atoms at non. def. surfaces
    43     1     1     1   -15     0     0     2
  1.0000E+00  1.0000E+04  0.0000E+00  0.0000E+00  1.0000E+01
    10
    44     1     1     1   -15     0     0     2
  1.0000E+00  1.0000E+04  0.0000E+00  0.0000E+00  1.0000E+01
    10
```

Number of tallies
Index of surface
Number of energy bins (negative: log binning)
ISPOPT=2: Functional expansion tally
Energy range 1 eV to 10 keV
Degree of Legendre expansion

Legendre polynomial coefficients $a_1 \ldots a_{10}$

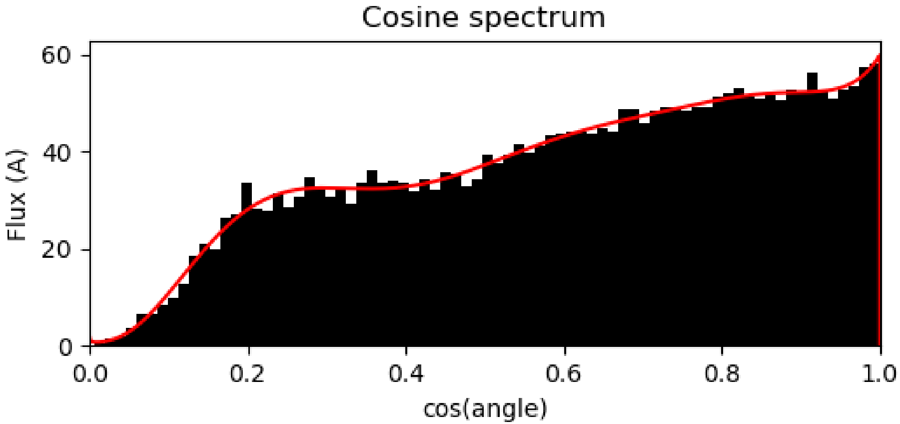
eirene.out:

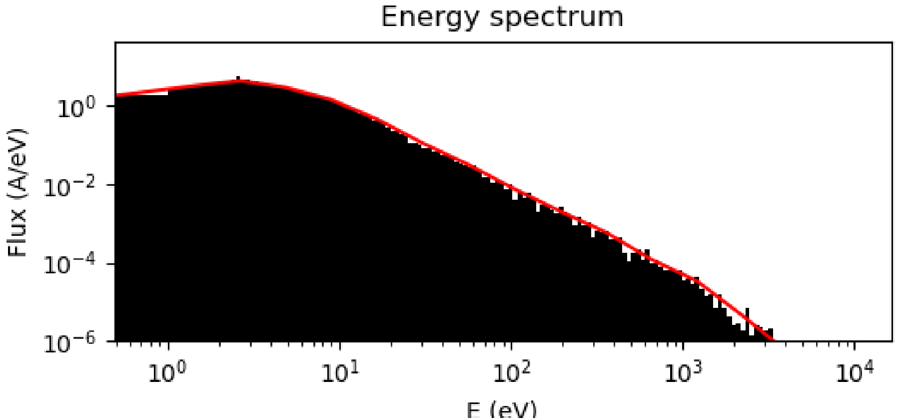
```
 LEGENDRE EXPANSION TALLY FOR ADDITIONAL SURFACE     43
  BIN   B-LEFT      B-RIGHT     COEFFICIENT
     0  0.0000E+00  1.0000E+00
 -3.2220E-03  5.7639E-02 -4.7795E-01  3.2590E+00 -2.0349E+01  1.2136E+02 -7.0498E+02  4.0308E+03 -2.2821E+04  1.2842E+05
 .......................................
     1  1.0000E+00  1.8478E+00
  7.6463E-02 -4.2559E-01  2.3846E+00 -1.3470E+01  7.6491E+01 -4.3513E+02  2.4725E+03 -1.4009E+04  7.9081E+04 -4.4462E+05
     2  1.8478E+00  3.4145E+00
 -1.6258E-01  8.5502E-01 -4.1910E+00  2.1008E+01 -1.0607E+02  5.4091E+02 -2.7836E+03  1.4452E+04 -7.5666E+04  3.9937E+05
     3  3.4145E+00  6.3096E+00
 -4.2213E-02  2.0578E-01 -9.4519E-01  4.4150E+00 -2.0772E+01  9.8492E+01 -4.7026E+02  2.2595E+03 -1.0919E+04  5.3039E+04
```

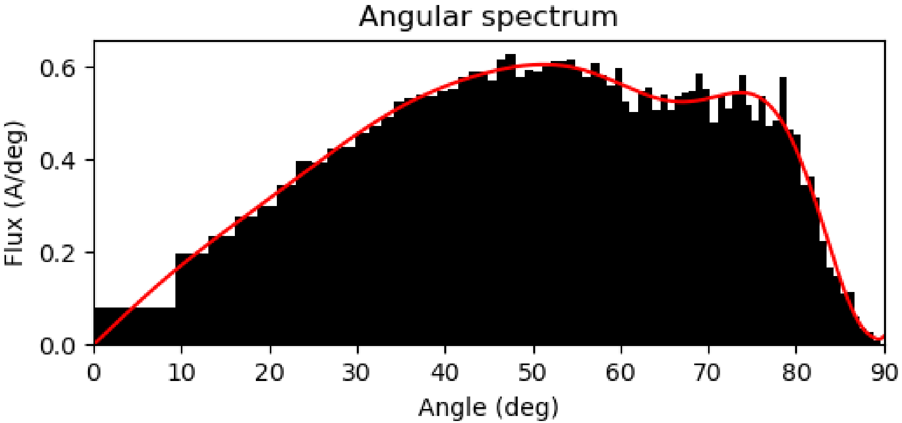
In case of questions, read the EIRENE manual or contact h.kumpulainen@fz-juelich.de

Functional expansion validated using JET cases, comparison with histogram binning

- Smooth analytic functions provide better angular resolution and lower noise with the same atom trajectories as the histogram method

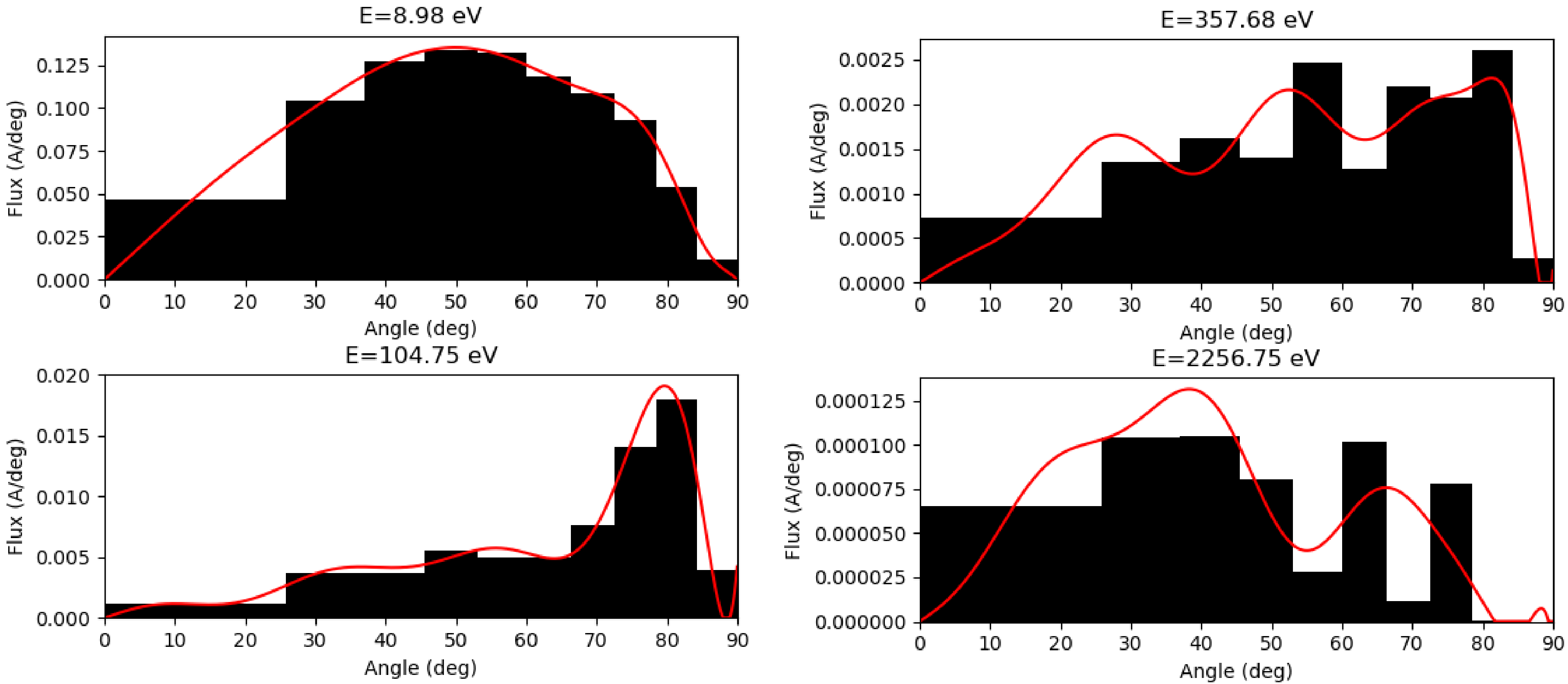






JPN 94606 at 50-51 s (H-mode), run588s3, outer vertical divertor

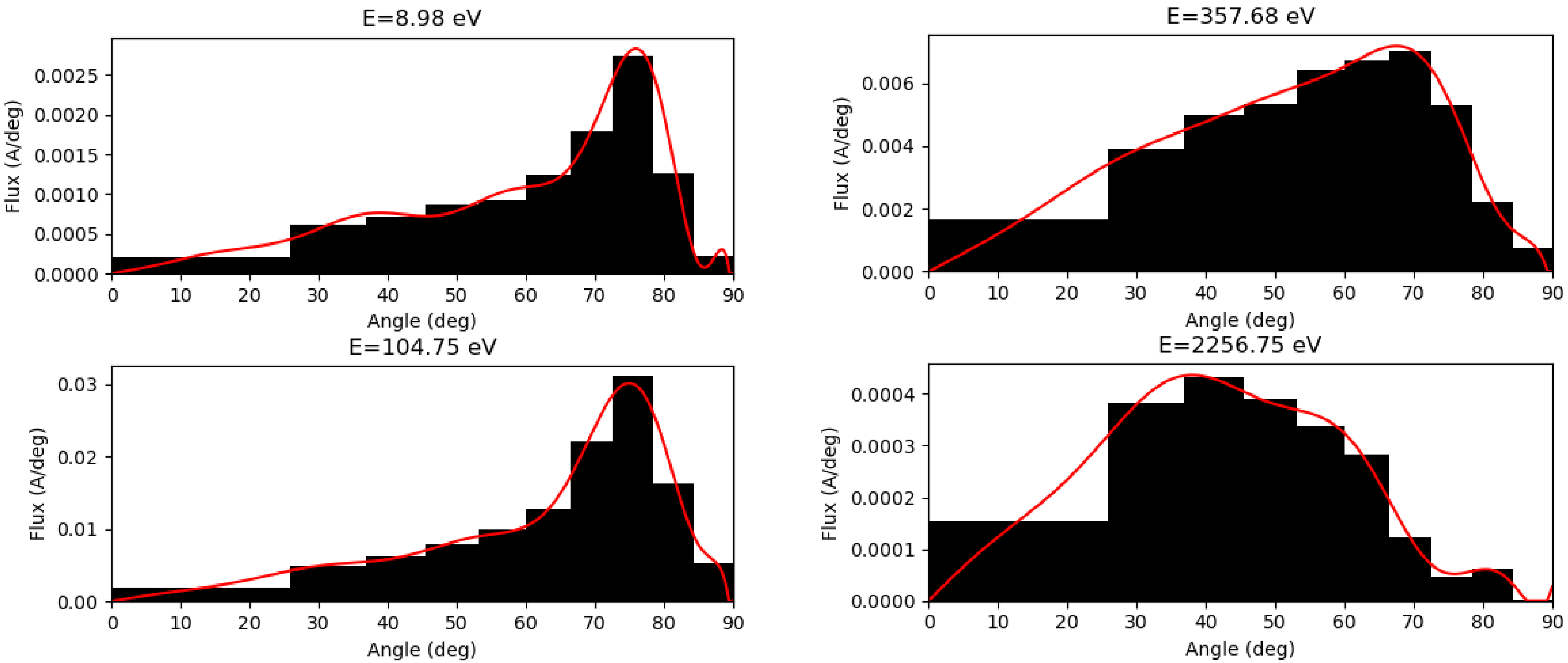
JET outer vertical divertor: E = 100 eV almost tangential, <50° peak at E > 1 keV



Significant MC noise with the histogram method especially at E=2256.75 eV

JPN 94606 at 50-51 s (H-mode), run588s3, outer vertical divertor

JET main chamber: >70° peak at low energies, <50° peak at E > 1 keV

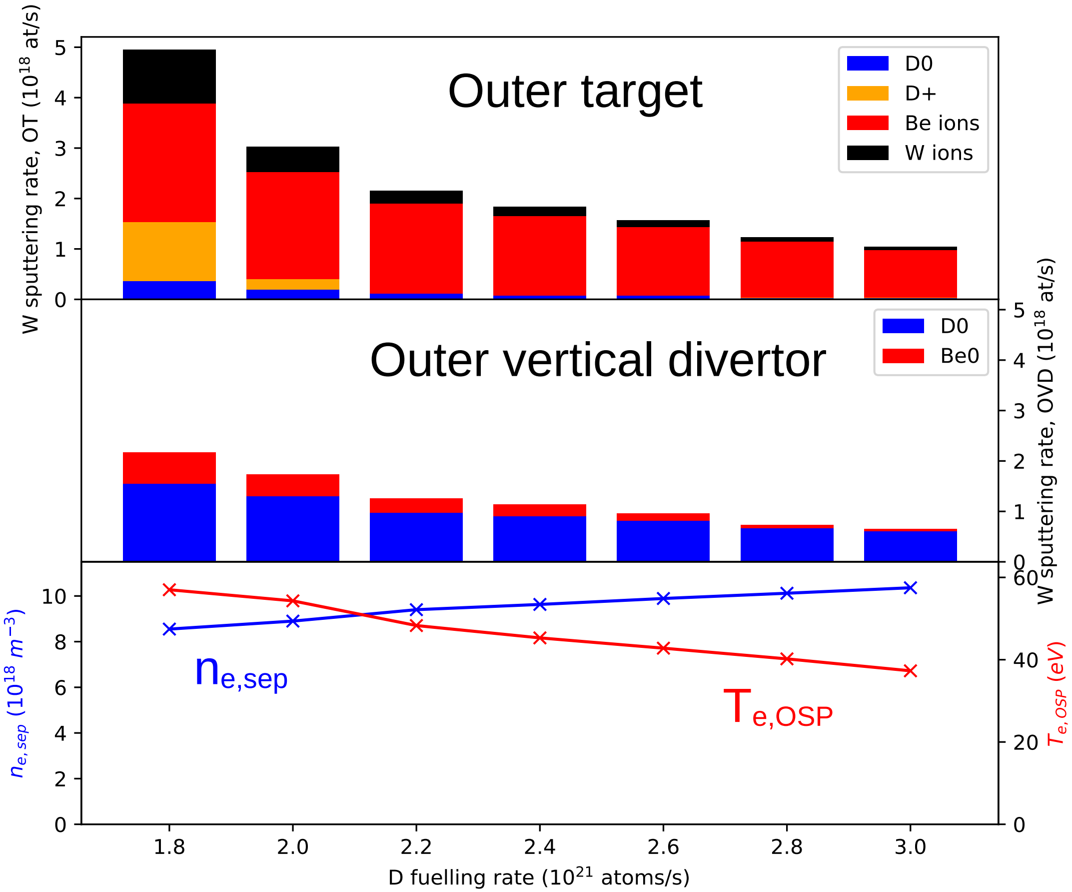


Correct implementation and post-processing of functional expansion tallies verified by comparison against histogram binning

JPN 81472 at 49-50 s, run581o (L-mode)

Fuel CX atoms are the main cause of W erosion in non-plasma-wetted regions

- Largest causes of gross W erosion in JET:
  - Be ions (L-mode and inter-ELM)
  - D ions (intra-ELM)
  - Seeding impurities in heavily seeded pulses
- W erosion rate density (atoms/m^{2}s) due to CXN is typically ~1% of the peak W source at the LFS target
- Integrating over the area of all W components, the predicted CXN contribution is >10% of all W sputtering

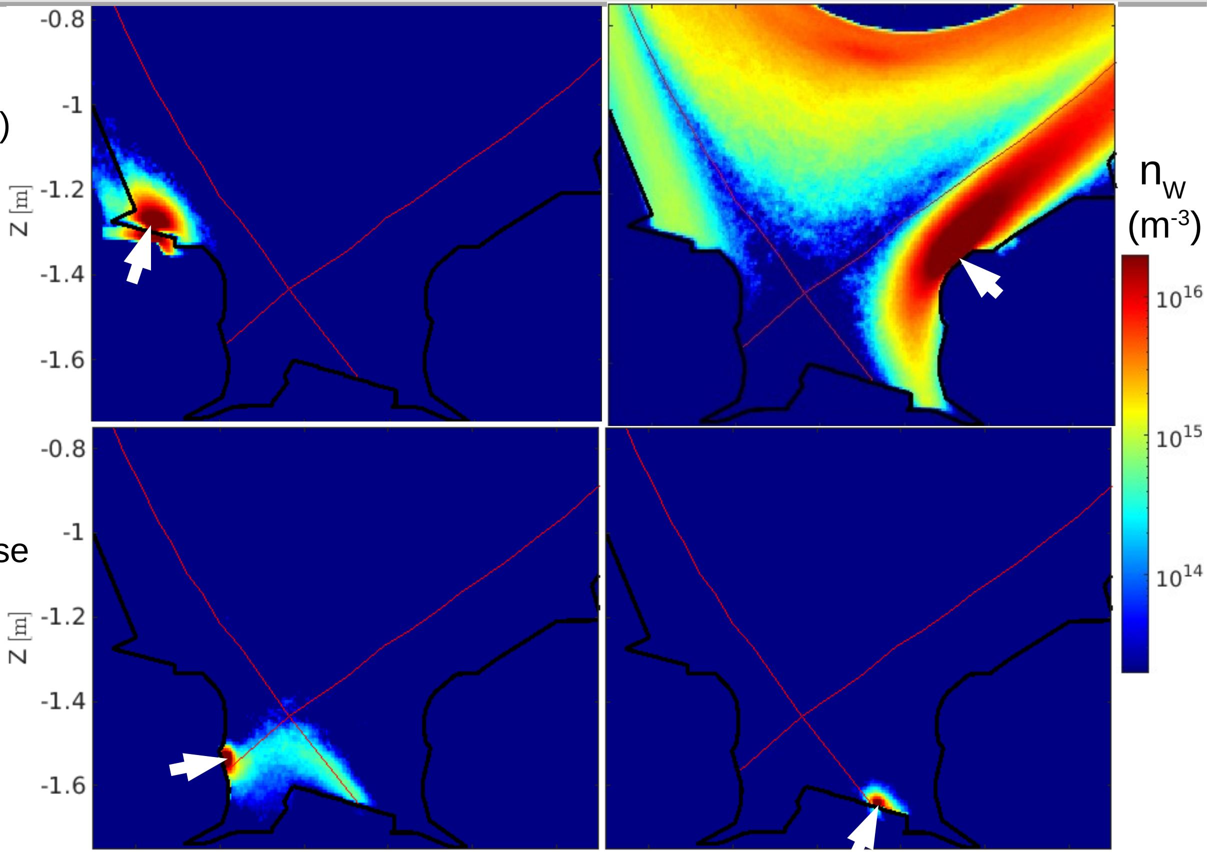


JPN 81472-81474 (L-mode)
H. Kumpulainen PhD thesis, 2023

ERO2.0 predicts near-perfect divertor screening of W, except near the outer divertor entrance

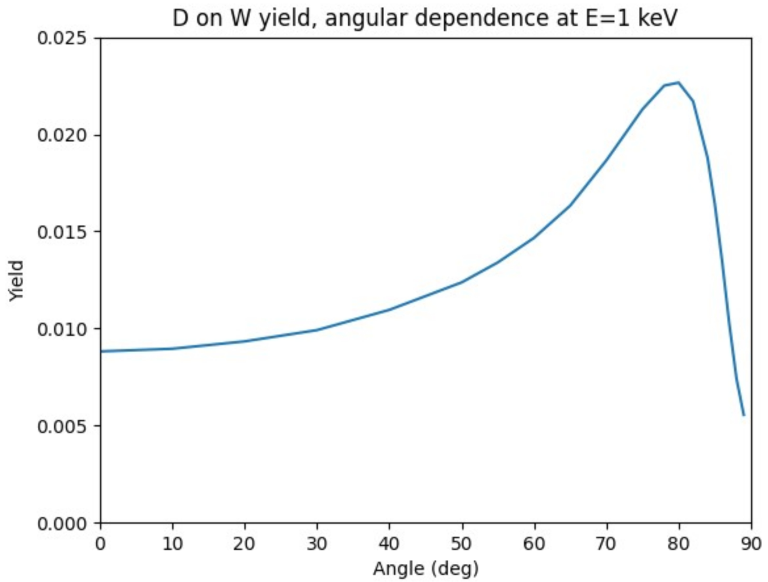
- Artificial W injection sources (no sputtering) placed in the JET divertor to assess W screening of different source locations
- Same W source in each location:
  10^{20} W atoms/second, initial energy 10 eV
- Only W sources near and above the outer divertor entrance have a non-negligible probability of reaching the core plasma

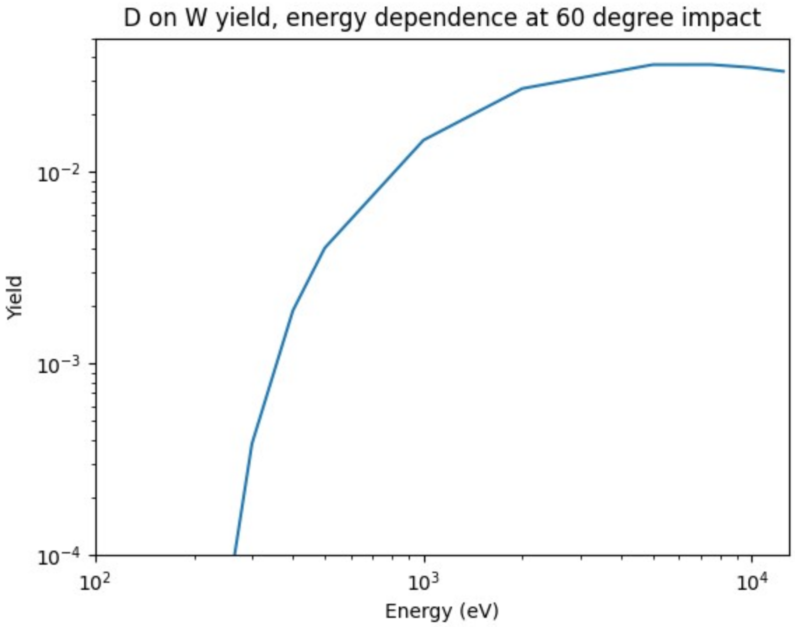
  → Erosion by CXN is the dominant cause of W radiation in JET



JPN 81472 at 49-50 s (L-mode)
H. Kumpulainen et al. PPCF 2024

D-on-W sputtering yields are sensitive to both impact angle and energy

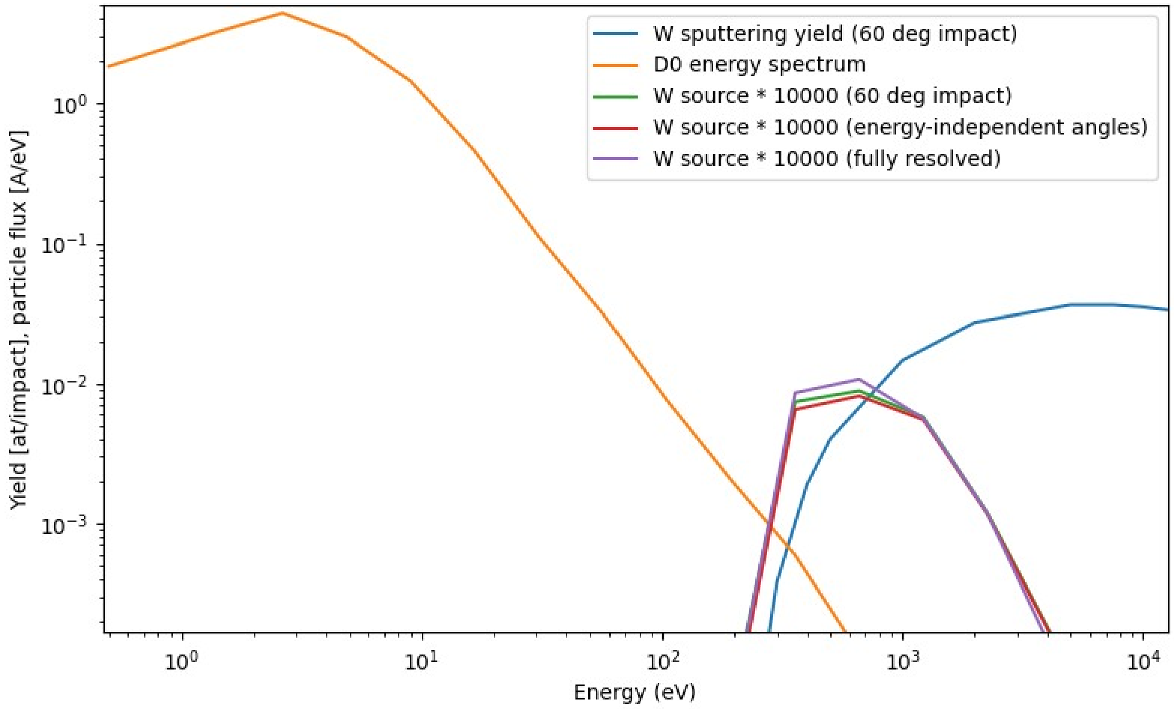




Yields calculated by SDTrimSP6

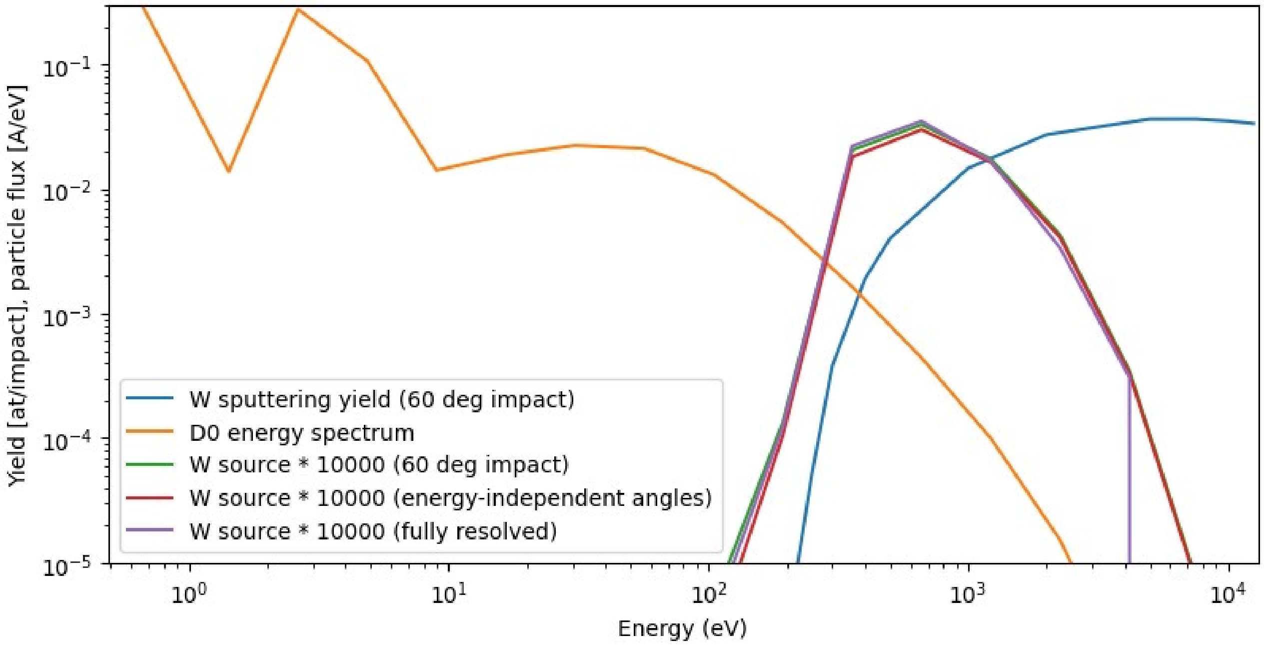
JET outer vertical divertor, H-mode: 22% higher W source with fully resolved angles

- W source due to CXN fluxes calculated with 3 different assumptions on the angular distribution



JPN 94606 at 50-51 s (H-mode), run588s3, outer vertical divertor

Hypothetical full-W JET main chamber, L-mode: 13% higher W source with resolved angles



JPN 81472 at 49-50 s (L-mode), run581o, main chamber
W source calculated assuming full-W wall

Conclusions

- New EIRENE option implemented for simultaneous co-dependent energy and angular spectra, tested and available in the ‘develop’ branch

- Using functional expansion tallies with a Legendre polynomial basis, the obtained spectra have arbitrarily high angular resolution and reduced Monte Carlo noise compared to histogram binning

- The most common predicted CXN impact angles in the JET outer vertical divertor range from 70°-85° ($E \approx 100$ eV) to 20°-50° ($E > 1000$ eV)

- L-mode and H-mode test cases indicate a moderate increase (22%, 13%) in W erosion by CXN (and W core radiation) due to the co-dependence of energy and angular CXN spectra