INTERFACING EIRENE NEUTRAL ENERGY AND ANGULAR DISTRIBUTIONS INTO ERO2.0

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Outline

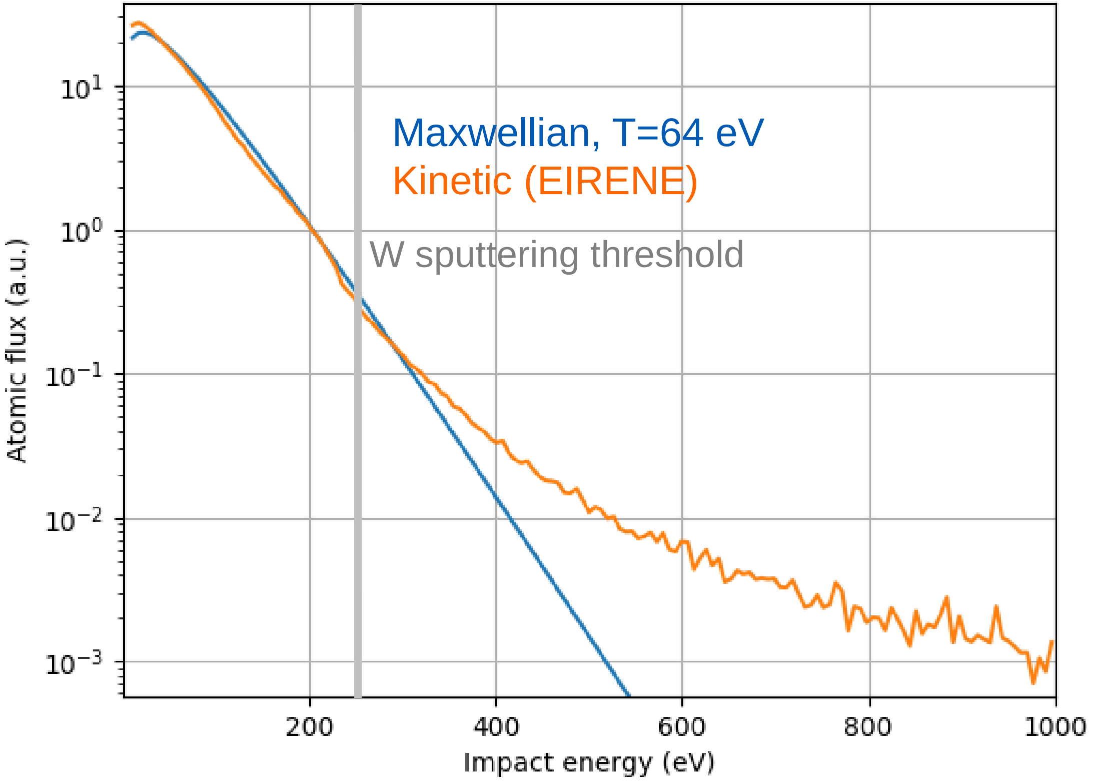
- EIRENE implementation of bivariate energy-angular distributions and functional expansion tallies
- Post-processing and converting EIRENE output to ERO2.0 input data
- Example use case: W erosion by incident D and T atoms in JET ELMy H-mode
- Conclusions

Kinetic treatment of CXN is needed for predicting the erosion of W

- The CXN impact energy distribution is highly non-Maxwellian above 300 eV
- The Maxwellian low-energy range is irrelevant for W sputtering due to the energy threshold

  → Using a fluid CXN description or assuming a “mean impact energy” may under- or overestimate the W erosion rate by orders of magnitude
- The impact angle is correlated with the impact energy → bivariate distribution

Energy spectrum of D^0, JET outer target [1]
L-mode #81472, 9 seconds



[1] H.A. Kumpulainen et al., PPCF 2024

Bivariate energy-angular spectra recorded in EIRENE as functional expansion tallies [1]

- Approach:

  1) Define 15 energy bins with logarithmic binning intervals

  2) Compute the Legendre polynomial expansion of the impact angle cosines for each energy bin
     - 10^{th} degree polynomials used here

  3) Store the Legendre expansion coefficients in the EIRENE output file

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

Degree of expansion

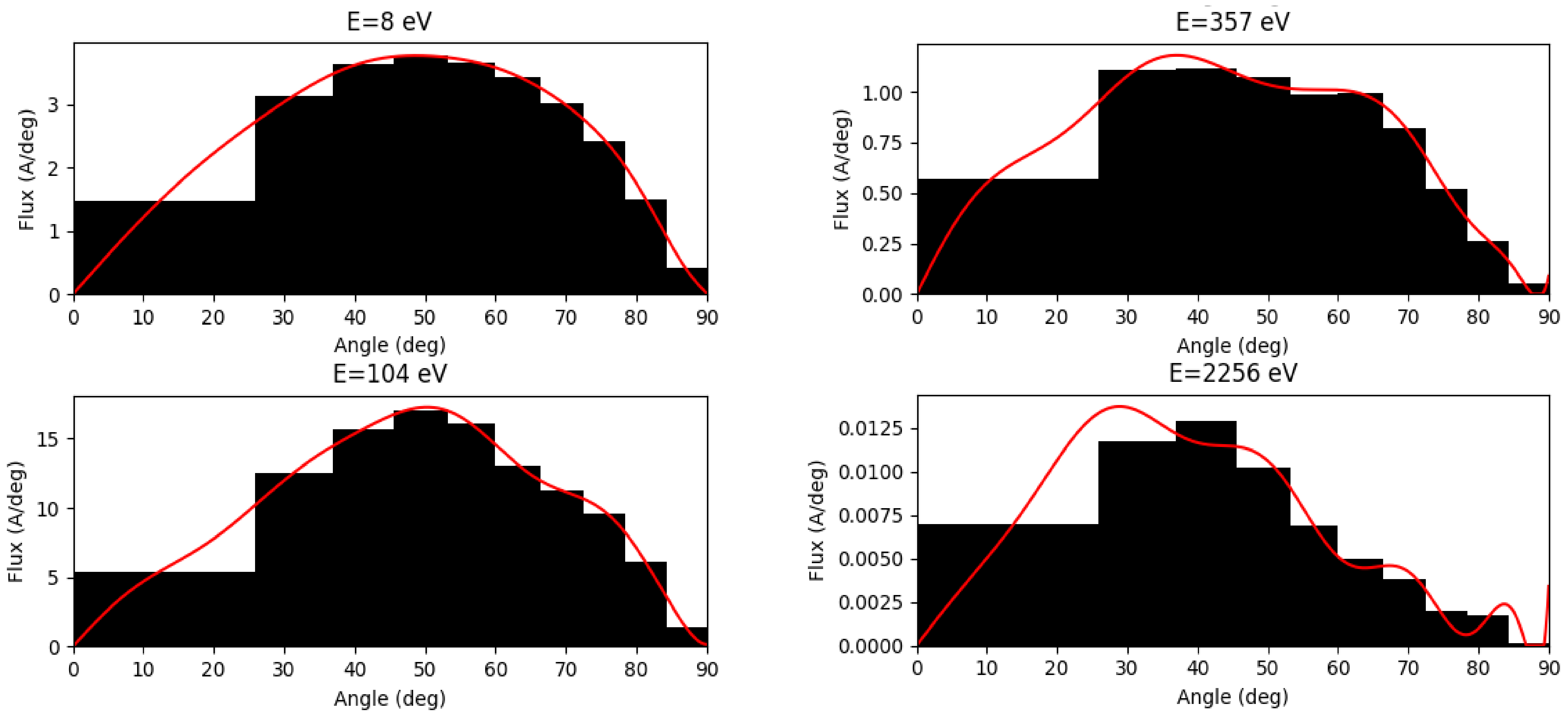
$$f(\theta) = \sum_{n=0}^{\mathrm{ISPLDEG}} a_n \cdot \pi sin(\theta) \cdot L_n(2cos(\theta) - 1)$$

Legendre expansion coefficient — Legendre polynomial of degree n

- No angular binning: less trajectories needed for accurate results
- The distribution function is smooth and can be evaluated at arbitrarily high angular resolution

[1] H.A. Kumpulainen et al., 21st ICPP conference (2024)

JET outer vertical divertor: shallower angles at lower energies, 30°-40° peak at E > 1 keV



JPN 81472 at 9-10 s (L-mode)

Workflow for importing atomic energy and angular spectra from EIRENE to ERO2.0

- Obtain a background plasma solution (eg. SOLPS-ITER, EDGE2D-EIRENE, …)
- Run EIRENE standalone with the desired surface tallies added into the input file (details on the next slide)
- Extract the atomic impact spectra from eirene.output into fluxes.h5 (addEnergyAngleSpectra.py)
- Run ERO2.0 with psi.neutrals.incidenceEnergyModel=3 and psi.neutrals.incidenceAngleModel=1

How to set up functional expansion tallies in EIRENE

- 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 $a_1 \dots a_{10}$

- 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, then ask h.kumpulainen@fz-juelich.de

Description of the ERO2.0 input file format for neutral distributions

- HDF5 file “fluxes.h5” with datasets for the wall contour and the atomic impact spectra for each plasma facing component

```
HDF5 "fluxes.h5" {
FILE_CONTENTS {
 group      /
 group      /2D_contour
 group      /2D_contour/contour
 dataset    /2D_contour/contour/R
 dataset    /2D_contour/contour/Z
```

```
 dataset    /div_360deg_tile0/spectra/D/0
 dataset    /div_360deg_tile1/spectra/D/0
```

- Each “spectra” dataset contains attributes for
  - “counts”: total flux in each energy bin
  - “energy_high”, “energy_low”: energy bin upper & lower bounds
  - “nBins”: number of energy bins
  - “nTerms”: number of Legendre expansion terms (= expansion degree + 1)

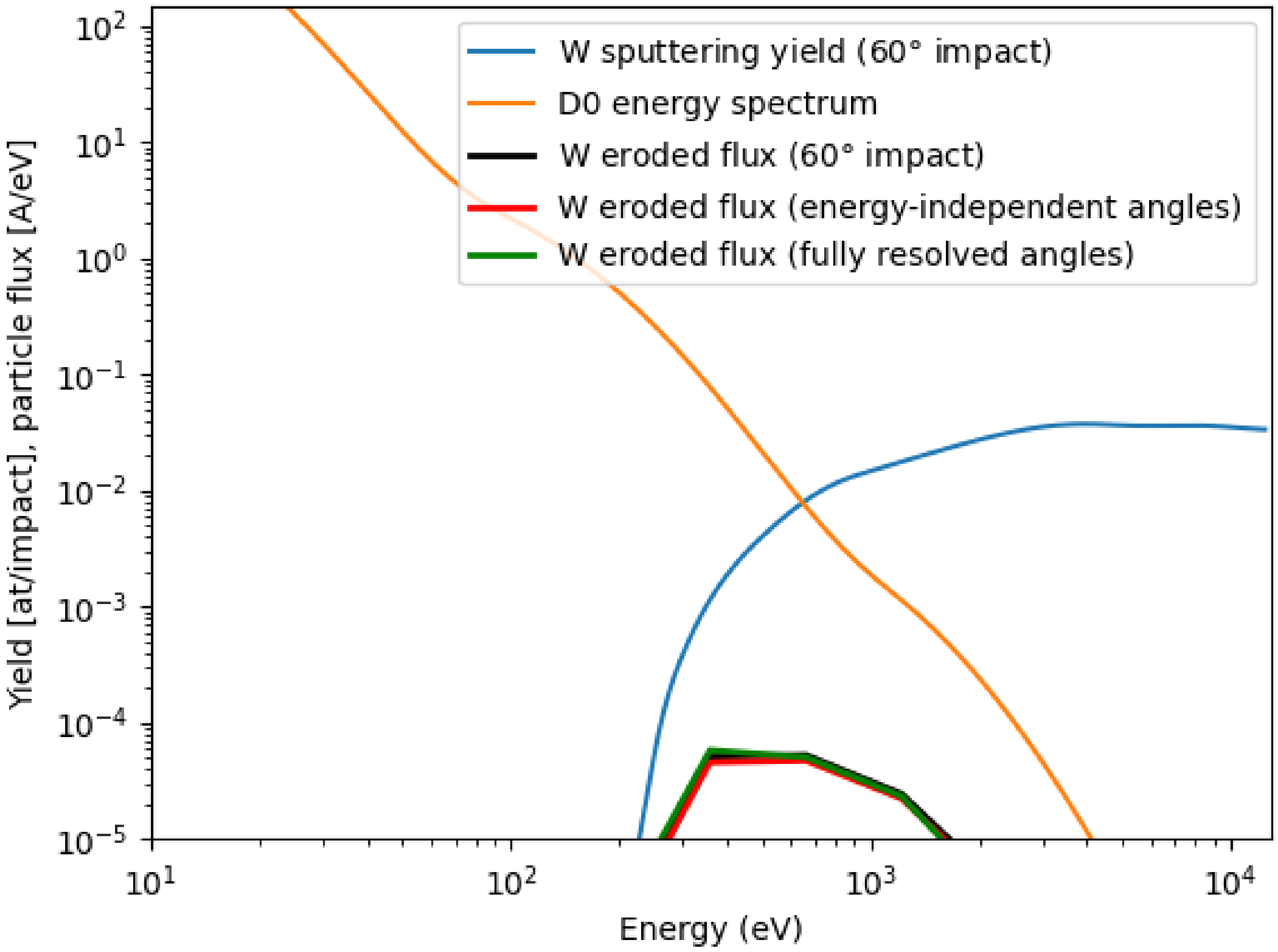
- The dimensions of the “spectra” dataset are (nBins, nTerms)

```
DATASET "/div_360deg_tile1/spectra/D/0" {
   DATATYPE  H5T_IEEE_F64LE
   DATASPACE  SIMPLE { ( 17, 11 ) / ( 17, 11 ) }
   DATA {
   (0,0): 1.1293, 0.47558, -0.079194, -0.12621, -0.11943, 0.064209, 0.009761,
   (0,7): -0.018972, 0.071732, 0.028789, -0.11995,
   (1,0): 2.4078, 1.0812, -0.26844, -0.18291, -0.11012, 0.00052389, 0.18377,
   (1,7): 0.11429, -0.071717, -0.12318, 0.022814,
```

```
ATTRIBUTE "counts" {
   DATATYPE  H5T_IEEE_F64LE
   DATASPACE  SIMPLE { ( 17 ) / ( 17 ) }
   DATA {
   (0): 1.1293, 3.5371, 11.706, 3.338, 0.62696, 0.58718, 0.47279, 0.28429,
   (8): 0.11354, 0.026697, 0.0029323, 0.00015673, 8.8795e-06, 5.1991e-07,
   (14): 5.9973e-08, 9.6969e-09, 0
   }
}
ATTRIBUTE "energy_high" {
   DATATYPE  H5T_IEEE_F64LE
   DATASPACE  SIMPLE { ( 17 ) / ( 17 ) }
   DATA {
   (0): 1, 1.8478, 3.4145, 6.3096, 11.659, 21.544, 39.811, 73.564, 135.94,
   (9): 251.19, 464.16, 857.7, 1584.9, 2928.6, 5411.7, 10000, inf
   }
}
ATTRIBUTE "energy_low" {
   DATATYPE  H5T_IEEE_F64LE
   DATASPACE  SIMPLE { ( 17 ) / ( 17 ) }
   DATA {
   (0): 0, 1, 1.8478, 3.4145, 6.3096, 11.659, 21.544, 39.811, 73.564,
   (9): 135.94, 251.19, 464.16, 857.7, 1584.9, 2928.6, 5411.7, 10000
   }
}
ATTRIBUTE "nBins" {
   DATATYPE  H5T_STD_I32LE
   DATASPACE  SCALAR
   DATA {
   (0): 17
   }
}
ATTRIBUTE "nTerms" {
   DATATYPE  H5T_STD_I32LE
   DATASPACE  SCALAR
   DATA {
   (0): 11
   }
}
```

W erosion rate calculated from the atomic impact distributions and the sputtering yield

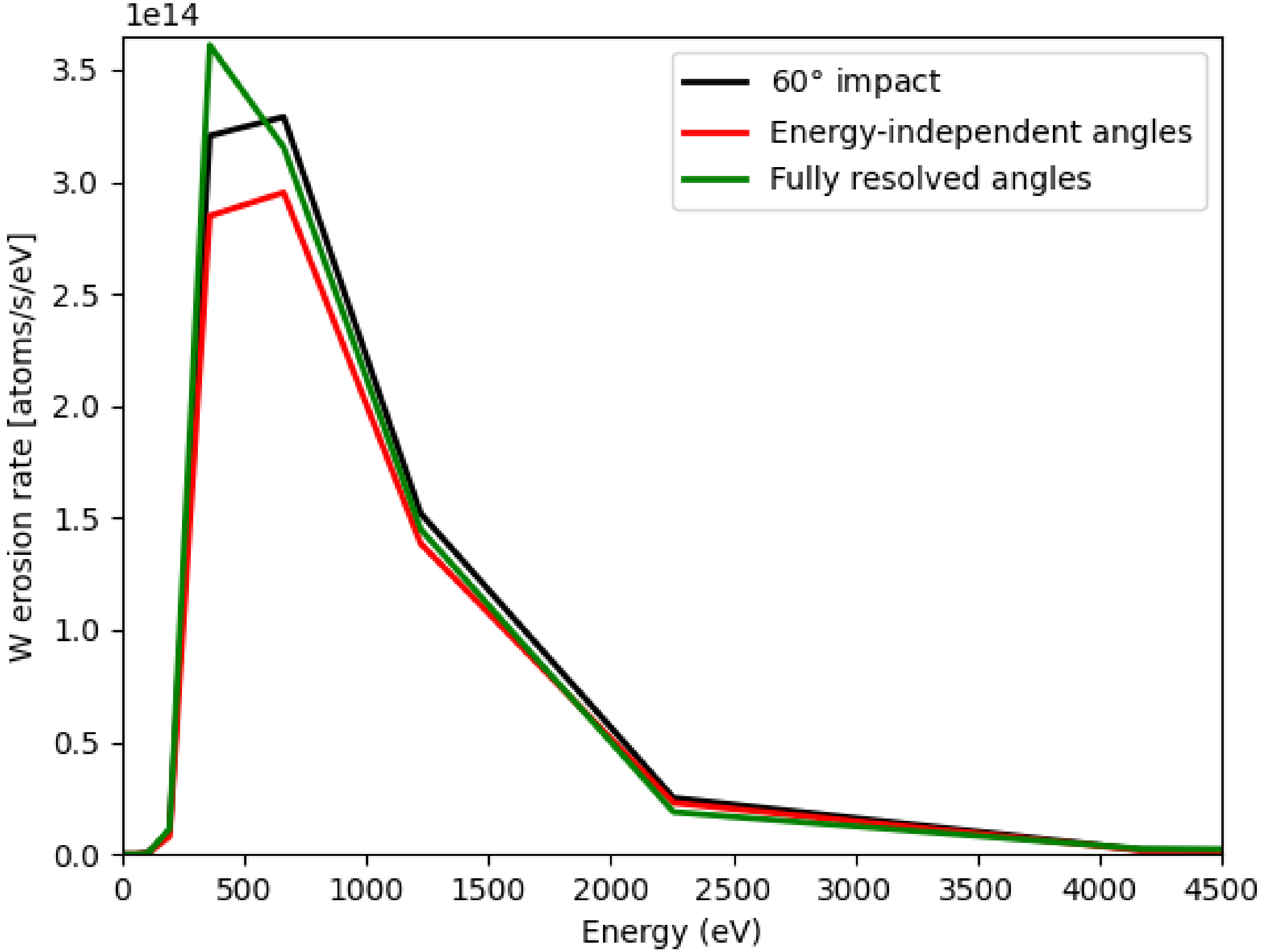
- D^0 impact energies 300 to 2000 eV contribute the most to W sputtering
- W source due to CXN fluxes calculated with 3 different assumptions on the angular distribution



JPN 94606 at 10-11 s (inter-ELM H-mode), outer vertical divertor

W erosion rate calculated from the atomic impact distributions and the sputtering yield

- D^0 impact energies 300 to 2000 eV contribute the most to W sputtering
- W source due to CXN fluxes calculated with 3 different assumptions on the angular distribution
- Fully resolved energy-angular distributions result in 10-20% more W sputtering than assuming energies and angles independent

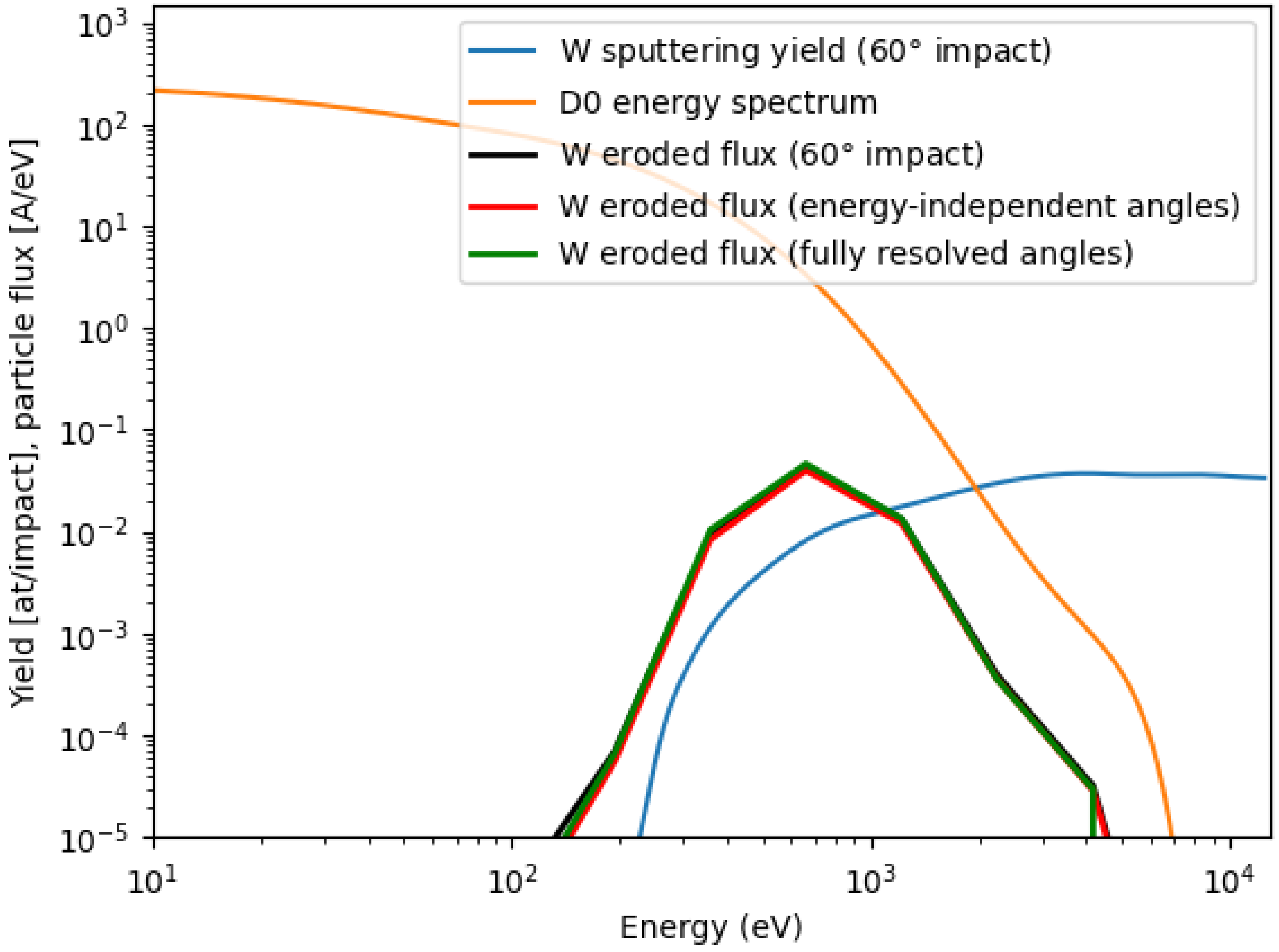


JPN 94606 at 10-11 s (inter-ELM H-mode), outer vertical divertor

W erosion rate calculated from the atomic impact distributions and the sputtering yield

- D^0 impact energies 300 to 2000 eV contribute the most to W sputtering
- W source due to CXN fluxes calculated with 3 different assumptions on the angular distribution
- Fully resolved energy-angular distributions result in 10-20% more W sputtering than assuming energies and angles independent
- During an ELM, W erosion by atoms is briefly increased by > factor of 100 (also fast reflections, not only CXN)

  → The sub-millisecond ELM is a larger W source than the 25 ms inter-ELM



JPN 94606 at 10-11 s (intra-ELM H-mode), outer vertical divertor

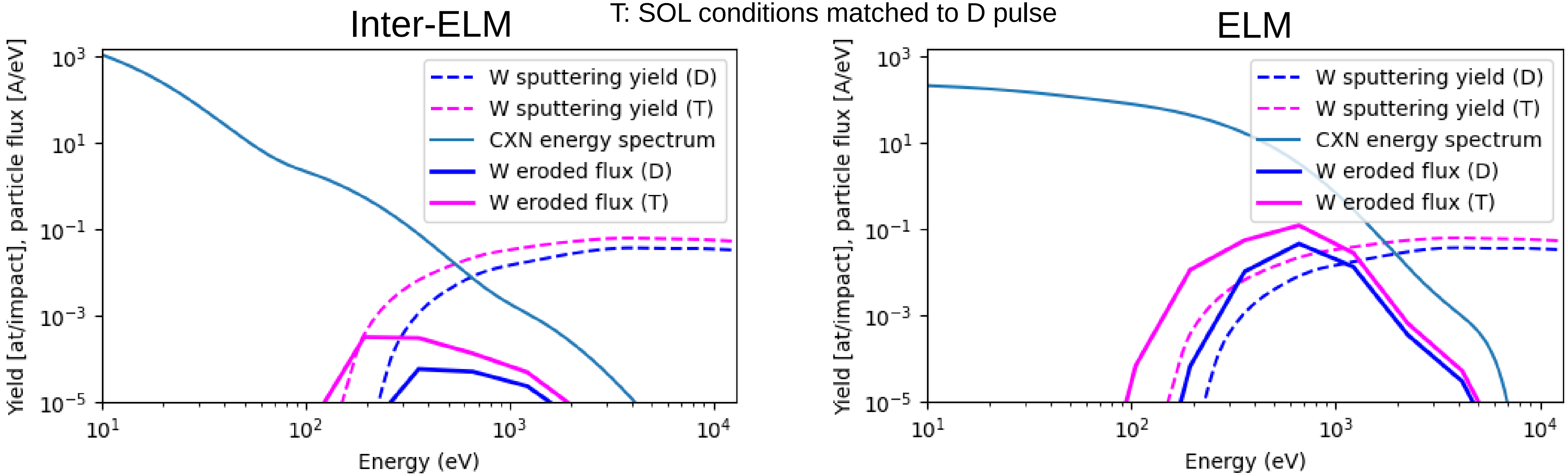
W erosion by CXN in T is higher than in D by a factor of 3 (ELM) to 6 (inter-ELM)

- The ELM-averaged W influx is dominated by the ELM-induced W source
- CXN which erode W are mostly created inside the separatrix in the inter-ELM phase, but in the SOL during ELMs

W erosion by CXN, JET LFS divertor entrance

D: #94606 (10 s), P_{aux}=18 MW

T: SOL conditions matched to D pulse



Conclusions

- Bivariate energy-angular atomic impact spectra simulated in EIRENE using functional expansion tallies and used in ERO2.0

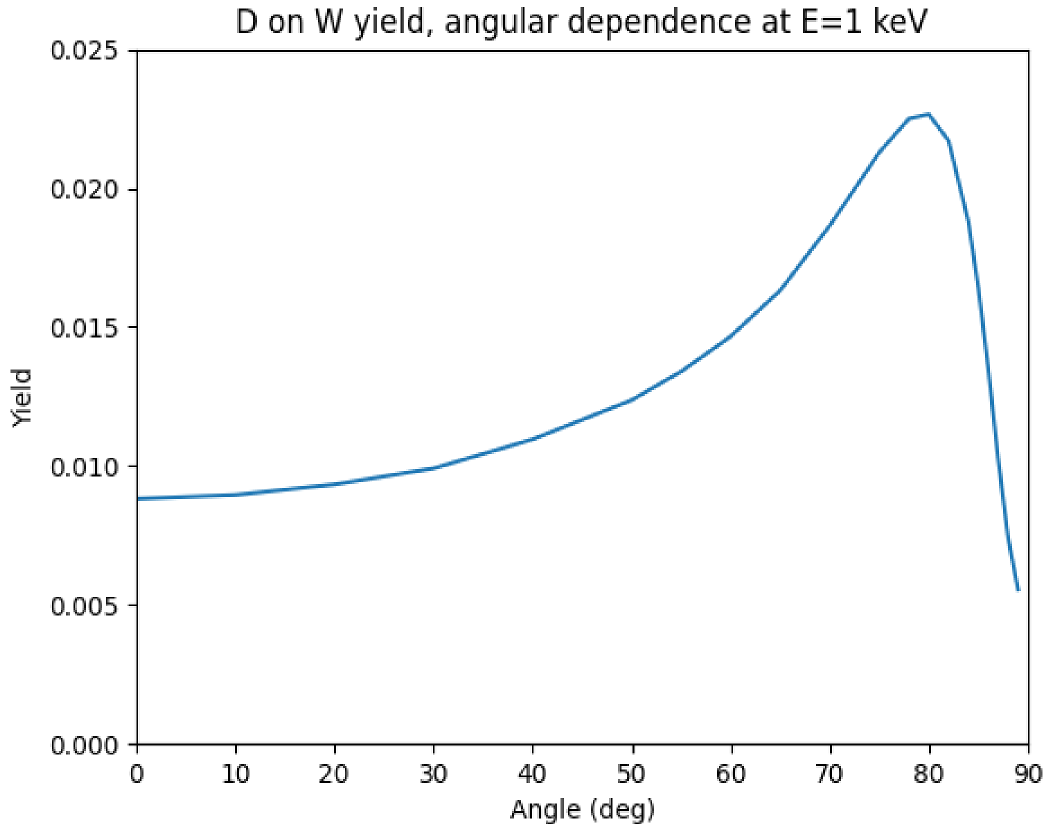
- JET L-mode and H-mode simulations indicate a 10% to 20% increase in W erosion by CXN and W core radiation due to the correlation between energy and angular CXN spectra

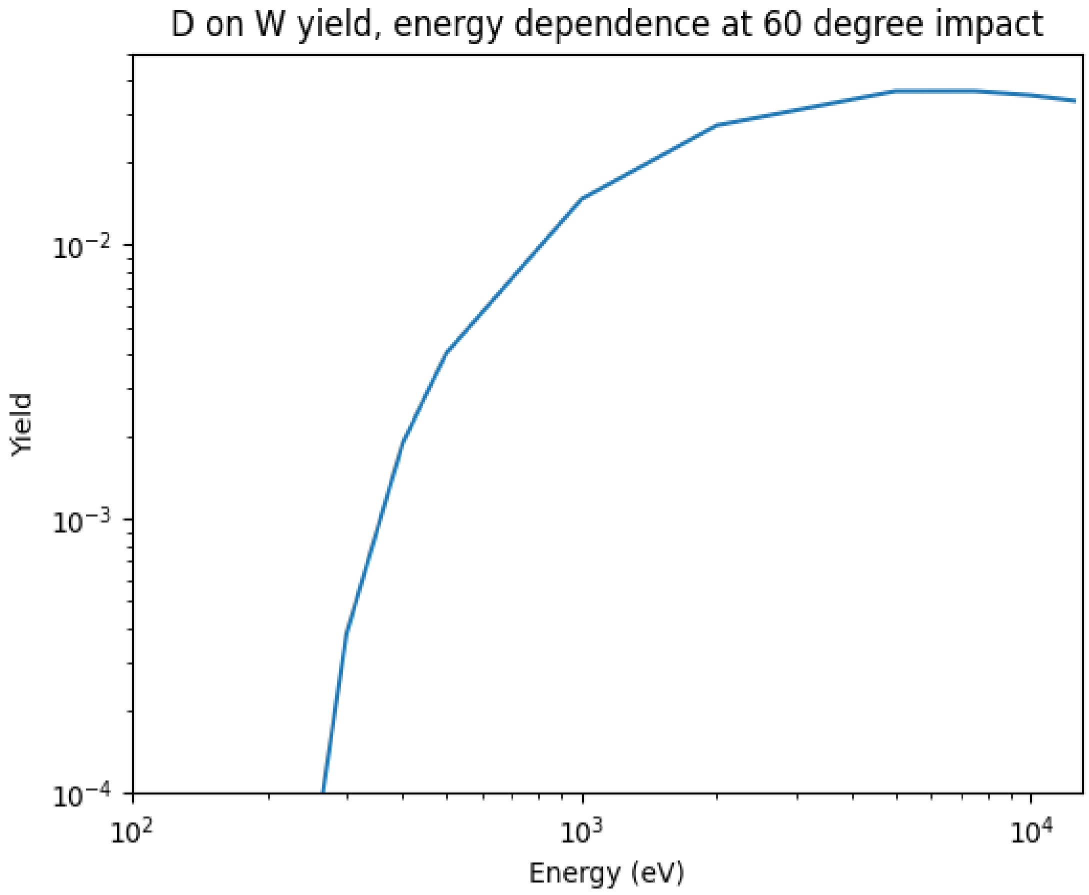
- A 60° effective impact angle is a fair approximation for W sputtering by CXN in JET if angular spectra are unavailable

- EIRENE and ERO2.0 simulations indicate that the erosion of unscreened W components at the LFS divertor entrance is higher in T than in D by a factor of 3 (intra-ELM H-mode) to 6 (inter-ELM), proportional to the W influx to the core

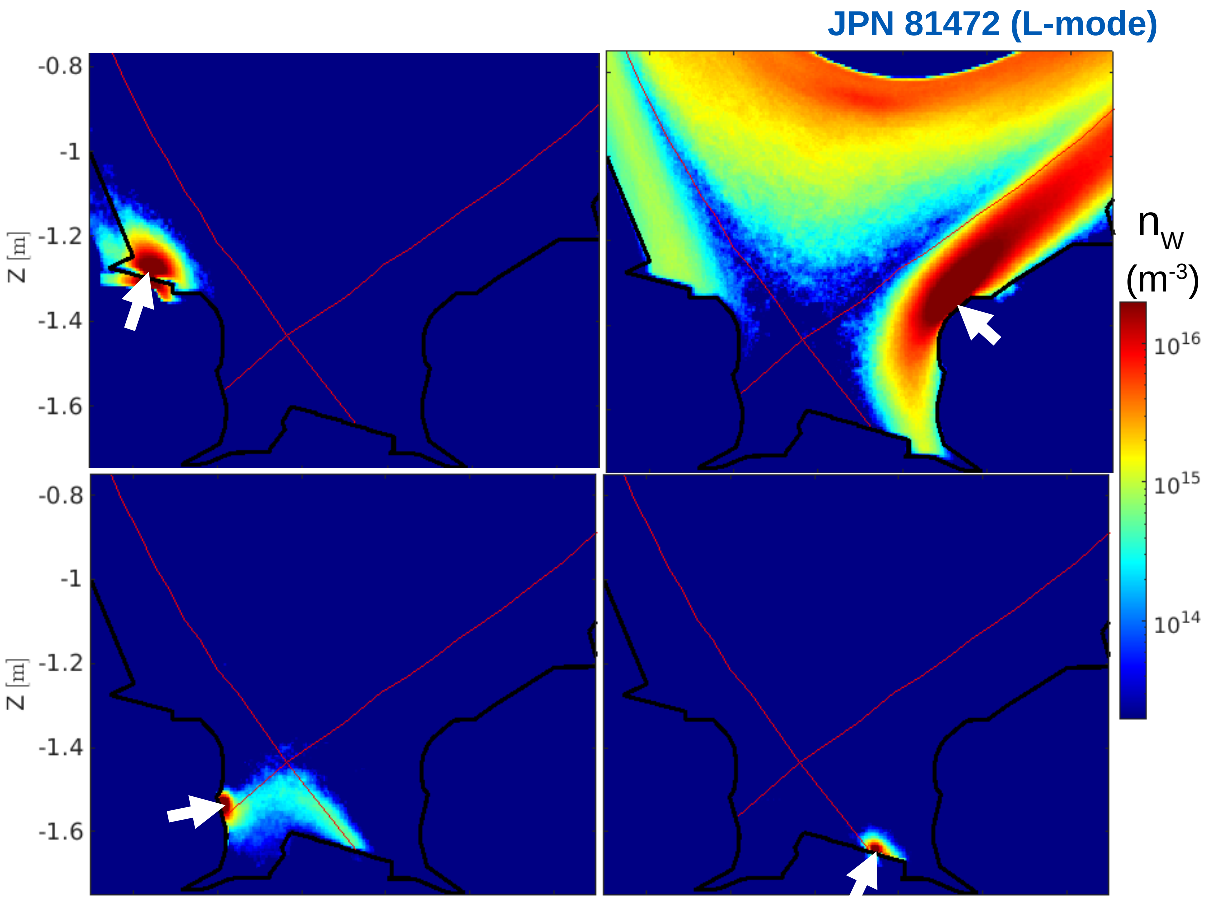
Additional slides for discussion

D on W sputtering yields



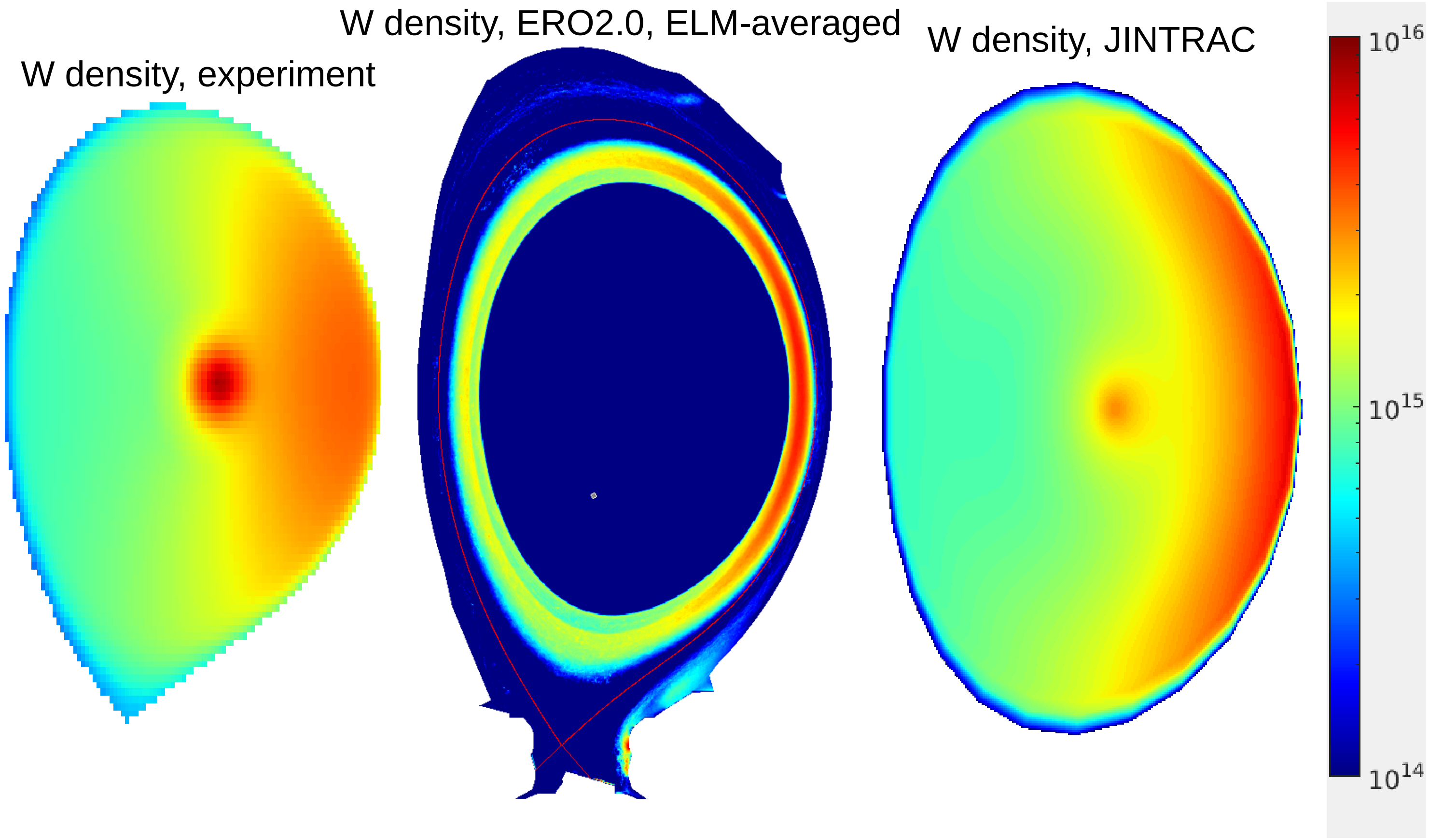


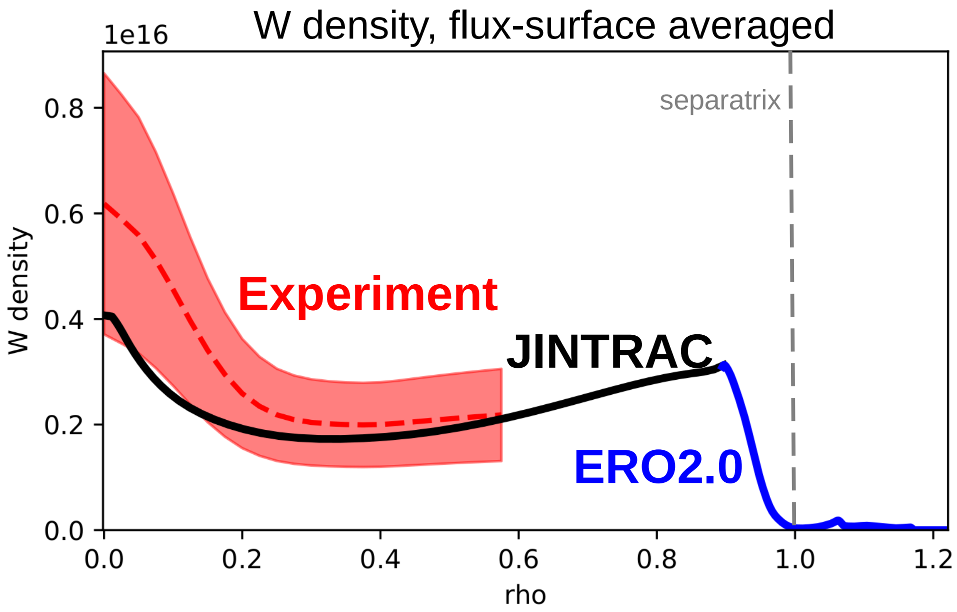
W sources at divertor targets and HFS shoulder are fully screened (ERO2.0)



ERO2.0 modelling in D reproduces the W density in the core plasma

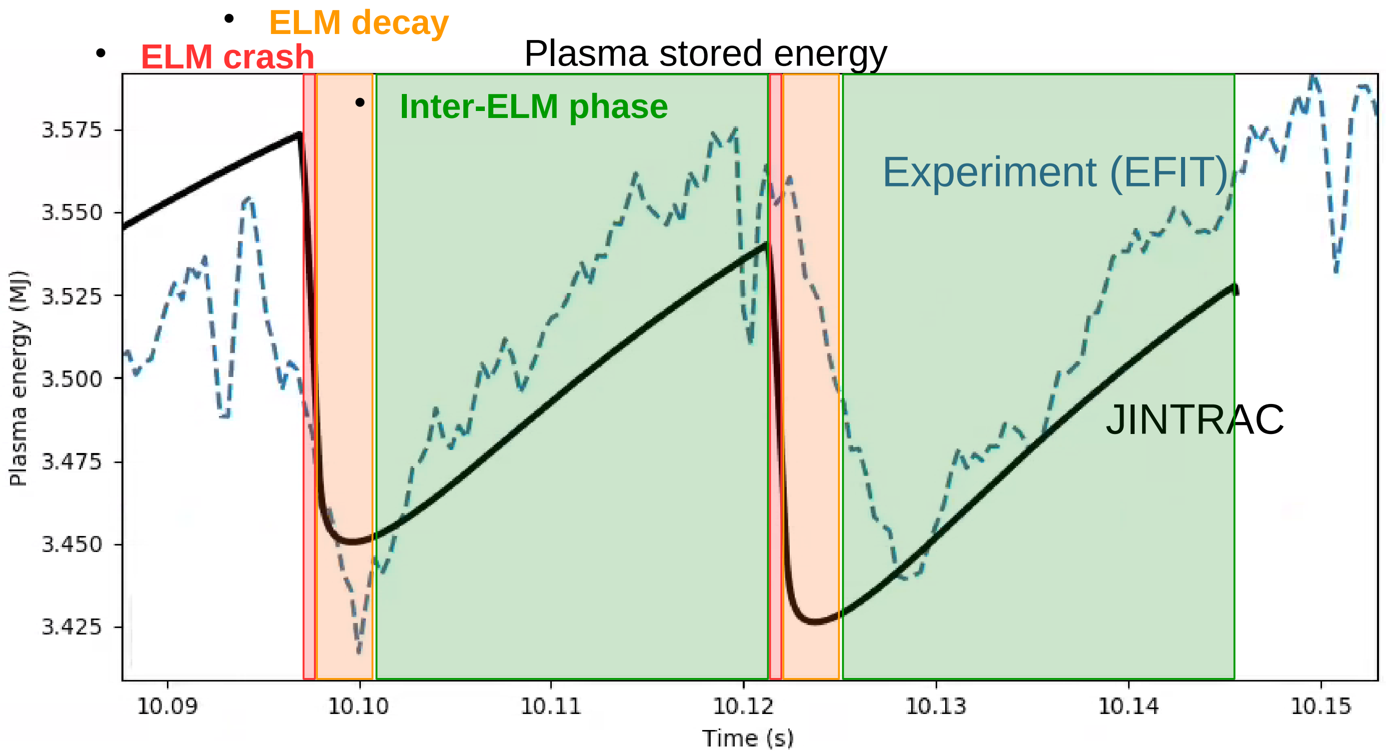
JPN 94606 at 10 s (P_{aux} = 18 MW)





H.A. Kumpulainen et al., PPCF 2024

JINTRAC time-dependent background plasma



Kinetic treatment of CXN is needed for predicting the erosion of W

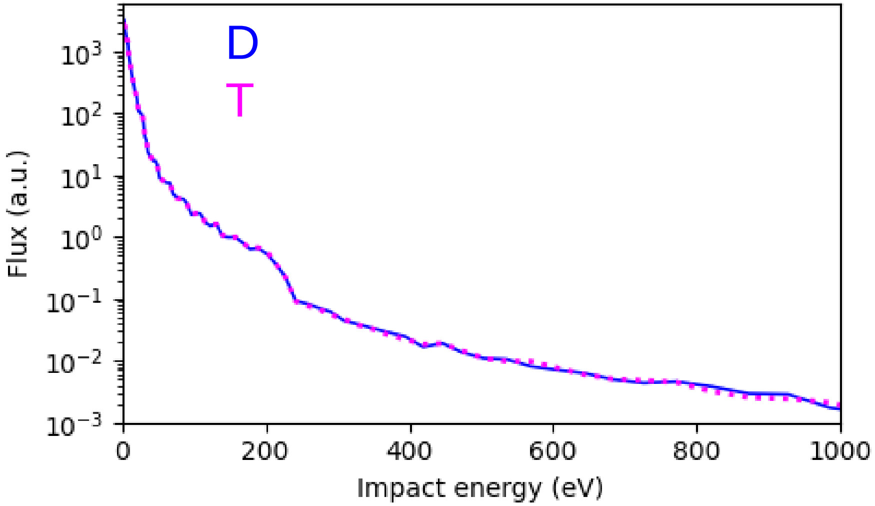
- The CXN impact energy distribution is highly non-Maxwellian above 300 eV
- The Maxwellian low-energy range is irrelevant for W sputtering due to the energy threshold

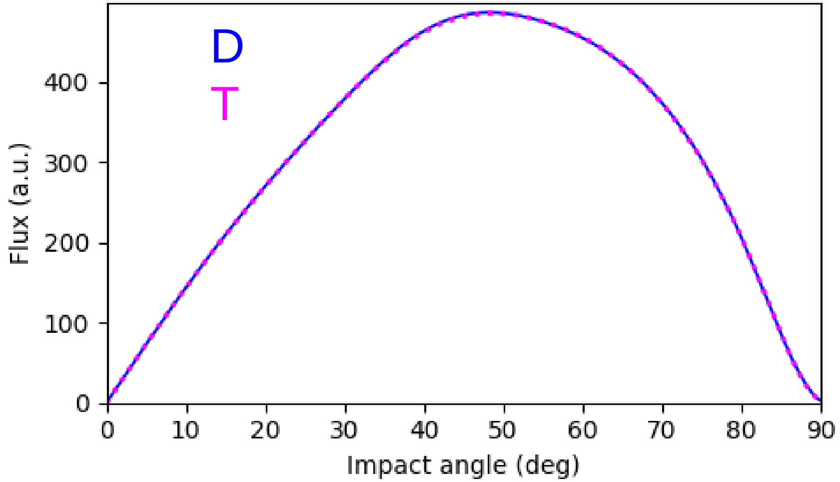
  → Fluid CXN descriptions may under- or overestimate the W erosion rate by orders of magnitude

- Bivariate energy-angular CXN distributions recently became available in EIRENE [1]
- Imposing the same plasma profiles for D and T in EIRENE, no isotope effect on the CXN impact energies and angles
  - Only the sputtering yield changes if SOL conditions are matched

CXN energy and angular distributions (EIRENE)

JET outer vertical divertor, D inter-ELM H-mode #94606 (11s)

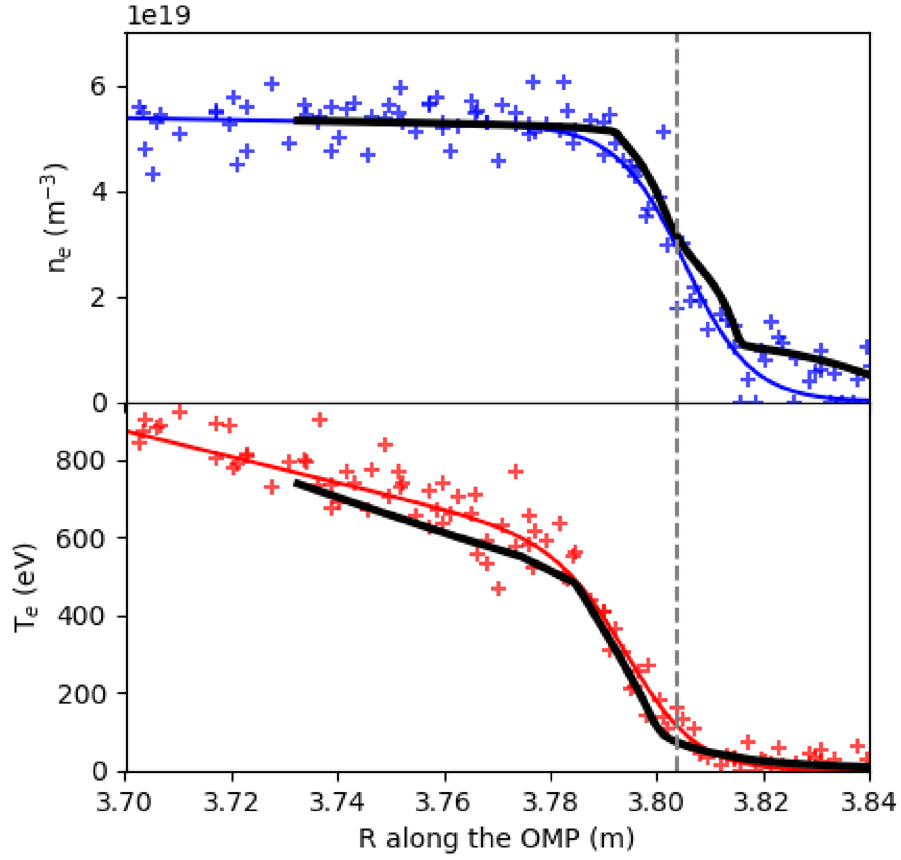


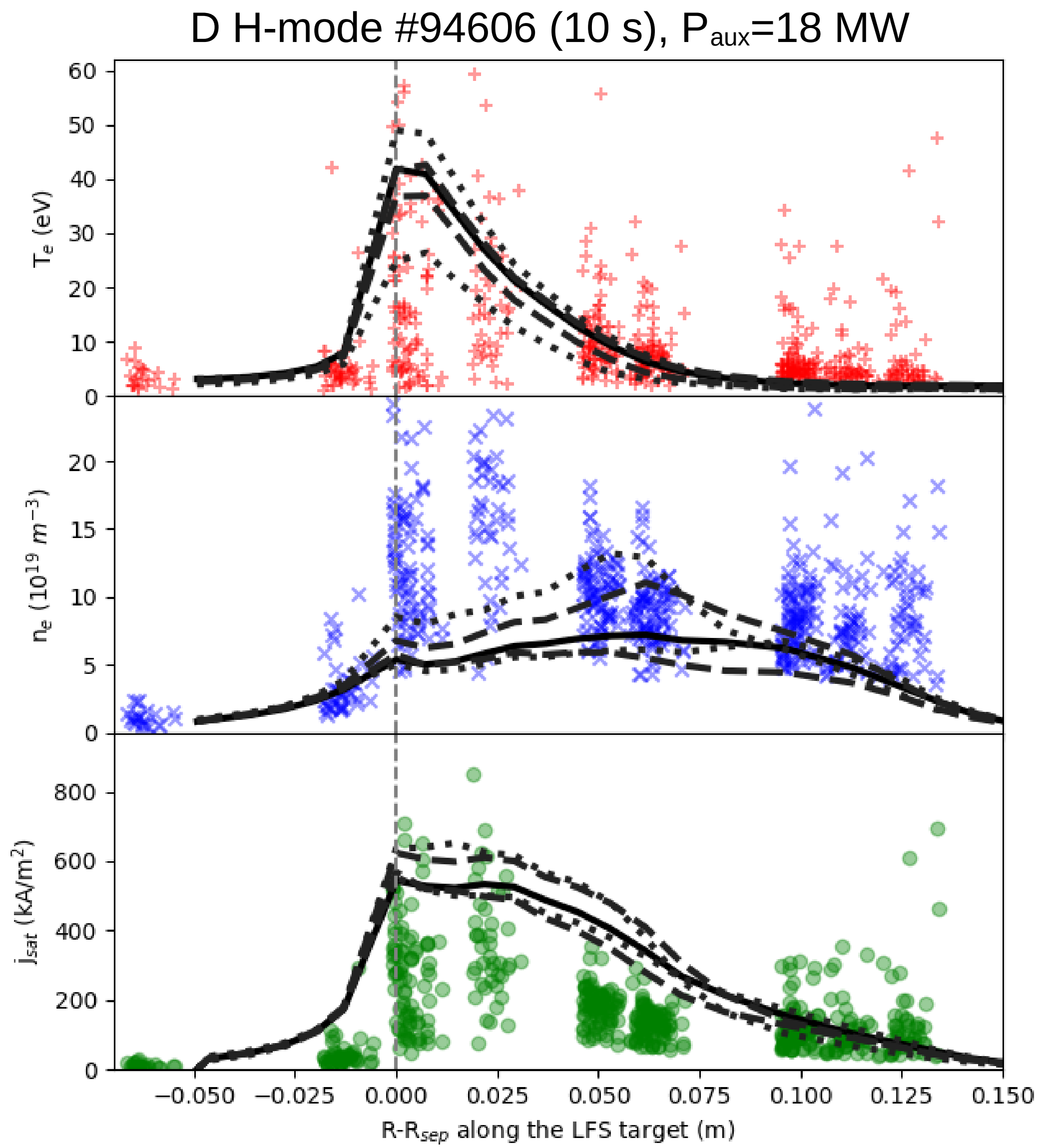


[1] H.A. Kumpulainen et al., 21st ICPP conference (2024)

JÜLICH Forschungszentrum

EDGE2D-EIRENE plasma solution validated against outer target and mid-plane measurements





H.A. Kumpulainen et al., NME (2022) 33 101264