Global tungsten erosion and impurity migration modeling for the DEMO with the ERO2.0 code

IAEA Technical Meeting on Tungsten and Hydrogen in Edge Plasmas

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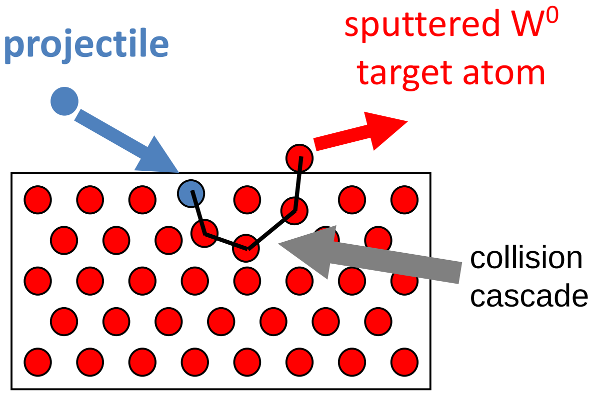
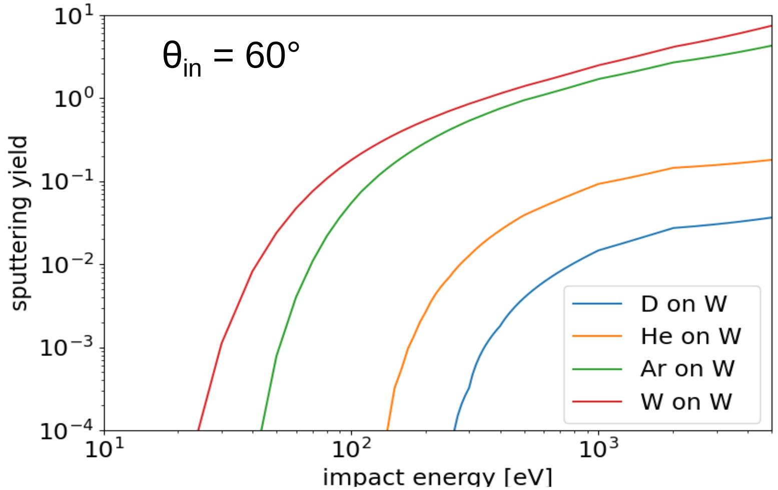
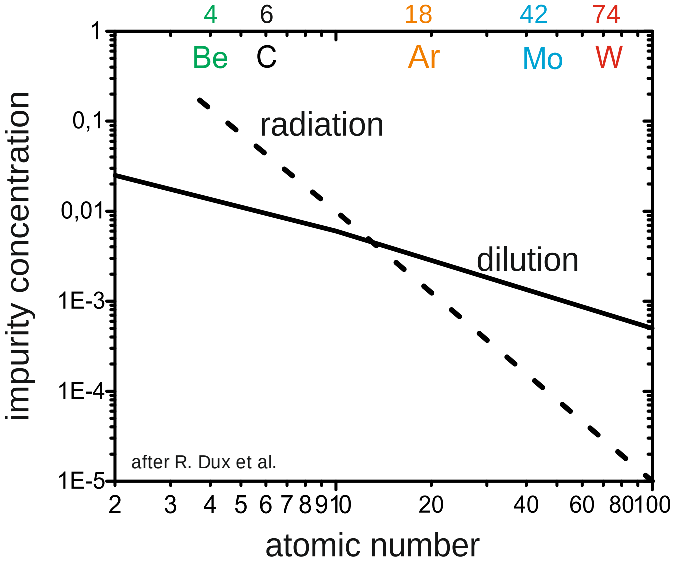
Plasma-facing materials in fusion devices

Tungsten as a prominent candidate

- high melting point
- low sputtering yield due to large mass
- large probability of prompt re-deposition due to generally short ionization mean free paths







after R. Dux et al.

- stability of core plasma requires low W concentration of < 10^{-5}
- dedicated modelling required in particular for future full-W devices such as ITER and DEMO

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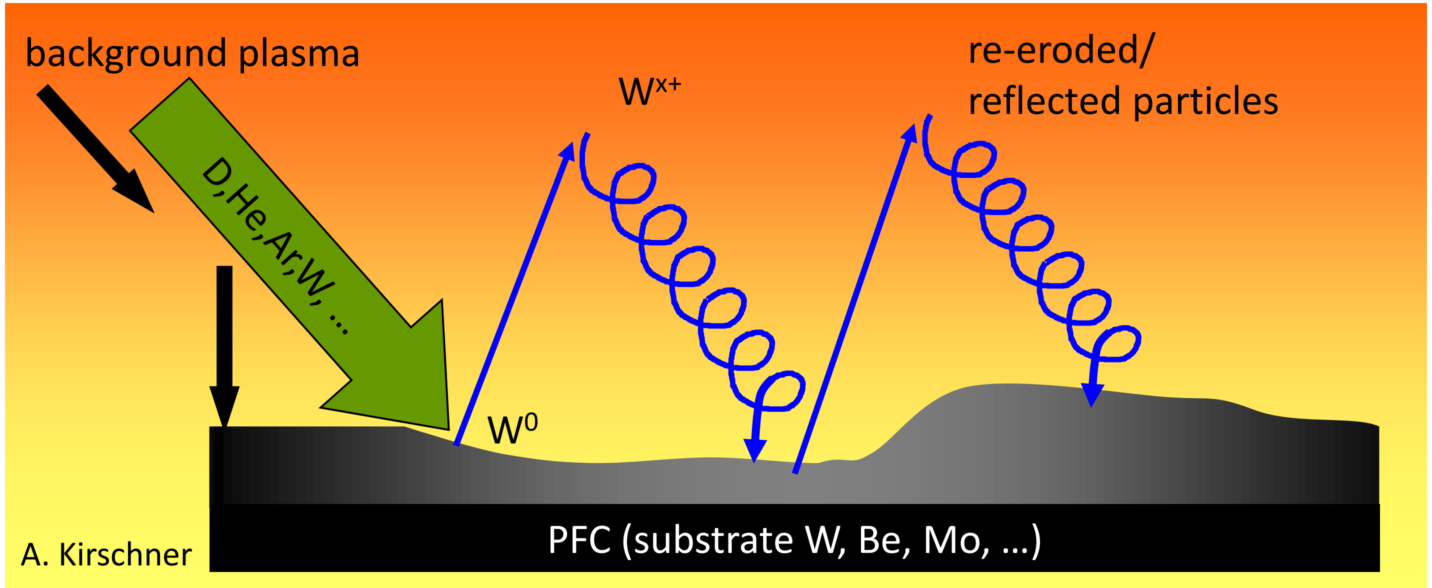
Simulation code ERO2.0

3D Monte-Carlo tool for PWI and global impurity migration studies



[1] A. Kirschner et al., Nuclear Fusion **40**, 989 (2000)
[2] J. Romazanov et al., Physica Scripta **T170**, 014018 (2017)

plasma-wall interaction (PWI):

- physical sputtering/reflection
- (re-)erosion and (re-)deposition
- material mixing

impurity transport:

- Lorentz force (including E x B)
- ionization, recombination
- friction (Fokker-Planck), thermal force
- cross-field diffusion

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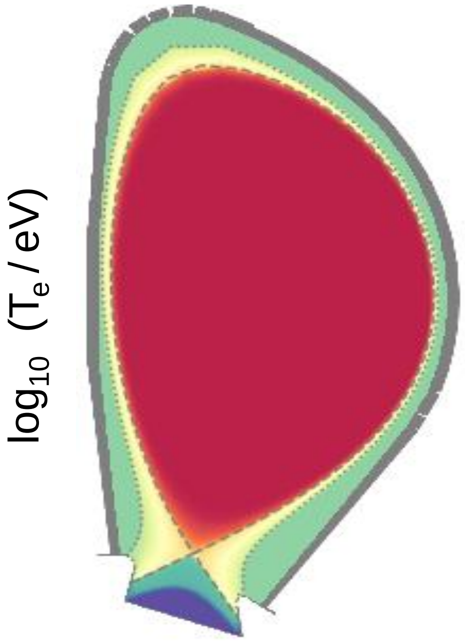
Tungsten data related to ERO2.0 modelling

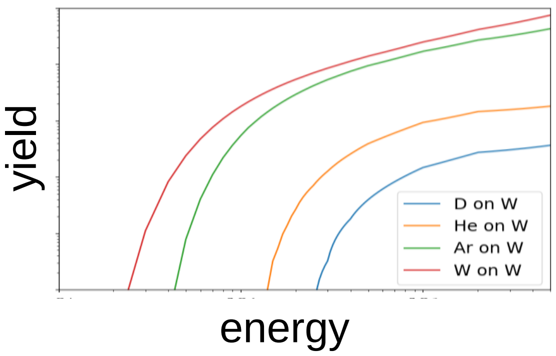
Schematic of ERO2.0 input

plasma + magnetic + neutral background



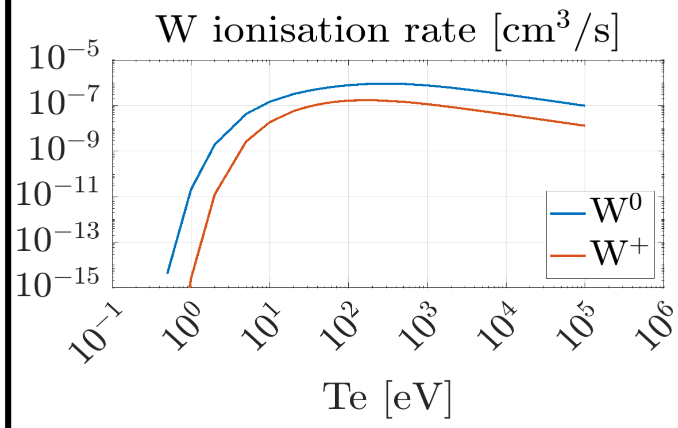
SOLPS-ITER, EMC3-EIRENE, ...

sputtering yields + reflection coefficients



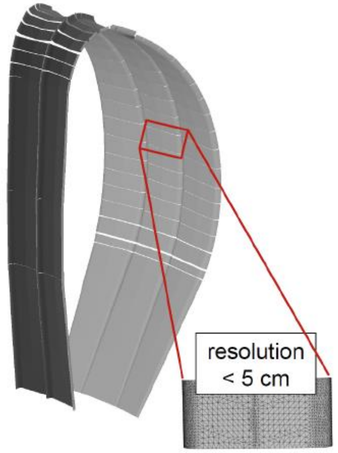
SDTrimSP, Molecular Dynamics, ...

atomic/molecular data



OPEN-ADAS, …

wall geometry



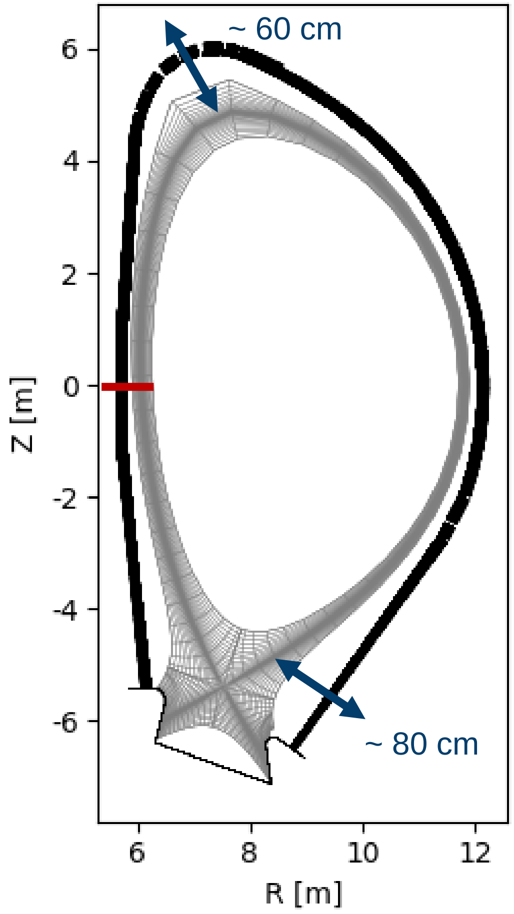
from technical drawings

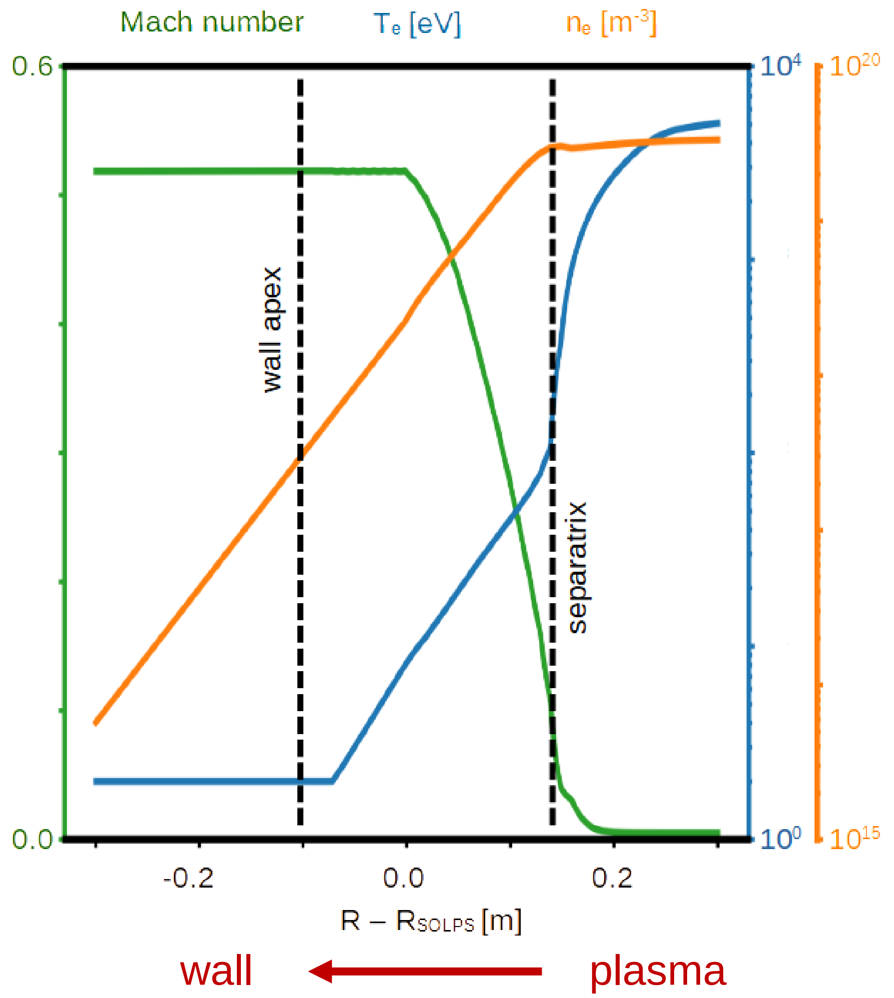
ERO2.0

SOLPS-ITER plasma background

DEMO case requires extrapolation

- background from SOLPS-ITER solution by F. Subba for DEMO [1]
- bridge void spaces up to about 80 cm
- current assumptions:
  - exponential decay for densities
  - exponential decay for temperatures, but restricted to $T_{min} = 2$ eV
  - uniform decay constant of 5 cm
  - ion parallel flow from local Mach number; Mach number constantly extrapolated





[1] F. Subba *et al.*, Nuclear Fusion **61**, 106013 (2021)

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SOLPS-ITER plasma background

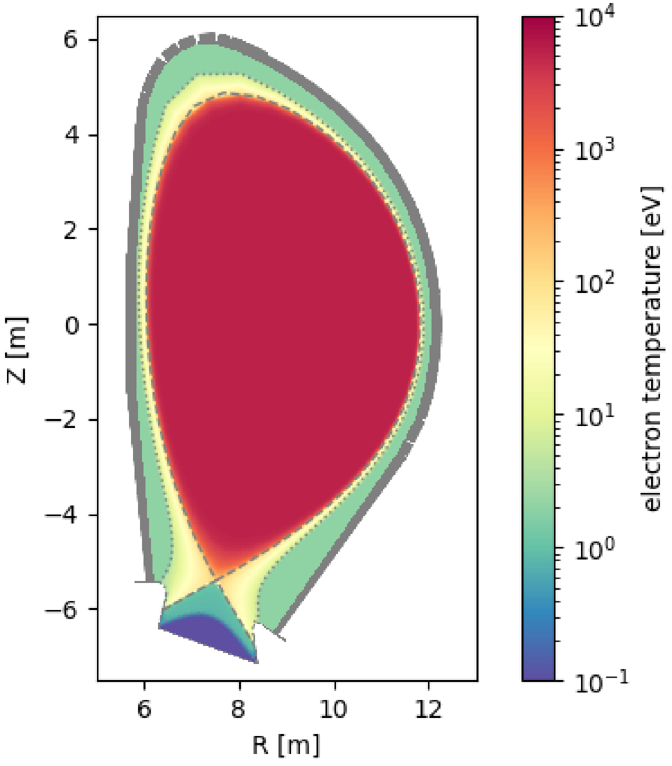
DEMO: Range of background plasma parameters

– – – – separatrix

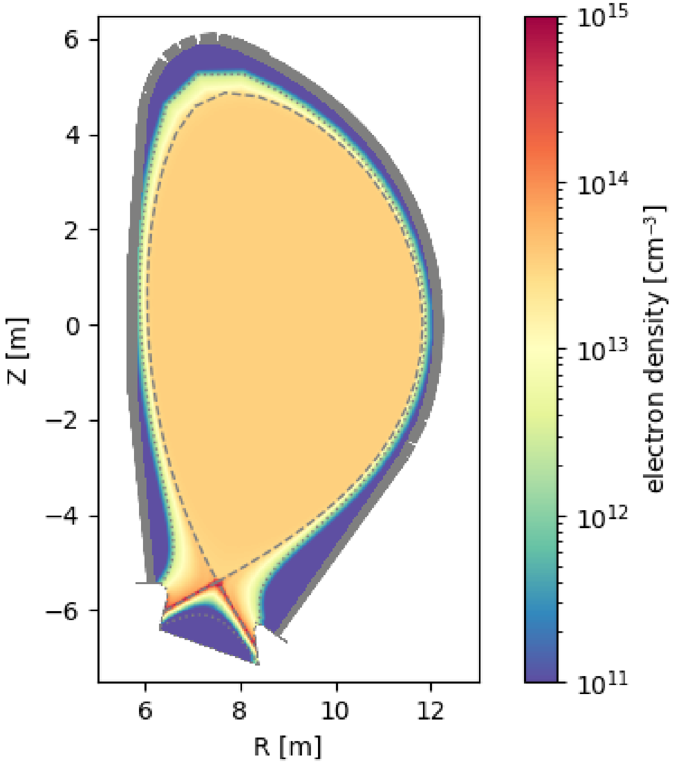
············ solps boundary

- DEMO covers wide range of electron temperatures and densities
- original SOLPS-ITER range:
  - T_e: ~ eV to 5 keV
  - n_e: ~ $4x10^9$ cm^{-3} to $3x10^{15}$ cm^{-3}
- lower parameter limits even smaller due to extrapolation
- parameter range should be covered by available tungsten data to model plasma-surface interaction and impurity transport accurately

electron temperature:



electron density:



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Plasma-surface interactions

Sputtering, reflection, and distribution of outgoing particles

- sputtering and reflection yields typically from in-house calculations using SDTrimSP

- MD simulations may be important to improve database at low impact energies
  - increasingly important for devices such as DEMO
  - TSVV-7 activities in that direction (see talk by Frederic Granberg)

- ERO2.0 typically uses simplified models for angular/energy distributions of sputtered/reflected particles:
  - polar angle: cosine-like
  - azimuth angle: uniform
  - energy: Thompson-like (sputtering), fixed value based on energy reflection coefficient (reflection)

experimental/modelling input data always appreciated
to study impact on global-scale simulations

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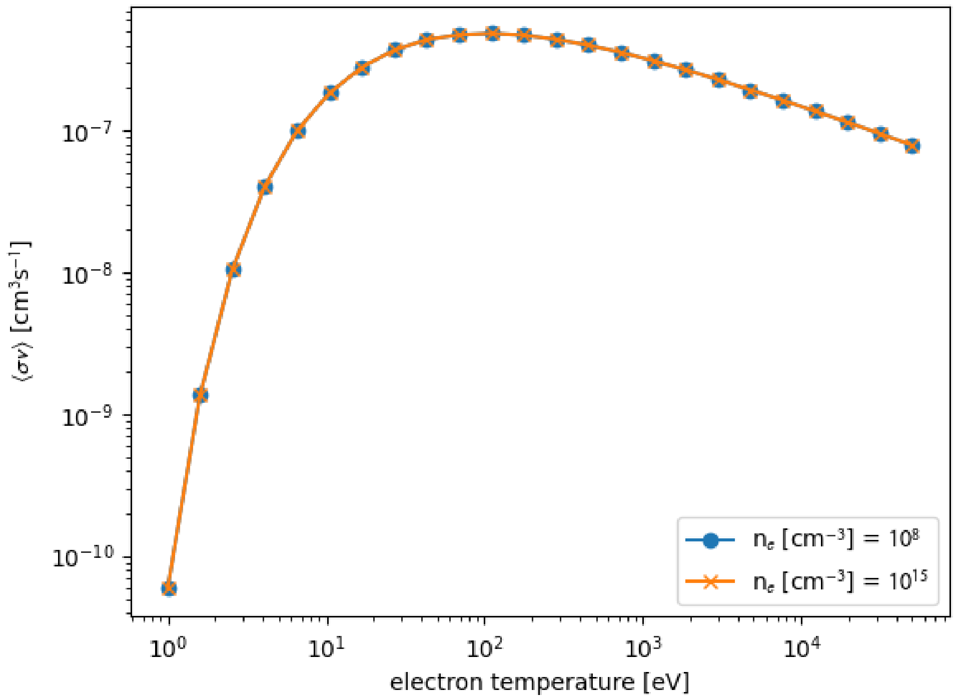
OPEN-ADAS data in ERO2.0

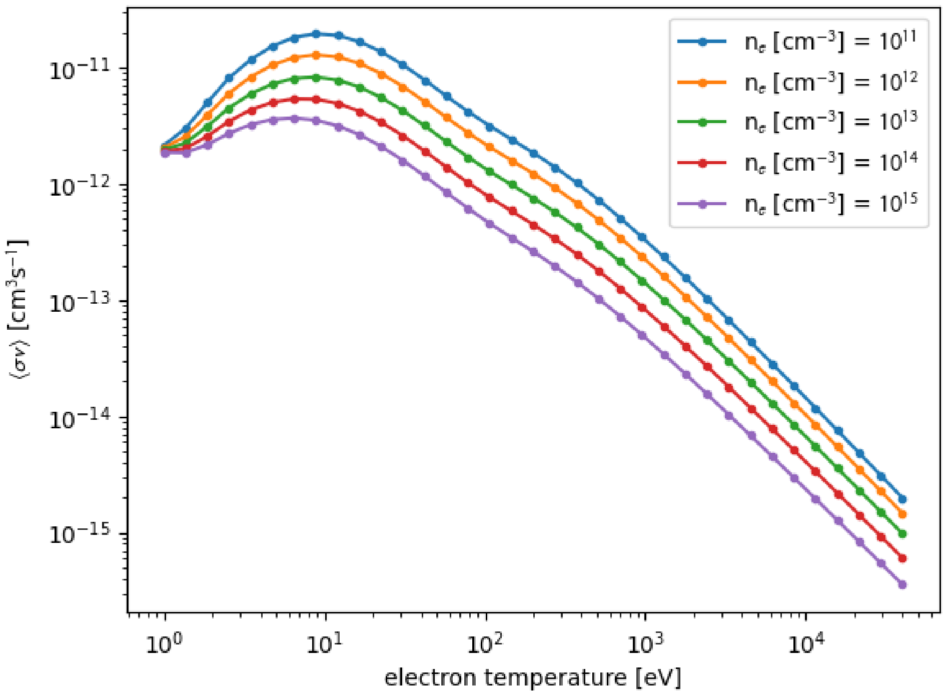
Tungsten ionization and recombination rate coefficients

$W^0 + e \rightarrow W^+ + 2e$



ionization rate coefficients do not show dependence on background electron density

$W^+ + e \rightarrow W^0$

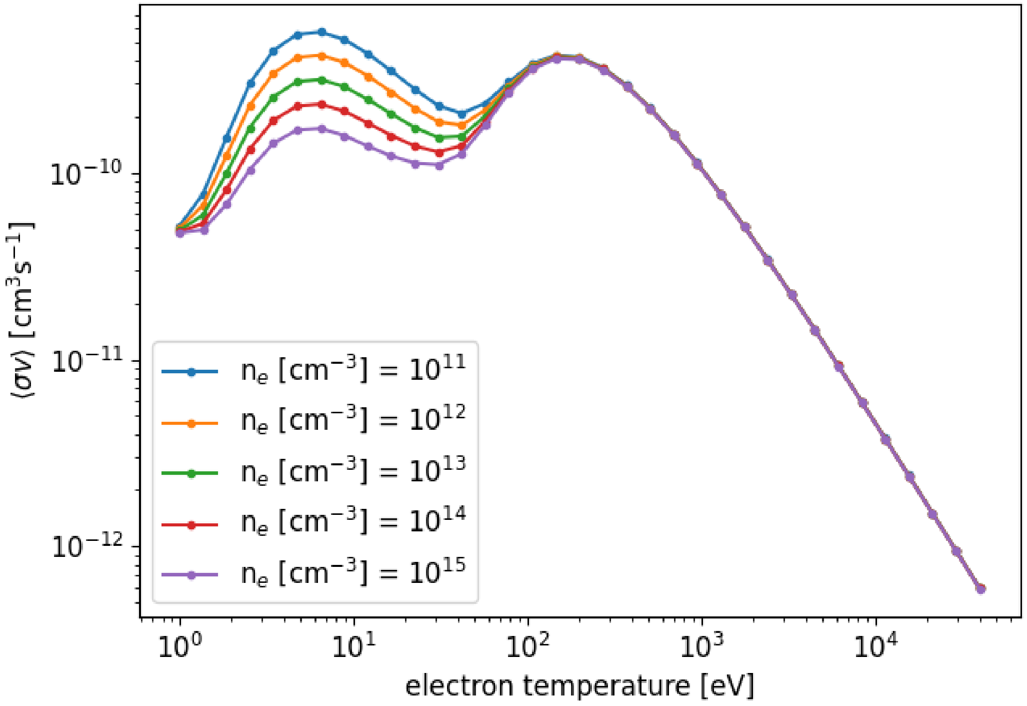


available recombination data do not cover entire range of background electron densities

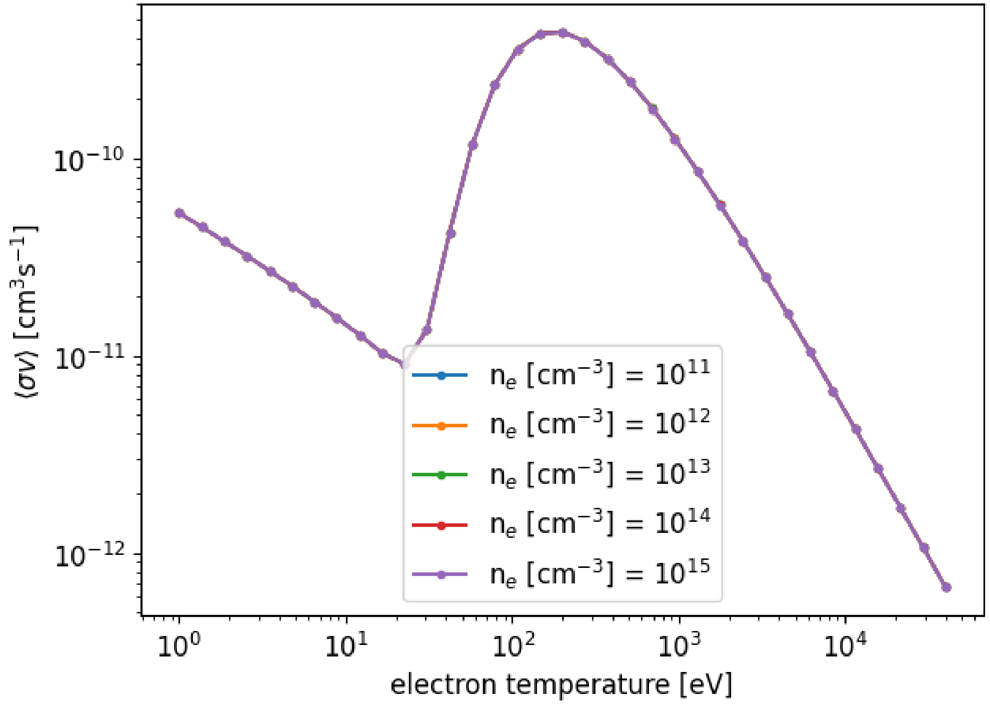
OPEN-ADAS data in ERO2.0

Tungsten recombination rate coeffiecients

$W^{13+} + e \rightarrow W^{12+}$



$W^{14+} + e \rightarrow W^{13+}$



large qualitative difference between recombination of W^{13+} and W^{14+} → why?

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What about …?

Processes not handled within ERO2.0

- W collisions with neutral background

  - can it become important?

  - example: hard-sphere approximation using van-der-Waals radii + 2 eV background temperature

$$\langle \sigma v \rangle = \sigma_{\text{hard sphere}}\, v_{\text{th}} \sim 10^{-8}\ \text{cm}^3\,\text{s}^{-1} > \langle \sigma v \rangle_{\text{ion}} \sim 10^{-9}\ \text{cm}^3\,\text{s}^{-1}$$

  - for collisions between hydrogen isotopes more sophisticated models exist
  → see Krstic and Schultz, *Atomic and Plasma-Material Interaction Data for Fusion*, Volume **8** (1998)

  - is there something similar for tungsten?

- is non-resonant W charge-exchange $W^0 + D^+ \rightarrow W^+ + D^0$ relevant in detached high-density divertors?
  → see also talk by David Tskhakaya

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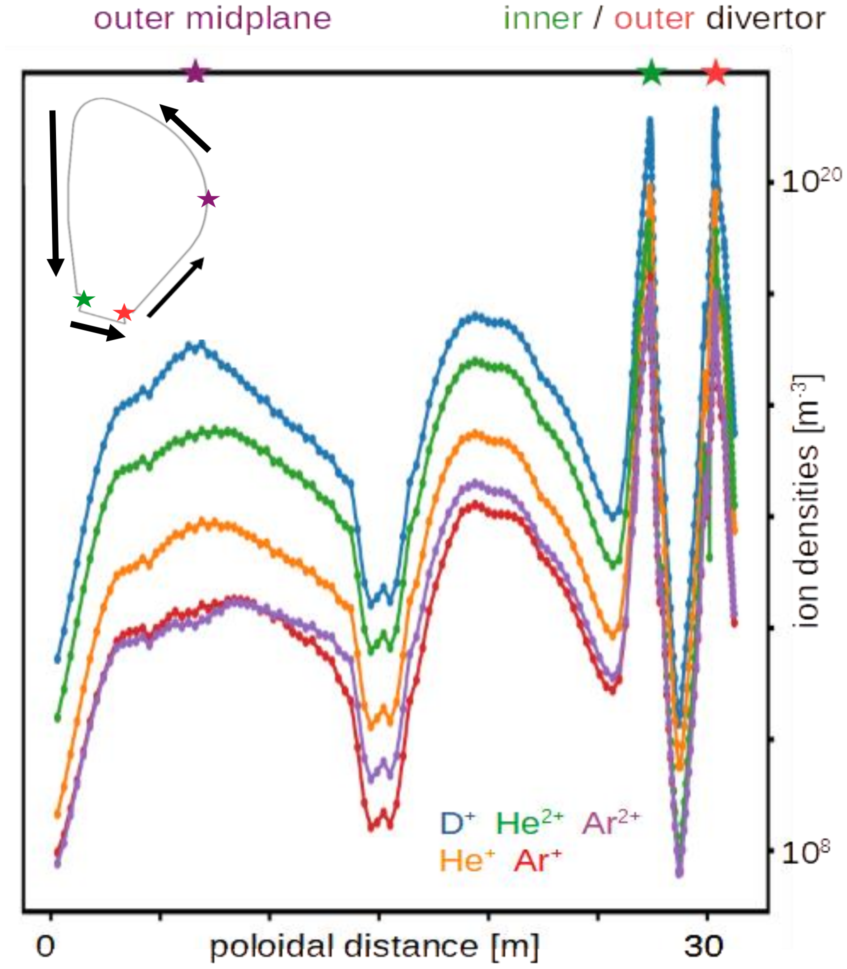
(Preliminary) ERO2.0 simulations for DEMO

Seeding impurities

Spatial distribution from SOLPS-ITER

- for the first time, ERO2.0 uses distributions for seeding impurities from a plasma edge simulation code
- large restructuring of code was needed
- main advantage:
  - more accurate estimates for background sputtering
  - spatially non-uniform charge state distributions possible



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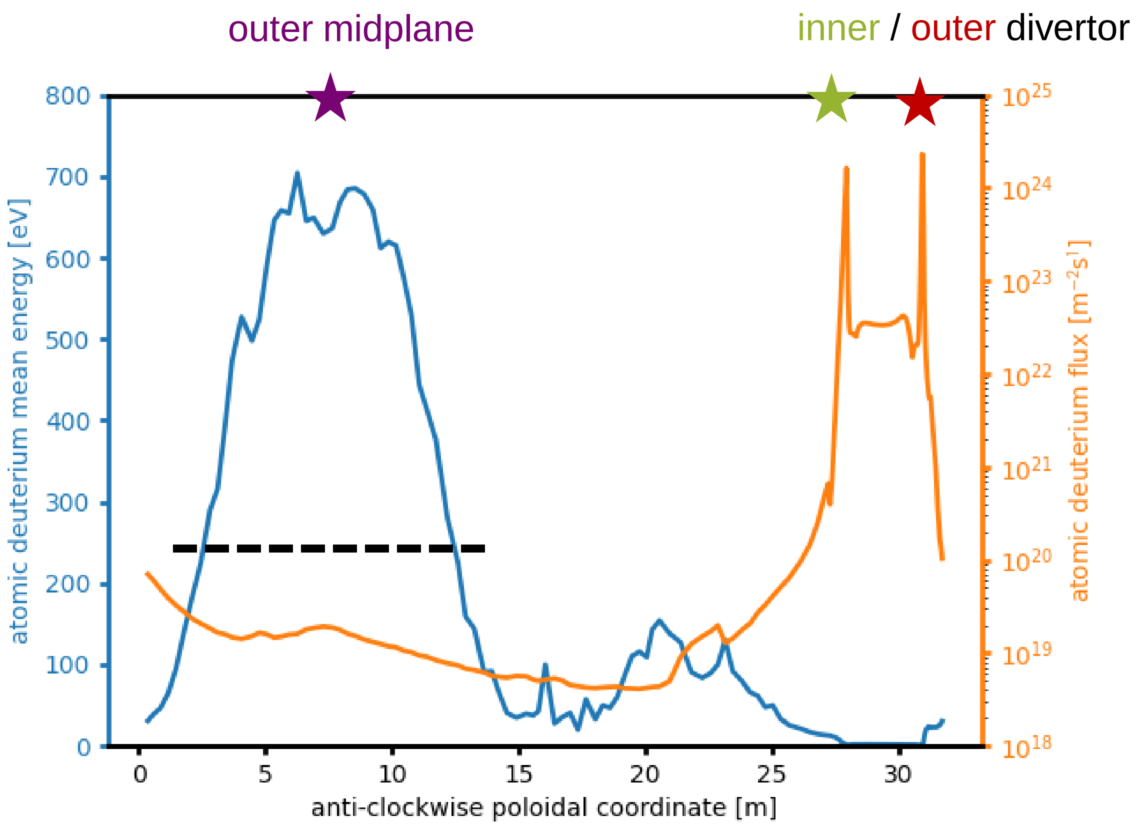
Charge-exchange neutrals

Poloidal profiles

- poloidal profiles of total atomic deuterium flux Γ_D and mean energies typically extraced from EIRENE

- standard approaches to calculate sputtering yield up to now:
  1) take mean energies and total flux Γ_D
  2) take mean energies and reduced flux (usually Γ_D /10) to account for high sputtering threshold of ~ 200 eV

- limitations due to strong energy dependence of yield on impact energy:
  - over- or under-estimation of total erosion rate?
  - deviations in spatial erosion patterns?



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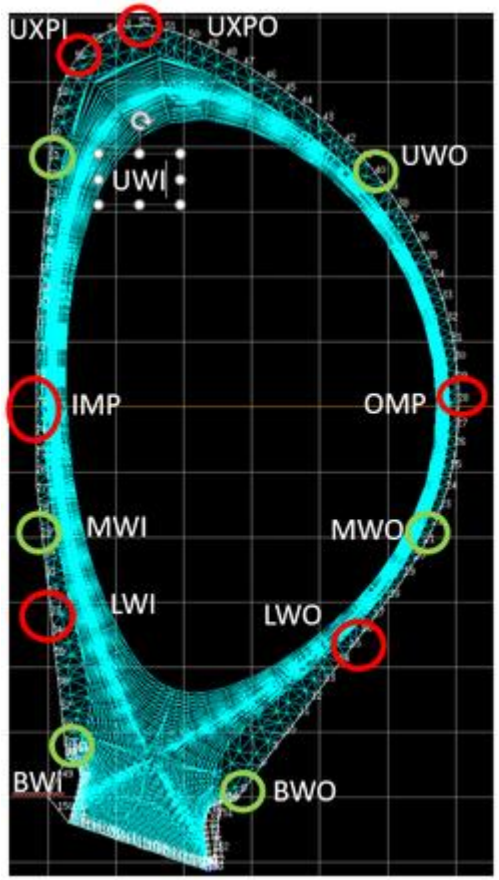
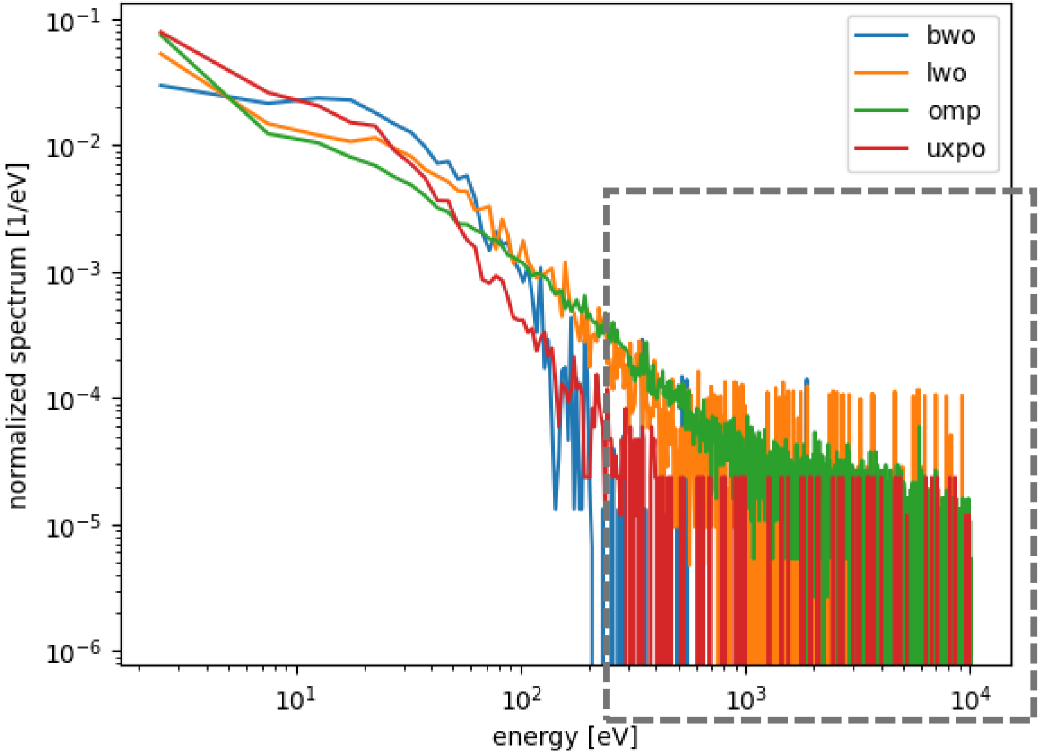
Charge-exchange neutrals

Energy distribution functions (EDFs)

- resolved energy spectra of D-CXN: a way to improve erosion calculations
- energy spectra at 12 different poloidal locations generated by Sven Wiesen
- spectra quite noisy; but the noise may contribute significantly
- effective yield at any surface element determined by interpolated effective yields of two neighbored spectra

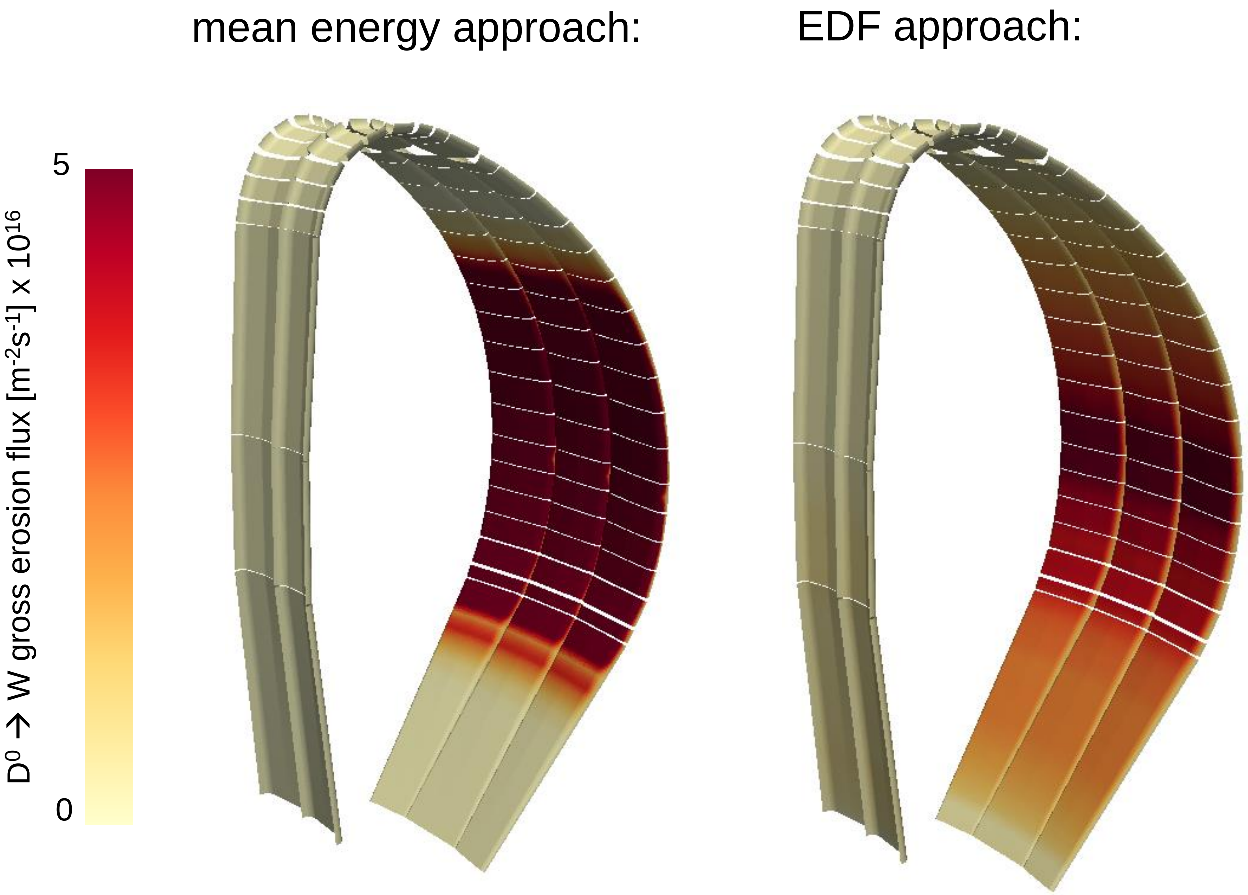


EDFs – Energy Distribution Functions



Tungsten gross erosion induced by CXN

Comparison of mean energy and EDF approach



	mean energy	EDF
peak flux [$m^{-2}s^{-1}$]	1.56×10^{17}	5.41×10^{16}
integrated rate [s^{-1}]	5.75×10^{19}	2.76×10^{19}

- EDF calculation reduces main chamber erosion by a factor 2-3 (peak flux or integrated rate)
- BUT: additional wall area locations will be subject to finite gross erosion
- EDF approach used in the following

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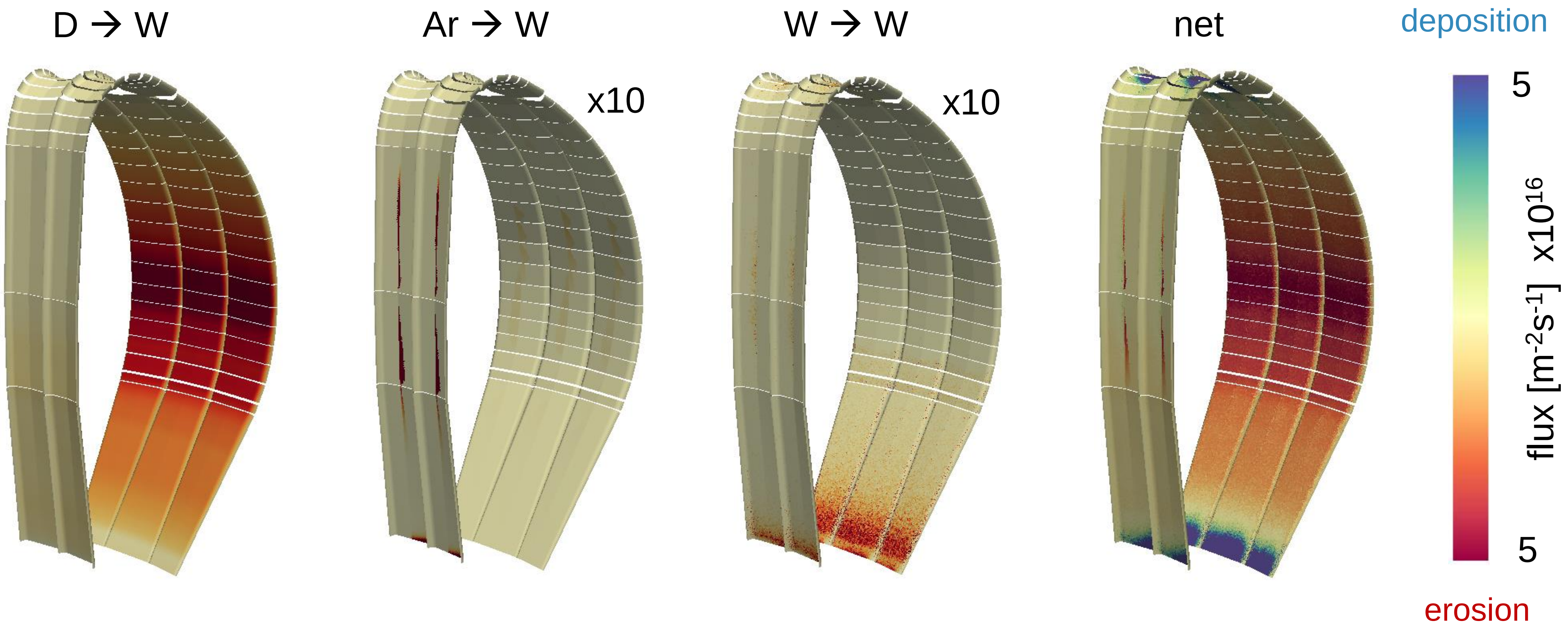
Erosion and re-deposition maps



[10^{18} atoms/s]	net	gross	… by D^0	… by Ar^{Z+}	… by W^{Z+}
main chamber	-16.4	28.3	27.6	0.3	0.4
divertor	15.0	86.8	-	57.8	28.9

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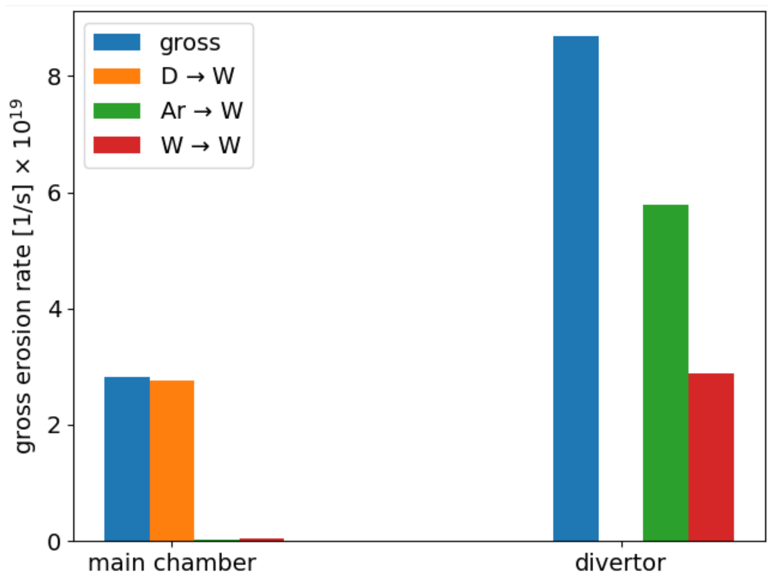
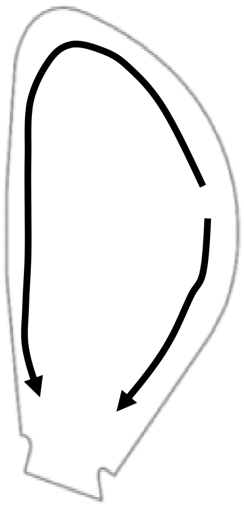
Summary

Key results for preliminary PWI-DEMO modelling



- W main chamber erosion dominated by CXN at low-field side

- W divertor erosion dominated by Ar ions and W self-sputtering
  → relative contribution: ~ 2/3 by Ar, ~ 1/3 by W



- strong W transport from main chamber into divertor due to long ionization mean free paths

- main deposition locations:
  - inner and outer divertor above strike lines up to shoulders
  - remote areas above outer divertor
  - top of the machine (upper X-point)

- large uncertainty in modelling due to large separation between plasma grid and wall

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Summary

Tungsten data needs

- ERO2.0 is a 3D code for PWI and impurity migration studies, which needs various W-related input data

PWI part:

- sputtering and reflection coefficients for various W-target combinations (H isotopes, He ash, B, seeding species)

- now, mainly SDTrimSP input (internal data generation possible), but MD data required to improve data especially for low impact energies

Impurity migration part:

- atomic rate coefficients needed in range determined by background
    - ionization rate coefficient (density dependence)
    - recombination rate coefficient (entire density range)

- relevance of non-resonant W charge exchange with H isotopes?

- when talking about full-W devices, one should not forget about boron data!

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Thank you for your attention!