The Decennial IAEA Technical Meeting
on Atomic, Molecular and Plasma-Material Interaction Data
for Fusion Science and Technology

Global 3D Modelling of Plasma-Wall Interaction in Fusion Devices
Applications and Data Needs in View of ITER and DEMO

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EUROfusion

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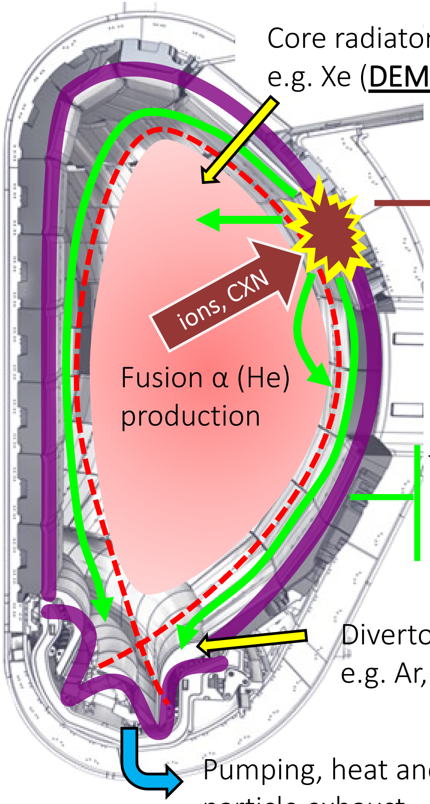
Outline

- Plasma-wall interaction (PWI) in fusion devices
- ERO2.0 code for PWI modelling
- Input data needs for PWI modelling
- Plasma solutions for PWI modelling
- ERO2.0 validation & applications
- Integral approach to PWI in EU-DEMO
- Summary in view of W wall in ITER and DEMO

Plasma-wall interaction (PWI) in fusion devices

full-W machine (here ITER)



Core radiator
e.g. Xe (DEMO)

Erosion of wall material(s) by
- plasma ions
- impurity ions
  - intrinsic (He, O)
  - seeded (Ar, Ne, N, Xe)
  - eroded (B, W) / self-sputtering
- charge-exchange neutrals (CXN)

Transport of eroded material(s)
- plasma flows towards divertor
- diffusion into core plasma

Divertor / X-point radiator
e.g. Ar, Ne, N

Pumping, heat and
particle exhaust

PWI-related issues

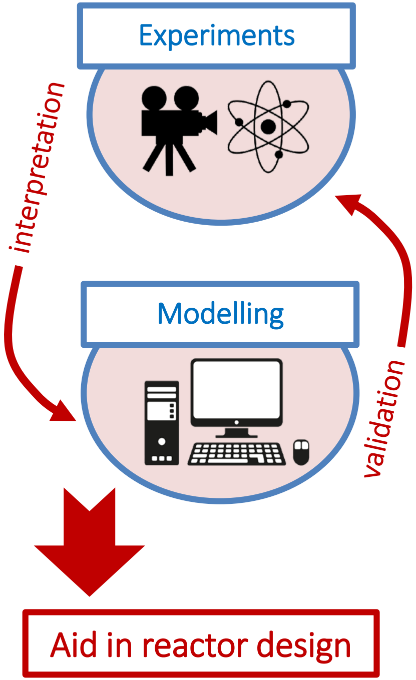
Erosion
- wall lifetime
- dust formation

Core impurity concentration
- fuel dilution
- radiative cooling

Implantation
- fuel retention
- material degradation

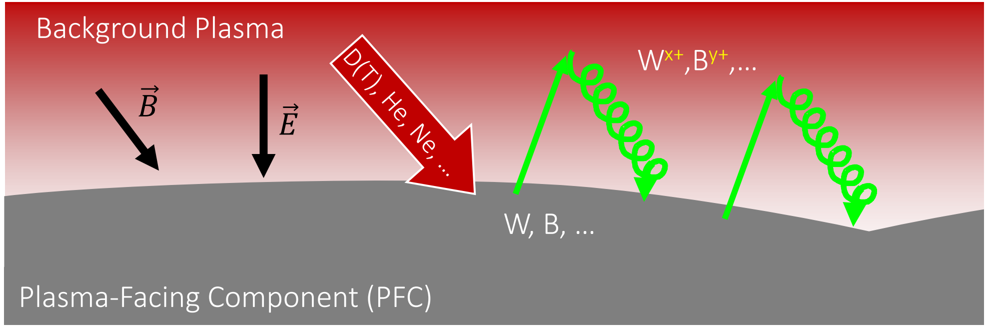
Deposition / co-deposition
- fuel retention
- dust formation

Role of modelling



ERO2.0 code for PWI modelling

JÜLICH Forschungszentrum



Plasma-material interaction + **Impurity transport**

- Reflection
- Physical sputtering
- Chemical erosion
- Deposition
- Material mixing
- Layer growth

- Lorentz force + drifts
- Ionization/Dissociation
- Recombination
- Friction (Fokker-Planck)
- Thermal force
- Cross-field diffusion

ERO2.0 – a 3D Monte-Carlo impurity tracing and plasma-surface interaction code

- Simulation volume up to full reactor-scale
- Optimized for high-performance computing (HPC)
- Realistic CAD 3D wall with high resolution incl. shaping
- Magnetic shadowing from field line tracing
- Full-orbit ion tracing + guiding center approximation
- Plasma sheath models (E field, ion impact energies and angles)
- Plasma-material data (SDTrimSP, Molecular Dynamics)
- Connection to atomic & molecular databases (e.g. ADAS)
- Material mixing model (homogeneous mixing)
- Local surface morphology evolution model
- Multi-stage approach to erosion/deposition in ports, e.g. for diagnostic mirrors

- **JET-ILW**
- **ITER**
- **DEMO**
- WEST
- EAST
- W7-X
- LHD
- DTT
- PSI-2
- GyM

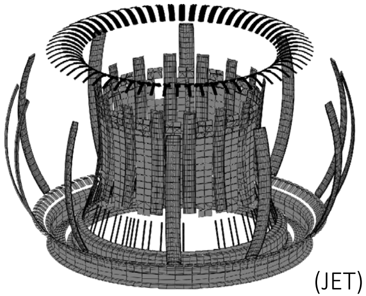
ERO: A. Kirschner et al., NF 40 (2000) 989
ERO2.0: J. Romazanov et al., PS T170 (2017) 014018

Input data for PWI modelling

device & scenario specific

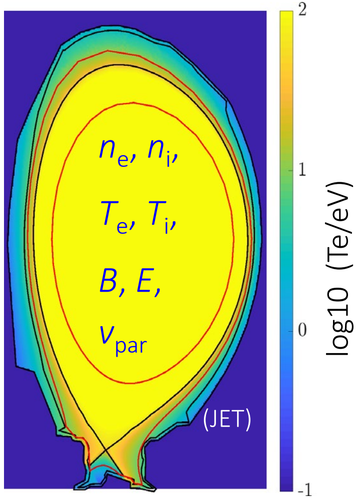
fundamental

wall geometry and materials



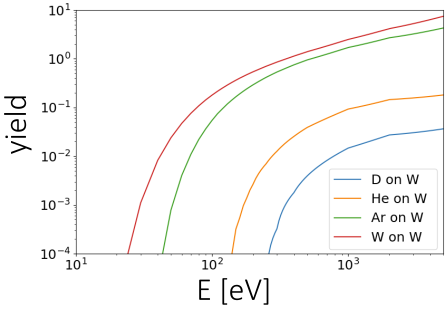
from technical drawings

plasma and neutrals background



SOLPS, EMC3-EIRENE, SOLEDGE-EIRENE, OEDGE

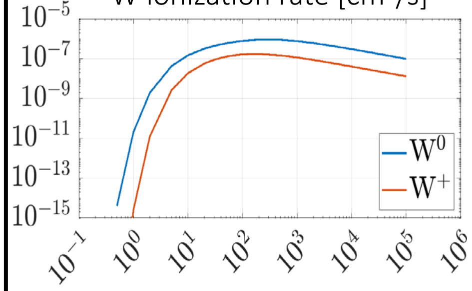
sputtering yields reflection coefficients



SDTrimSP, Molecular Dynamics

atomic & molecular data

W ionization rate [cm³/s]



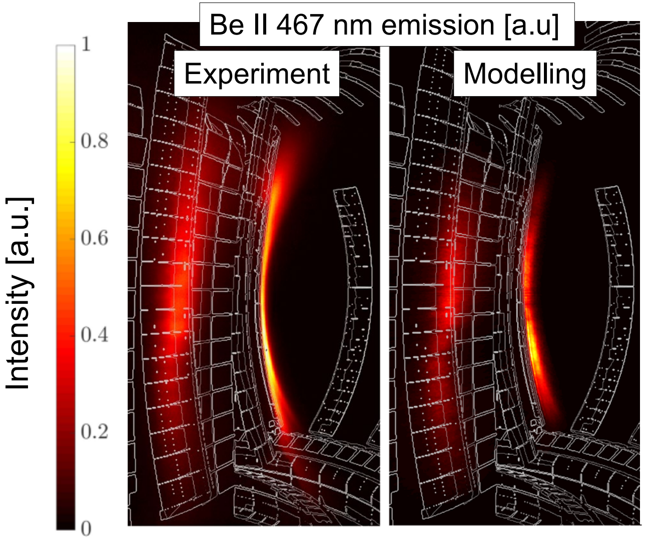
ADAS, GKU, ATOM

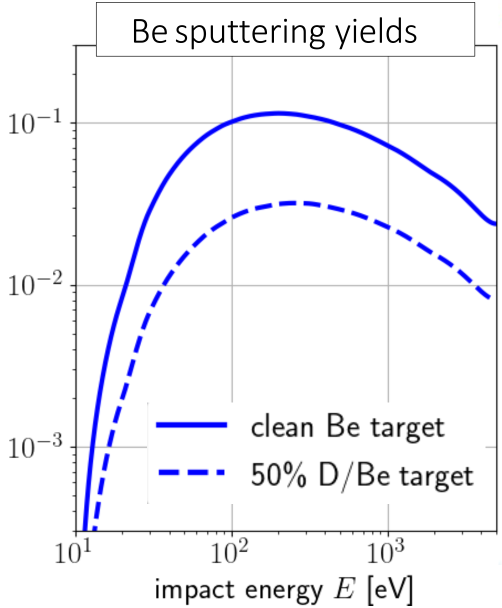
ideally, with known surface composition dependencies

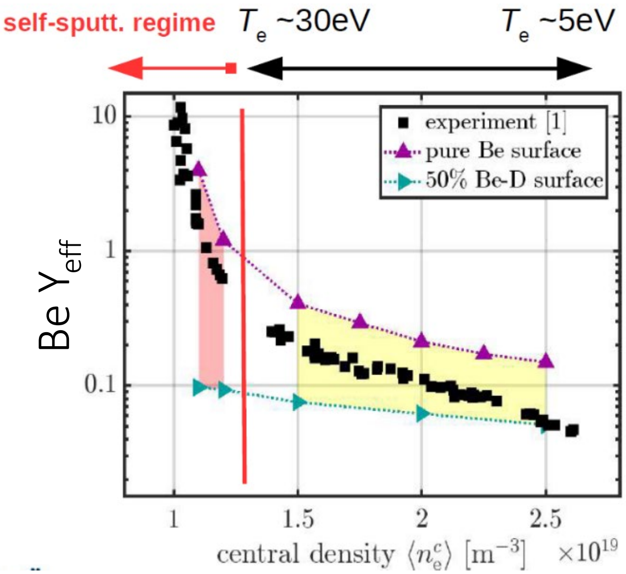
+ magnetic equilibrium / shadowing
+ energy / angular resolved fluxes

ERO2.0 modelling for JET-ILW

Effective Be erosion yields







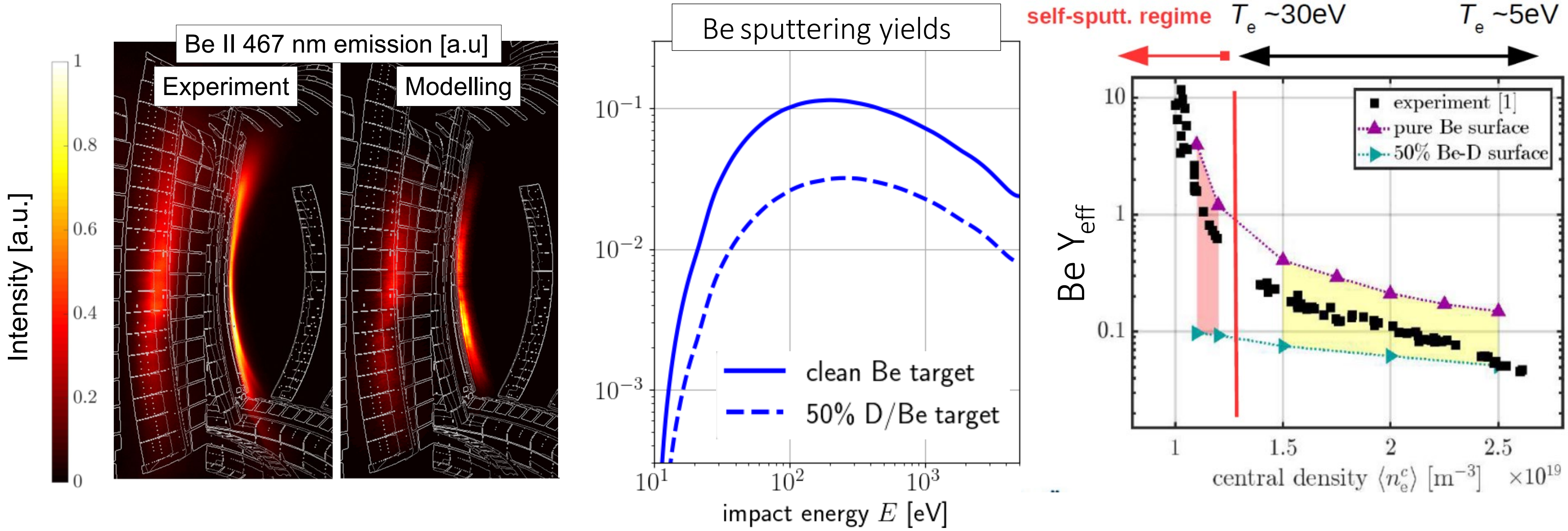
Good agreement of Be emission and effective erosion yields validates the models and data used

- Significant role of presence of D in Be surface
- Significant contribution of self-sputtering (high Z_{eff})
- Additional erosion mechanisms (CAPS, CXN)

J. Romazanov et al., NME 18 (2019) 331

ERO2.0 modelling for JET-ILW

Effective Be erosion yields

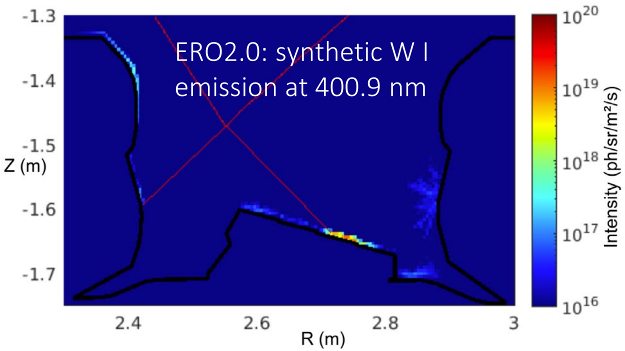


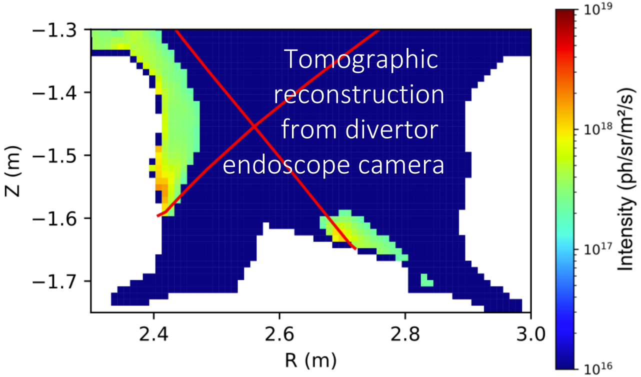
- Underlying modelling assumptions are possible reasons for discrepancies with experiment
- Parameter studies help identifying critical dependencies when models lack completeness

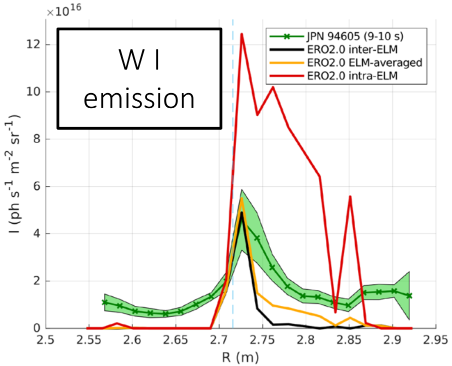
J. Romazanov et al., NME 18 (2019) 331

ERO2.0 modelling for JET-ILW

Validation of W erosion and transport simulations





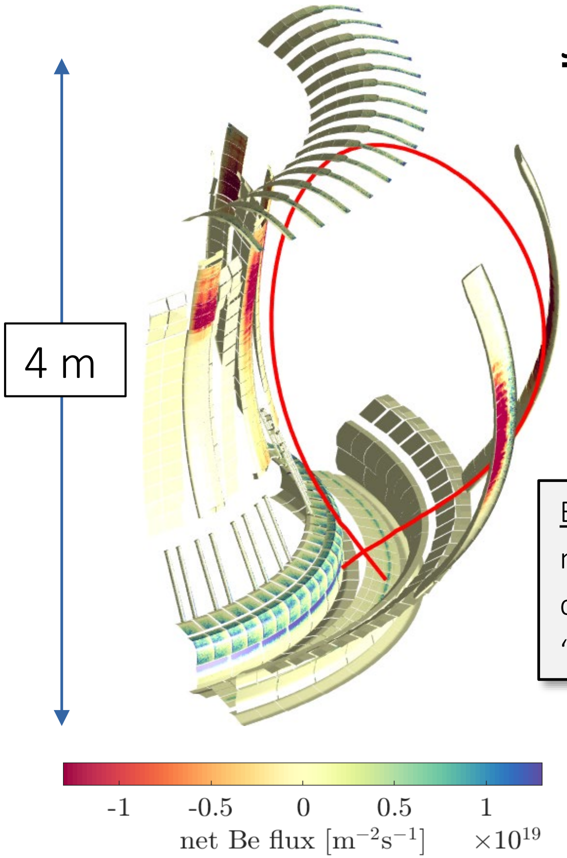


- W density in main plasma within factor 2 of experimental for a wide range of plasma scenarios
- ERO2.0 predictions of W erosion consistent with measured W I spectral line emission, but more localized, potentially due to uncertainties of W atomic data (e.g. **metastable states**)
- Virtually perfect divertor screening observed – **prompt re-deposition**, pre-sheath E field, main ion flow
- Influx into core mainly due to CXN erosion near LFS divertor entrance – much lower screening efficiency
- Critical SOL parameters: n_e, T_e, ion flow, **energy-resolved CXN fluxes**
- Multi-fluid plasma solution (EDGE2D-EIRENE) affected by **W charge-state bundling**

H. Kumpulainen et al., NME 33 (2022) 101264
H. Kumpulainen, PhD Thesis (2023)
https://urn.fi/URN:ISBN:978-952-64-1257-3

ERO2.0 modelling: JET-ILW vs ITER

JET

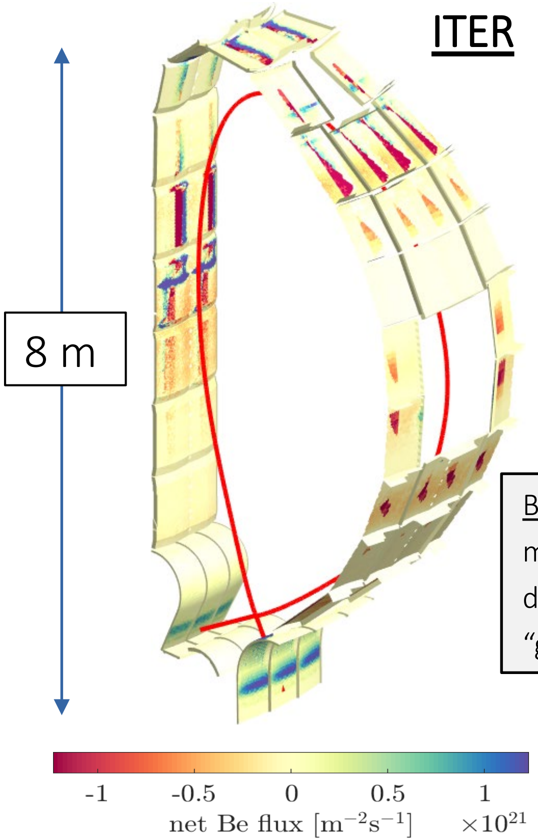


Balance of first wall Be erosion and deposition

Dominant Be deposition on inner divertor top surface

Be deposition:
main chamber: 18%
divertor: 58%
“gaps”: 24%

ITER



High confinement mode with zero SOL flow

Dominant Be re-deposition at main chamber wall

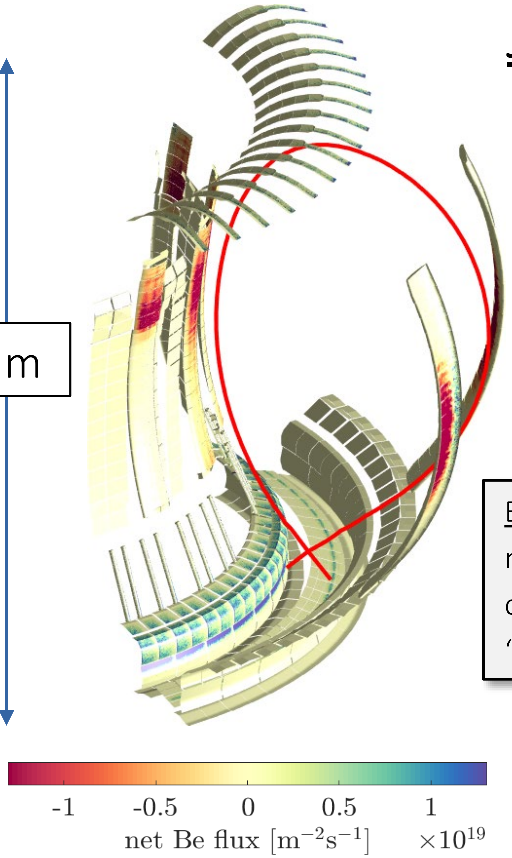
Be deposition:
main chamber: 90%
divertor: 10%
“gaps”: <1%

J. Romazanov NME2021, NF2022

ERO2.0 modelling: JET-ILW vs ITER

JET

4 m



Balance of first wall Be erosion and deposition

Dominant Be deposition on inner divertor top surface

Be deposition:

main chamber: 18%

divertor: 58%

"gaps": 24%

ITER

8 m

High confinement mode with zero SOL flow

Dominant Be re-deposition at main chamber wall

Be deposition:

main chamber: 90%

divertor: 10%

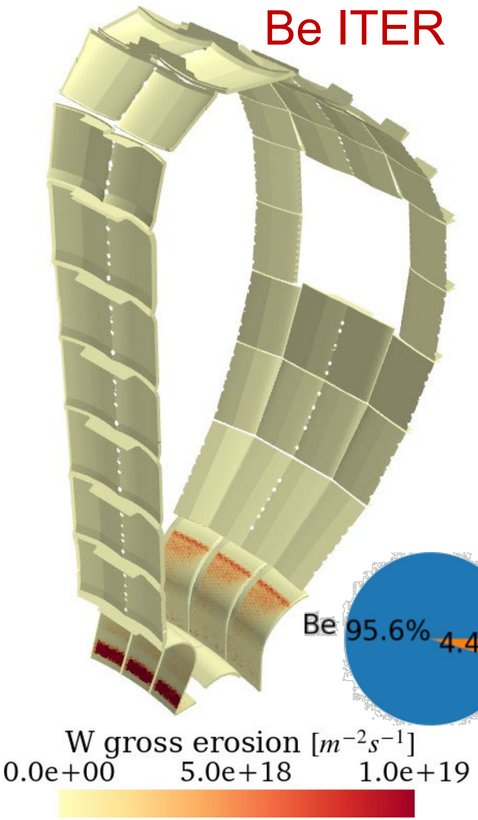
"gaps": <1%

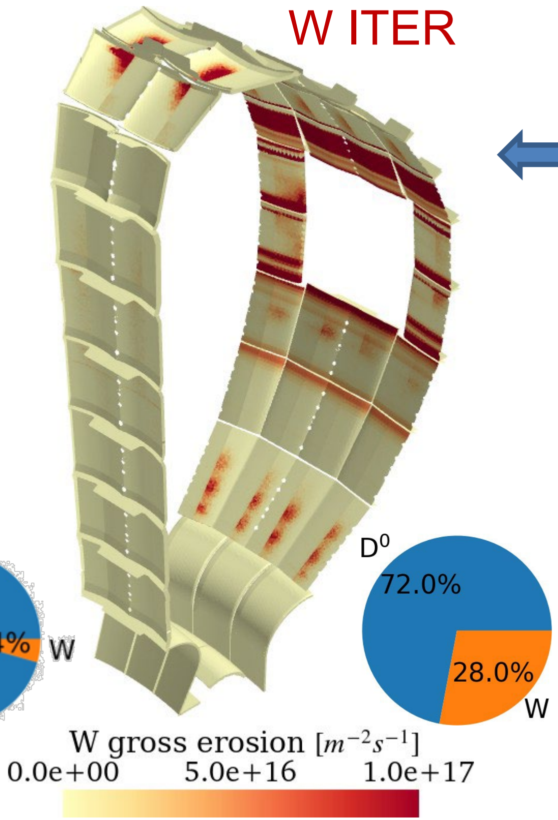
In ITER the dominant fuel retention (may have turned out) to be at the first wall and not in the divertor

J. Romazanov NME2021, NF2022

ERO2.0 modelling for ITER: Be vs W

ITER with Be: J. Romazanov et al., NF 62 (2022) 036011
ITER with W: A. Eksaeva et al., Phys. Scr. 97 (2022) 014001





Full-W ITER:

← pure D cases

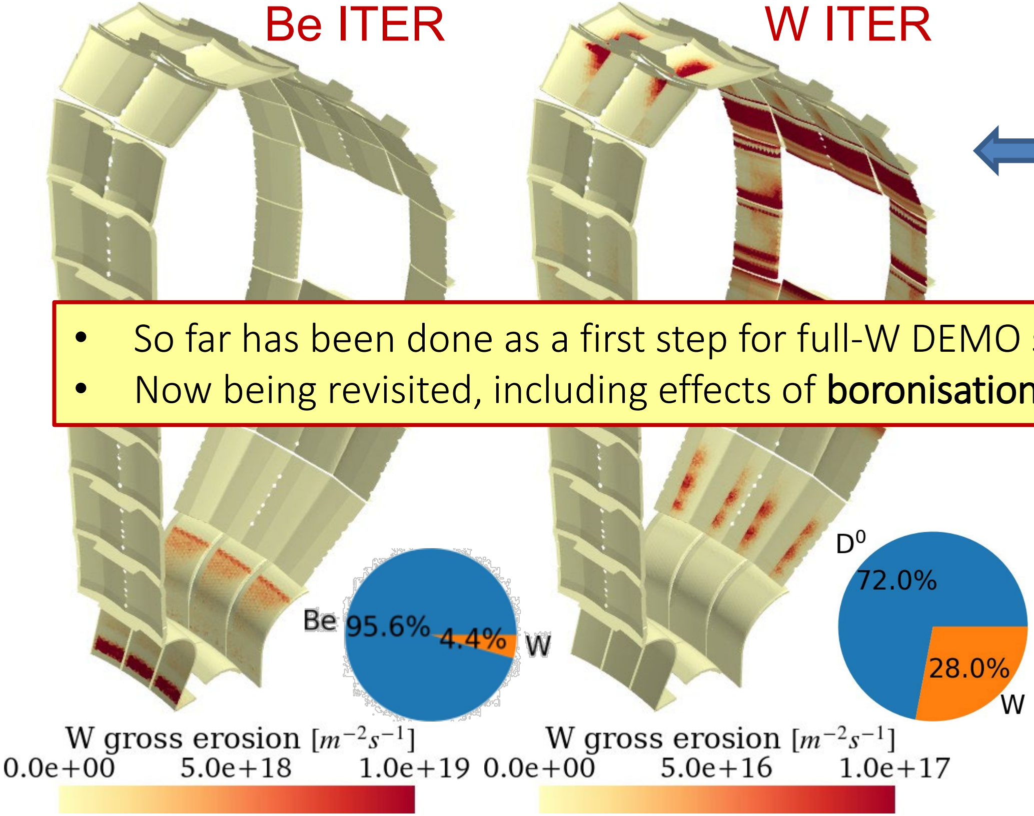
- Factor ~10 lower total erosion
- Main chamber erosion mostly by CXN
- Redeposition mostly in main chamber
- Flat far-SOL (high T_e) → fast W ionization
- No erosion by D in divertor (low T_e)

→ with seeded impurities

- Simplified assumption: constant concentration, single charge state
- Impurity and self-sputtering important in the divertor

ERO2.0 modelling for ITER: Be vs W

ITER with Be: J. Romazanov et al., NF 62 (2022) 036011
ITER with W: A. Eksaeva et al., Phys. Scr. 97 (2022) 014001



Full-W ITER:

pure D cases

- Factor ~10 lower total erosion
- No erosion by D in divertor (low T_e)

with seeded impurities

- Simplified assumption: constant concentration, single charge state
- Impurity and self-sputtering important in the divertor

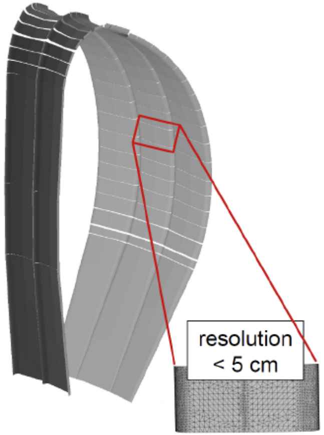
- So far has been done as a first step for full-W DEMO simulations (before ITER re-baselining)
- Now being revisited, including effects of **boronisation** layer lifetime and re-deposition

ERO2.0 modelling for DEMO

Critical input data

Wall geometry

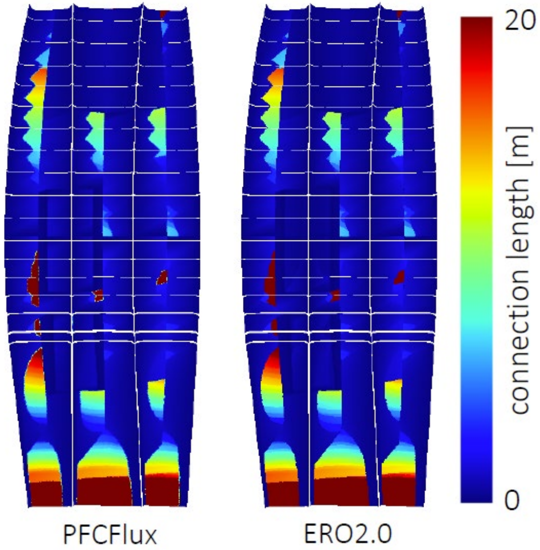
(baseline 2017)



EU-DEMO main chamber geometry as polygon mesh (~10^5 polygons)

Magnetic equilibrium

(baseline 2017)

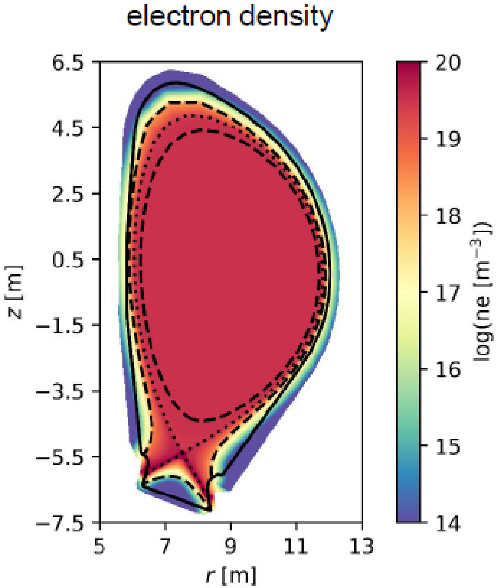


ERO2.0 magnetic shadowing validated

Plasma solution

F. Subba et al 2021 Nucl. Fusion 61 106013

(D, He, Ar)



C. Baumann et al. EPS 2023, PSI 2024

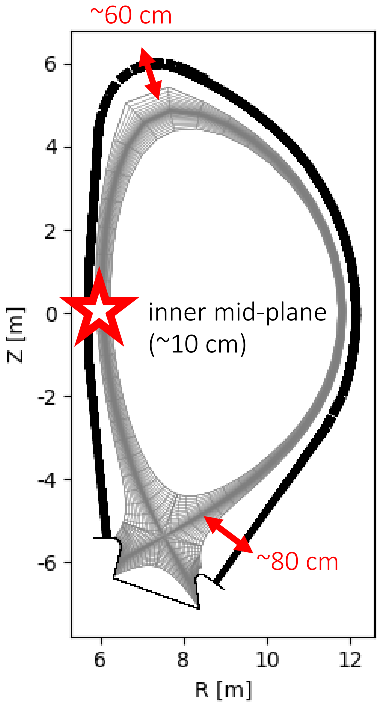
ERO2.0 modelling for DEMO

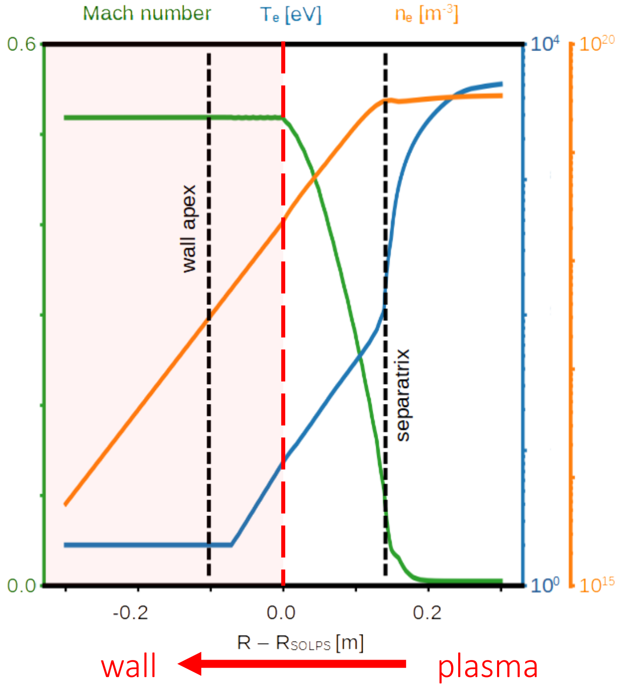
Large volume for extrapolation of plasma solution to the wall

Extrapolation introduces
large modelling uncertainties

Following assumptions used so far:

- Exponential decay for densities
- Exponential decay for temperatures; but capped by 2 eV / 5 eV / 10 eV
- Uniform decay constant of 5 cm
- Constant Mach number
- Ion flow velocity from local Mach number and plasma parameters





C. Baumann et al. EPS 2023, PSI 2024

ERO2.0 modelling for DEMO

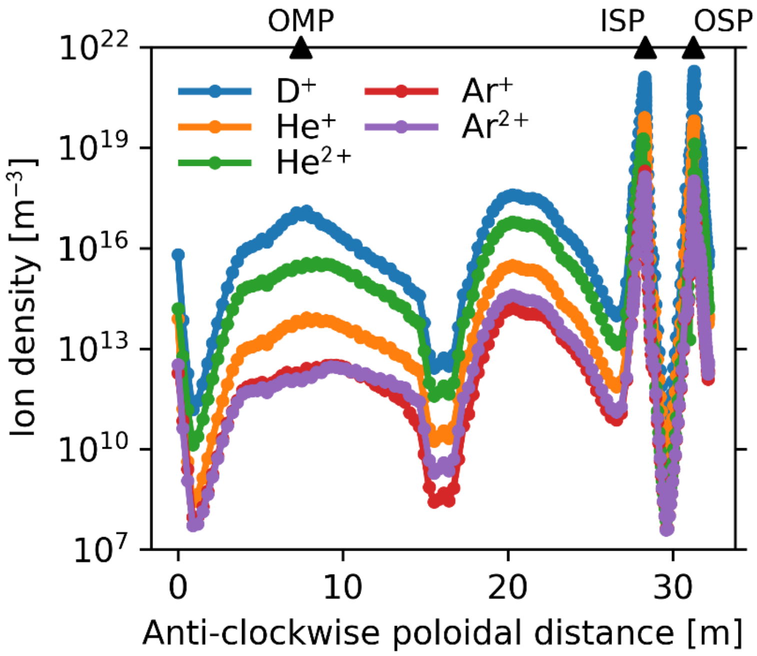
Charge-resolved spatially non-uniform impurity ion fluxes (He, Ar)

Essential for proper calculation of sputtering yields

Using the total flux with mean volumentric charge state leads to overestimation of gross erosion

Charged resolved spatially varying fluxes now implemented in ERO2.0 lead to significant reduction of divertor gross erosion by impurities

Remaining problem: impurity charge state distribution at the first wall is taken from outermost SOLPS nodes leads to overestimation of erosion



C. Baumann et al. EPS 2023, PSI 2024

ERO2.0 modelling for DEMO

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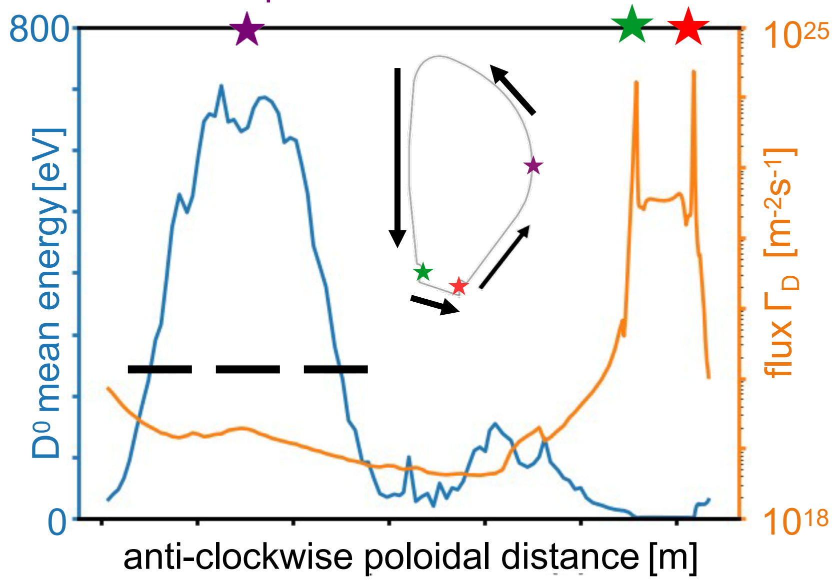
Charge-exchange fluxes and erosion in the main chamber

Standard SOLPS-ITER output: poloidal profiles and mean energies of neutral atoms at the wall



Simple approach to sputtering by CXN:

- Using the mean energy with the total flux may overestimate the flux and underestimate the erosion yield

Advanced appoach to sputtering by CXN:

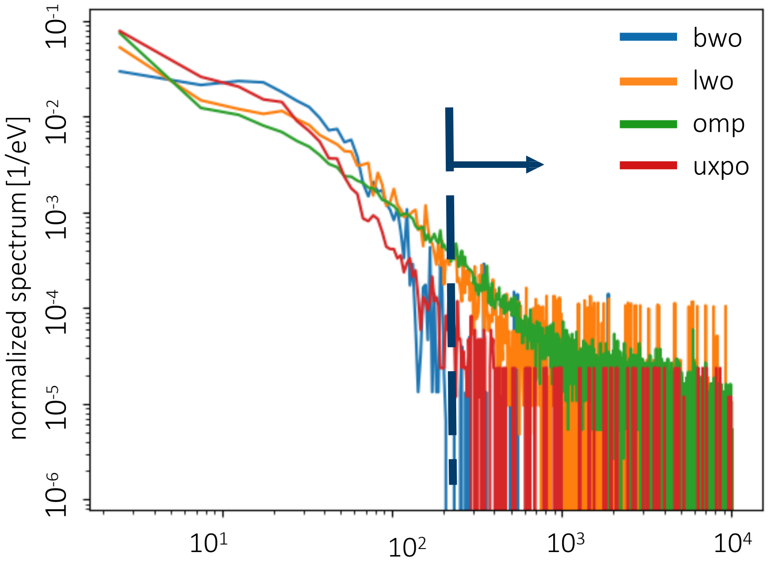
- EIRENE post-processig of the SOLPS-ITER solution to provide energy resolved (and ideally angular resolved) neutral fluxes

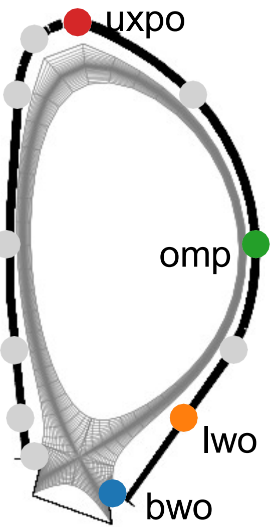
C. Baumann et al. EPS 2023, PSI 2024

ERO2.0 modelling for DEMO

Charge-exchange fluxes and erosion in the main chamber

EDFs – Energy Distribution Functions





Energy resolved spectra improve yield calculations

Available only for 12 poloidal locations (provided by S. Wiesen)

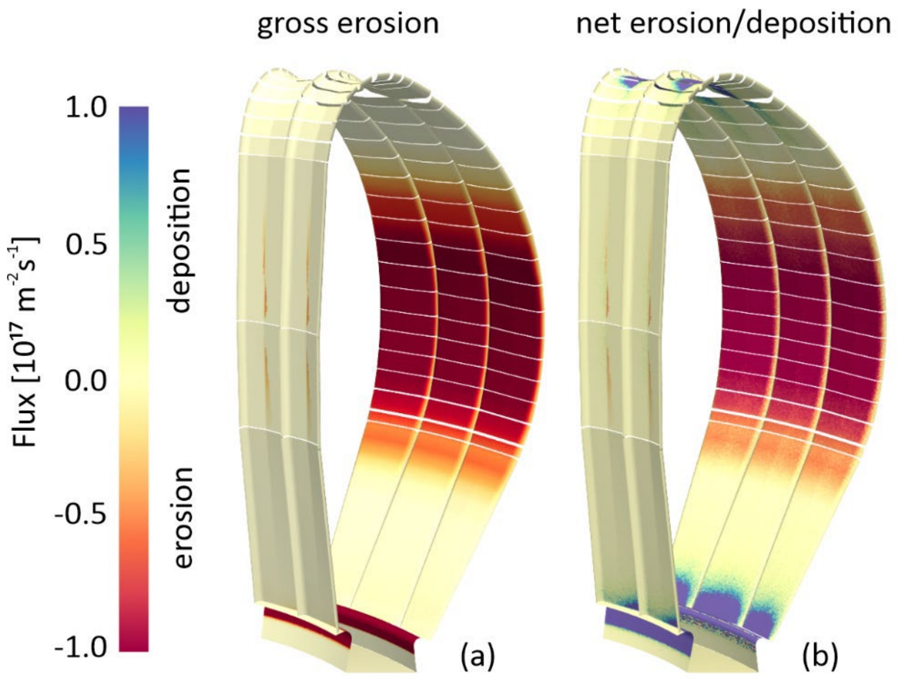
Interpolation is used by calculating effective erosion yield for each spectrum combined with poloidal flux profile

Angular resolved spectra still pending

C. Baumann et al. EPS 2023, PSI 2024

ERO2.0 modelling for DEMO

Example for the mean CXN energy approach

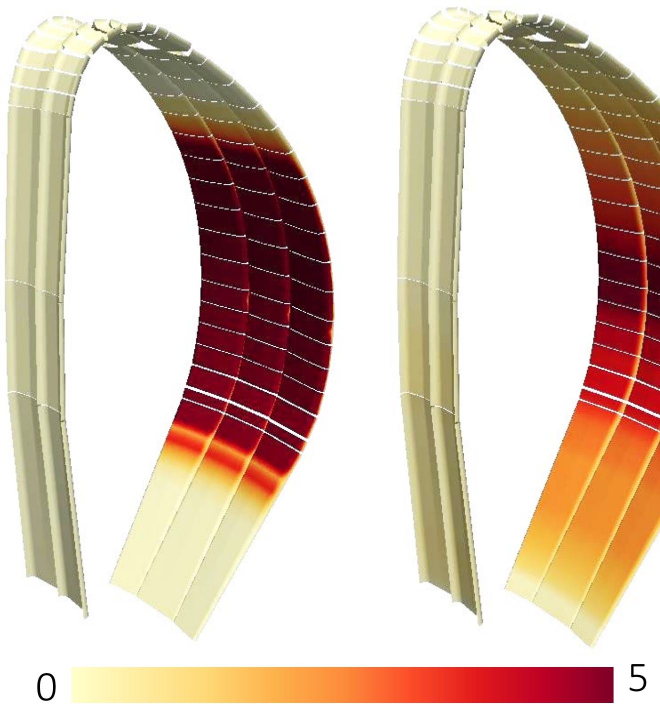


- Main chamber erosion dominated by neutrals
- Divertor erosion dominated by Ar and self-sputtering
- Strong transport from main chamber into the divertor due to long ionization mean free paths, no transport from divertor
- Main deposition locations:
  - inner and outer divertor above strike lines,
  - remote areas above outer divertor (wall gap),
  - top of the machine (upper X-point)

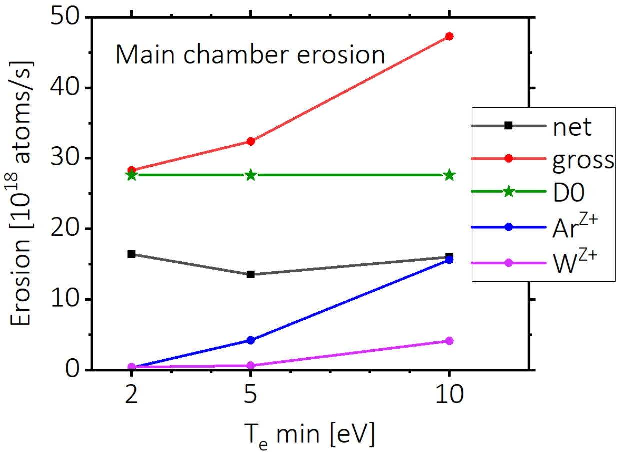
C. Baumann et al. EPS 2023, PSI 2024

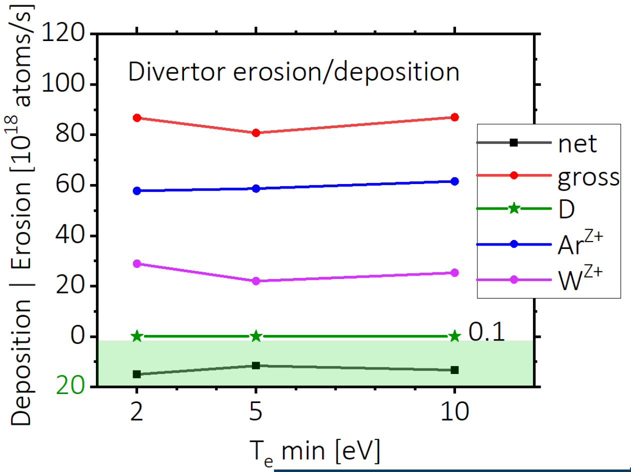
ERO2.0 modelling for DEMO

mean CXN energy vs EDF



$D^0 \rightarrow$ W gross erosion flux [10^{16} $m^{-2}s^{-1}$]





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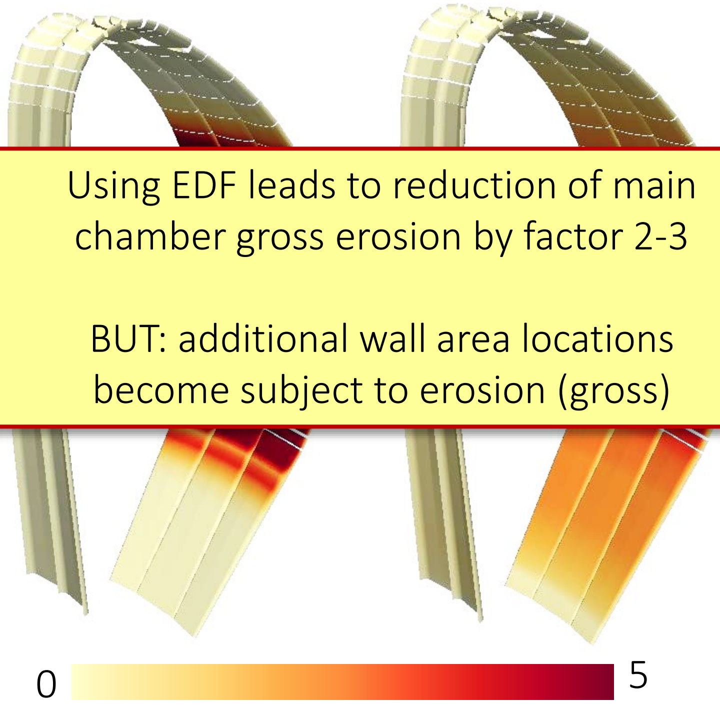
ERO2.0 modelling for DEMO

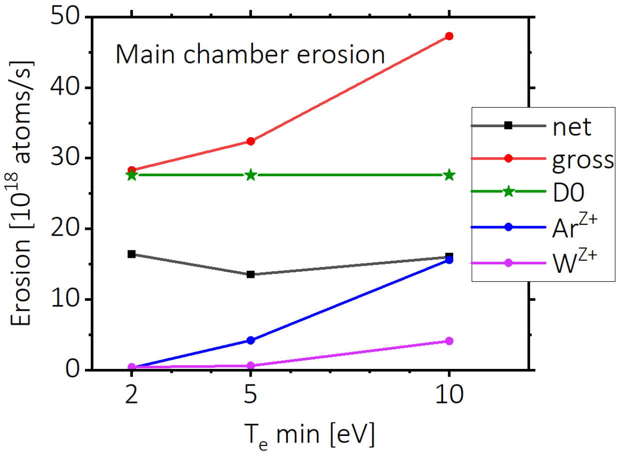
mean CXN energy vs EDF

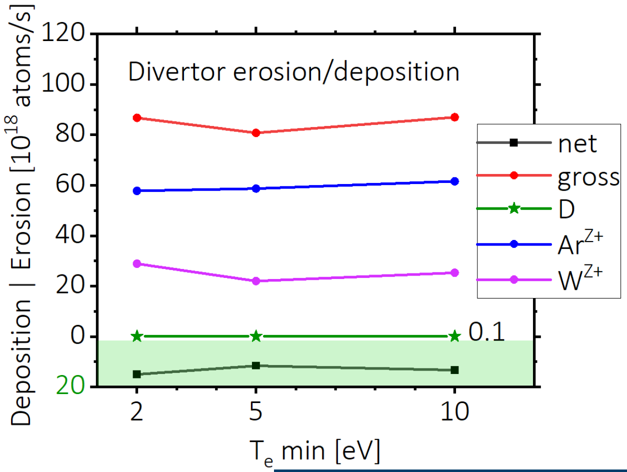


Using EDF leads to reduction of main chamber gross erosion by factor 2-3

BUT: additional wall area locations become subject to erosion (gross)

$D^0 \rightarrow W$ gross erosion flux [10^{16} $m^{-2}s^{-1}$]





C. Baumann et al. EPS 2023, PSI 2024

EUROfusion Theory, Simulation, Validation and Verification (TSVV) Task 7

Plasma-Wall Interaction in DEMO

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Plasma-Wall Interaction in DEMO

Objectives

- Assessment of steady-state W erosion rates for first wall and divertor
- Mapping of preferential W re/co-deposition locations
- Assessment of dust mobilization from likely dust production sites (dust survival rates and dust accumulation maps)
- Assessment of PFC response to transients: melting and splashing (melt-stability, likelihood of splashing, droplet-to-dust conversion)
- Assessment of W erosion rates for locations affected by transients
- Assessment of tritium in-vessel inventory & permeation rates (co-deposition, bulk retention with He-induced and neutron damage)

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Plasma-Wall Interaction in DEMO

Teams, codes and competences

FZJ	ERO2.0	Impurity transport and PWI: erosion-deposition mapping in steady-state
IPP Garching	SDTrimSP TESSIM, RAVETIME	PWI data: implantation, reflection, sputtering Fuel retention / Uncertainty quantification
KTH	MEMENTO MIGRAINE	Material response to transient heat loads: melting and splashing Dust & droplet mobilization and transport
IPP Prague	SPICE & BIT	Kinetic (PIC+MC) modelling of complex plasma sheath
JSI	BIT	Kinetic (PIC) modelling of dynamic SOL
CEA/USPN	MHIMS, FESTIM	Fuel retention (incl. 3D monoblock geometry)
VTT/Helsinki	MD, DFT, ML	Interatomic potentials development / MD modelling for PWI

a set of dedicated and validated codes

EUROfusion Theory, Simulation, Validation and Verification (TSVV) Task 7

Structure & workflows

External input: plasma background, wall geometry, material choice, steady-state and transient heat loads – interaction with other EUROfusion tasks and work packages

Post-processing / extraction of parameters (e.g. extrapolation, CX fluxes and distributions)

Local PWI
erosion, morphology

Kinetic plasma sheath
sheath collisionality, ion fluxes & distributions, heat loads, thermionic current

Global PWI in steady-state
erosion
impurity transport
deposition

Fuel
retention
co-deposition
n-damage

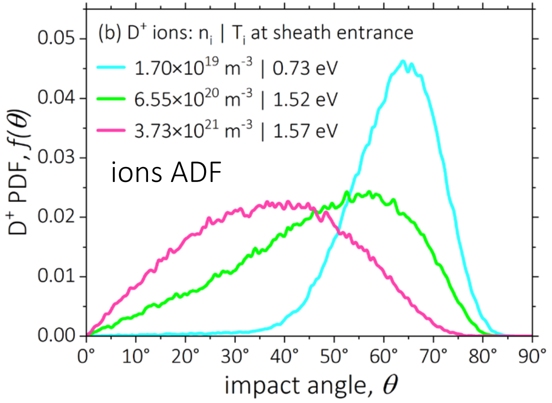
Dust
mobilization
transport
deposition

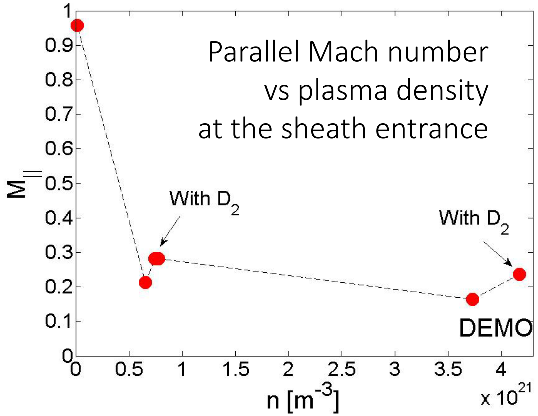
Transients
melting
splashing
droplet-to-dust

Advanced computing activities: standardization (e.g. IMAS), optimization for HPC

EUROfusion Theory, Simulation, Validation and Verification (TSVV) Task 7

PIC modelling (BIT1 code): high density divertor sheath (n_e up to $5\cdot10^{21}$ m^{-3})





Collisional sheath with a zoo of multi-step A&M processes:

- ← Modification of ion and neutral distribution functions (energies and angles of wall impact)
- ← Angular distributions of ions acquire shape similar to neutrals
- ↙ Parallel Mach number at sheath entrance is <1
- ↙ Boundary conditions of edge plasma simulations (e.g. SOLPS) use $M_{||} = 1$
- W prompt re-deposition decreases faster than gross sputter rate → increased net erosion rate
- Multi-step W ionization and W-D^+ charge-exchange at high density increase re-deposition (not much) but such collision cross-sections are largely unknown

D. Tskhakaya IAEA TM 2024, PSI 2024

EUROfusion Theory, Simulation, Validation and Verification (TSVV) Task 7

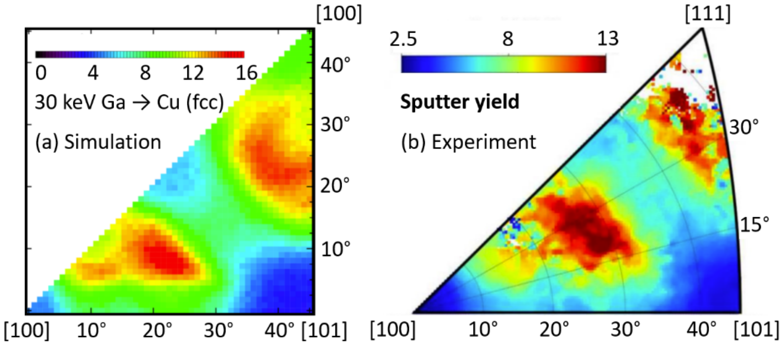
PWI data and new code capabilities

SDTrim-SP 1/2/3D

- **"Gyro-motion" extension:**
  - magnetic & electric field effects on impinging ions
  - e.g. for Y_{eff} of molten surface morphology

U. Von Toussaint

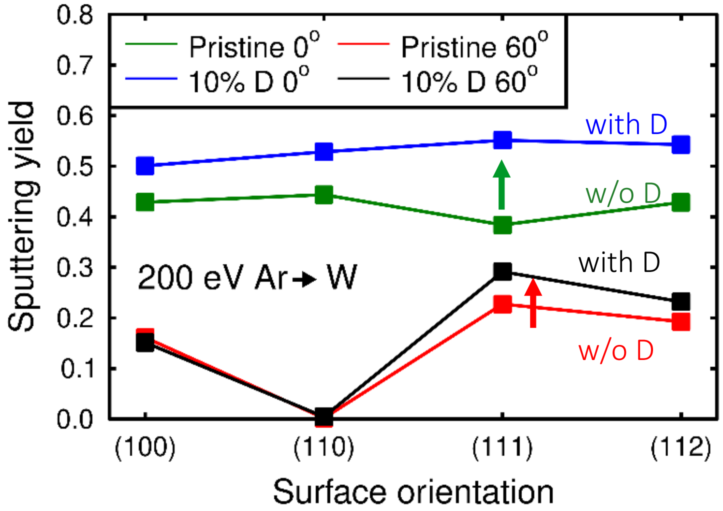
- **"Crystal" extension:**
  - More accurate description of polycrystalline surfaces



Sputtering data for D supersaturated W and W-O-D

- Ar case studies accomplished, D case in progress

F. Kporha, F. Granberg



Summary of critical questions in view of ITER and DEMO

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- PWI codes are capable of simulating full-W environments – rely on plasma solutions and fundamental data
- Key points for more consistent plasma backgrounds (far-SOL)
  - Wide-grid plasma codes (SOLEDGE3X, EMC3-EIRENE, SOLPS-ITER); turbulent transport?
  - New workflows in EIRENE for CXN distributions – high statistic requirement
  - Reducing uncertainties on SOL transport (ionization, recombination, diffusion, plasma flow)
  - Consequences of "diffusive" divertor sheath in view of edge coupling and impurity transport (edge code boundary conditions, prompt re-deposition, ion impact characteristics)
- Fundamental data needs

W

  - W atomic data – recombination at low n_e, qualitative differences between different W charge states, density dependence of ionization rate coefficients, H^+-W charge-exchange, multi-step ionization

B

  - Erosion yields for B and H/B layers (experiments), incl. low energies (Molecular Dynamics), B + O ?
  - Boron migration to shadowed areas, accumulation (in absence of B pumping) – dust issue ?
  - Fuel retention in and removal from co-deposited layers (diffusion, trapping, isotope exchange)