

“THEORY, SIMULATION, VERIFICATION AND VALIDATION”

TSVV TASK 7: PLASMA-WALL INTERACTION IN DEMO

WP PWIE Meeting | 27.03.2025

D. Matveev on behalf of TSVV-7 team





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Thrust 2 (WP PWIE) Facilitator: Sebastijan Brezinsek



Aims of the project

Establish an integrated modelling suite capable to treat complex 3D wall geometry to predict steady-state PWI in DEMO

Provide safety-relevant information for DEMO reference scenarios concerning first-wall erosion, dust, and fuel inventory

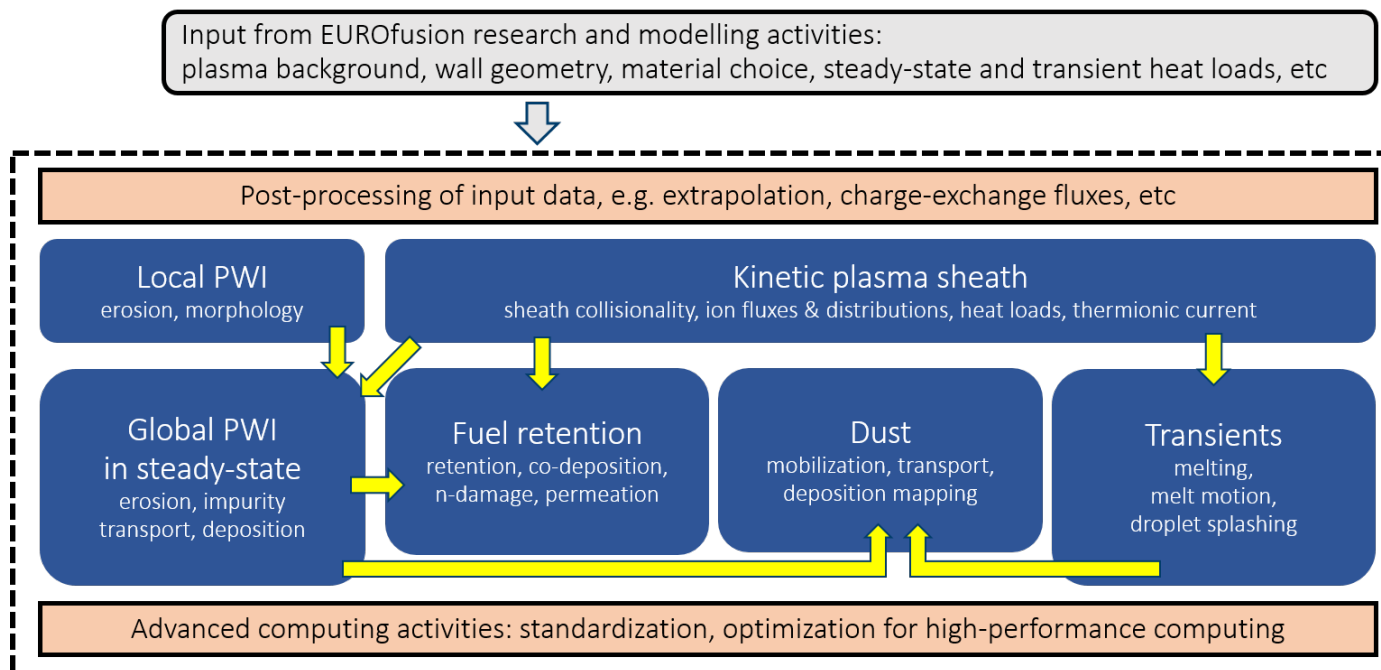
Develop and apply modelling capabilities to treat PWI in DEMO-relevant transients regarding their impact on PFC integrity



Objectives

Assessment of

- Steady-state W erosion rates
- Preferential W re-/co-deposition locations
- Dust mobilization, survival and accumulation
- PFC response to transients: melting, splashing
- W erosion for locations affected by transients
- Tritium inventory: co-deposition, bulk retention



Codes and model development

ERO2.0

→ PWI & impurity tracing

MIGRAINE

→ dust transport

MEMENTO

→ transient melting

- **BIT-1:** high density divertor sheath for ERO2.0
- **SPICE:** thermionic emission for MEMENTO heat & particle fluxes to shaped PFC
- **FESTIM & TESSIM:** - T retention & permeation
- **SDTrimSP, MD:** erosion yields, surface effects
- + Uncertainty quantification

Project overview paper

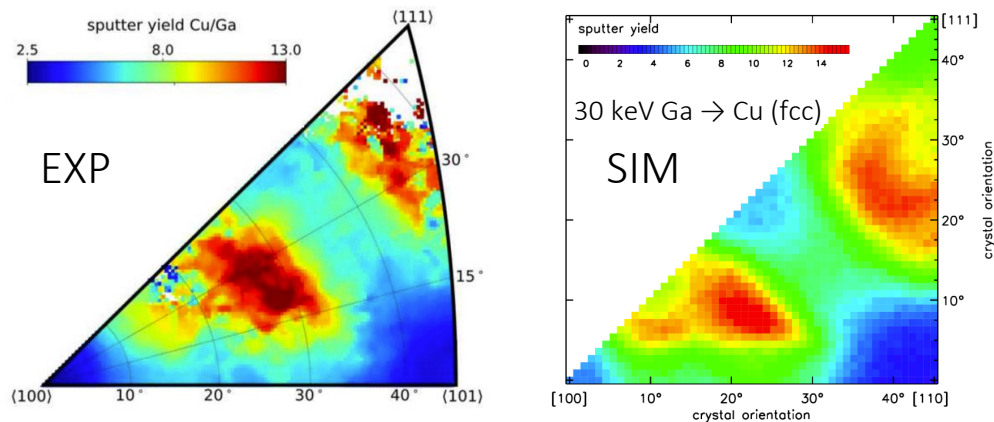
D. Matveev et al, Nucl. Fusion 64 (2024) 106043



PWI data and code capabilities improvement (in-brief)

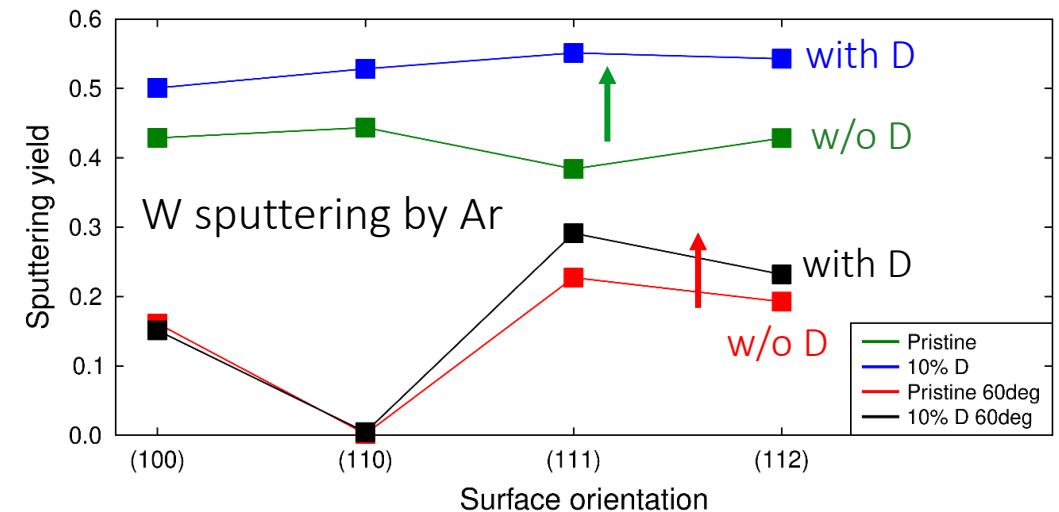
SDTrim-SP

- “Gyro-motion” extension:
 - magnetic & electric field effects on impinging ions
 - implemented and verified against computations
 - performance optimization, experimental validation
- “Crystal” extension:
 - validated against MD, MARLOWE and experiment



Sputtering data for D supersaturated W from MD

- Ar case studies accomplished: presence of D increases sputtering of W, strong grain orientation effect
- D and D₂ cases delayed by technical challenges (appropriate potential is slow, sputtering yield depends on the simulation cell depth, huge statistics required)
- Work on W-O / W-O-H potential development ongoing





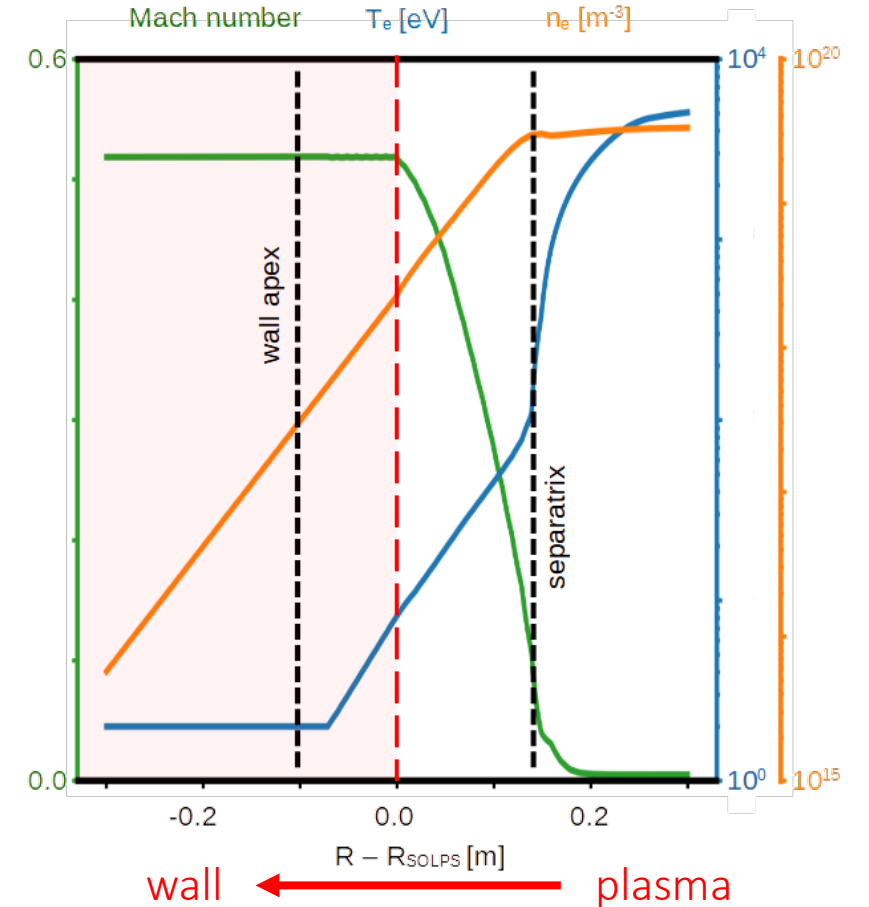
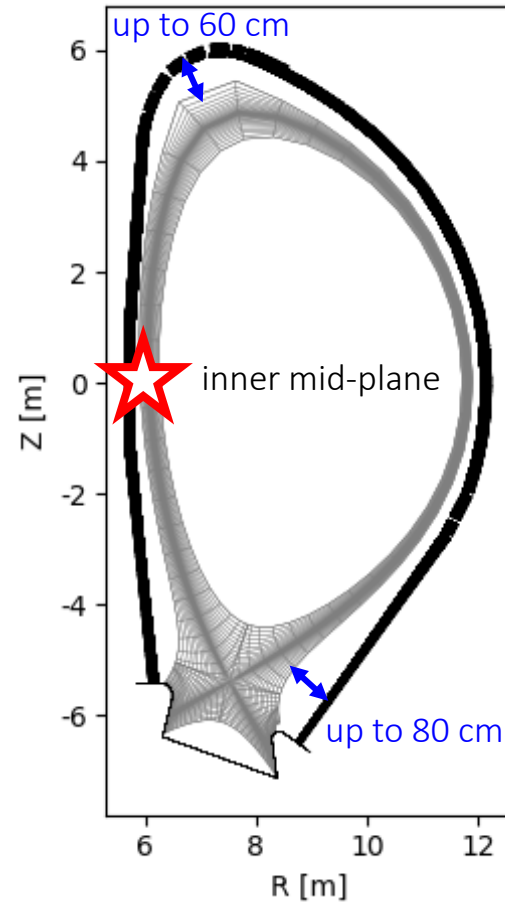
ERO2.0 modelling: erosion and deposition mapping

Unprecedentedly large volume for extrapolation of plasma solution to the wall

Large extrapolation volume introduces large modelling uncertainties

Following assumptions in far-SOL:

- Exponential decay for densities
- Exponential decay for temperatures; but capped at 2 eV, 5 eV or 10 eV
- Uniform decay constant of 5 cm
- Constant Mach number





ERO2.0 modelling: erosion and deposition mapping

Dominating role of charge-exchange (CX) fluxes on erosion in the main chamber

Normally only poloidal profiles and mean energies are available from SOLPS-ITER

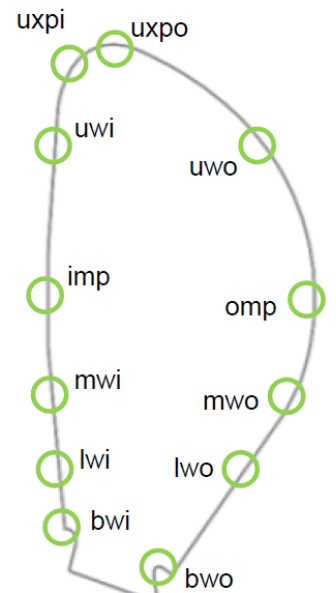
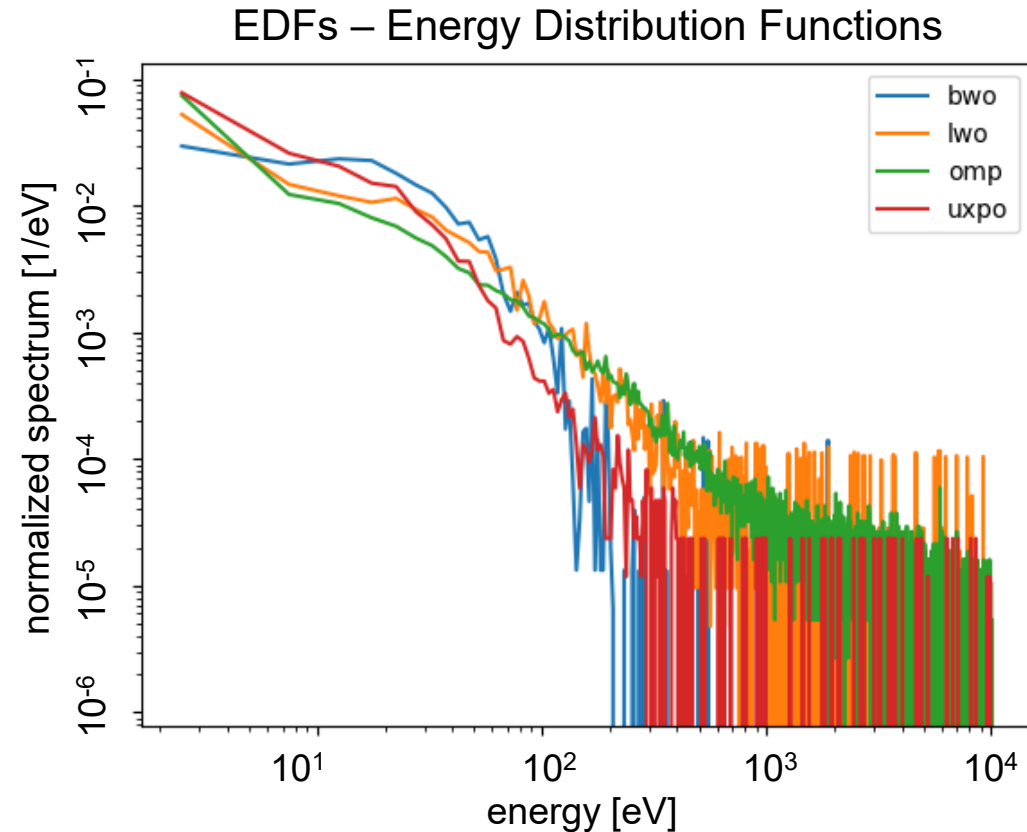
Former assumptions for sputtering:

- Using the **mean energy approach** (strong dependence of sputter yield on energy leads to incorrect erosion patterns)

Current approach - **EDF**:

- EIRENE post-processing of the SOLPS-ITER solution to provide **energy-resolved neutral fluxes** (angular-resolved in progress)

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

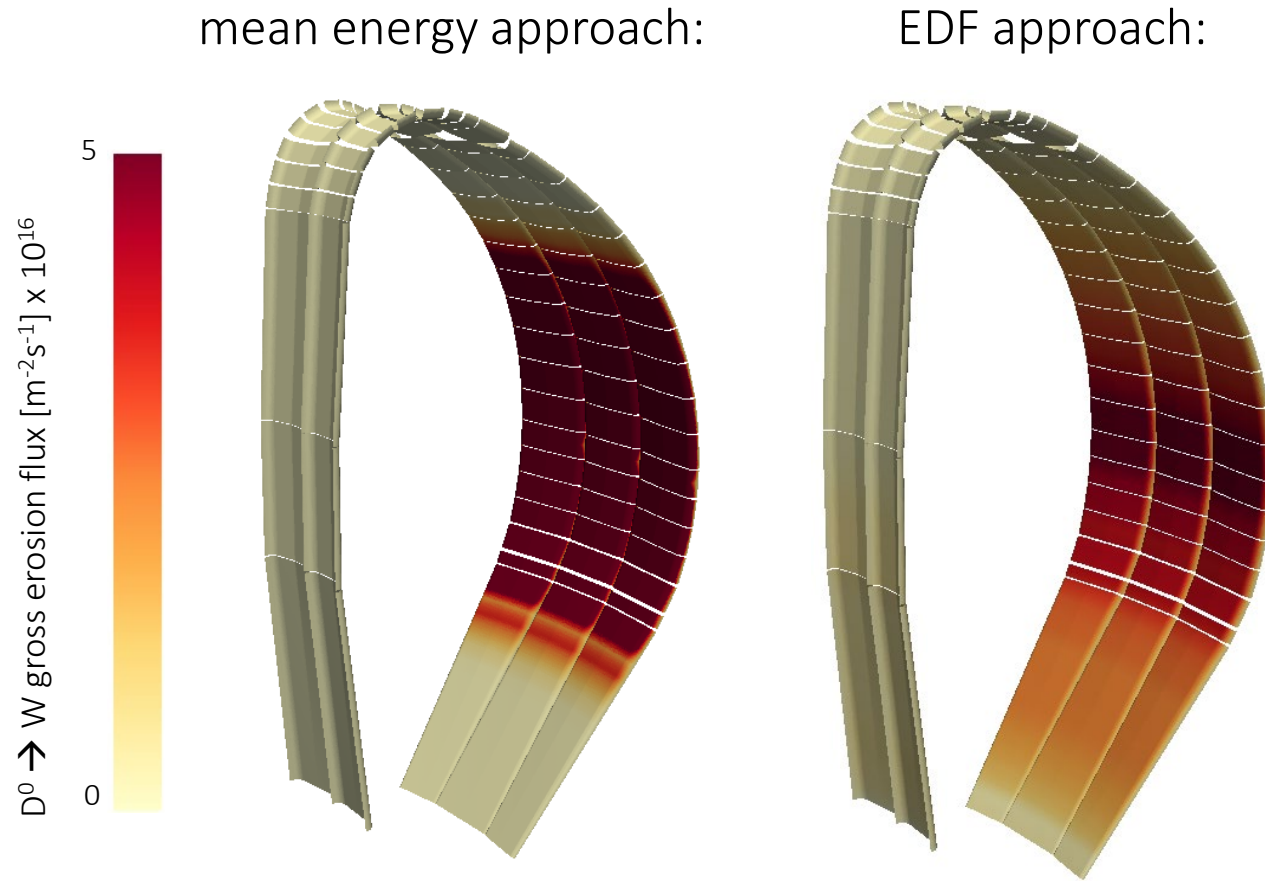


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ERO2.0 modelling: erosion and deposition mapping



Dominating role of charge-exchange (CX) fluxes on erosion in the main chamber (cont'd)



	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}

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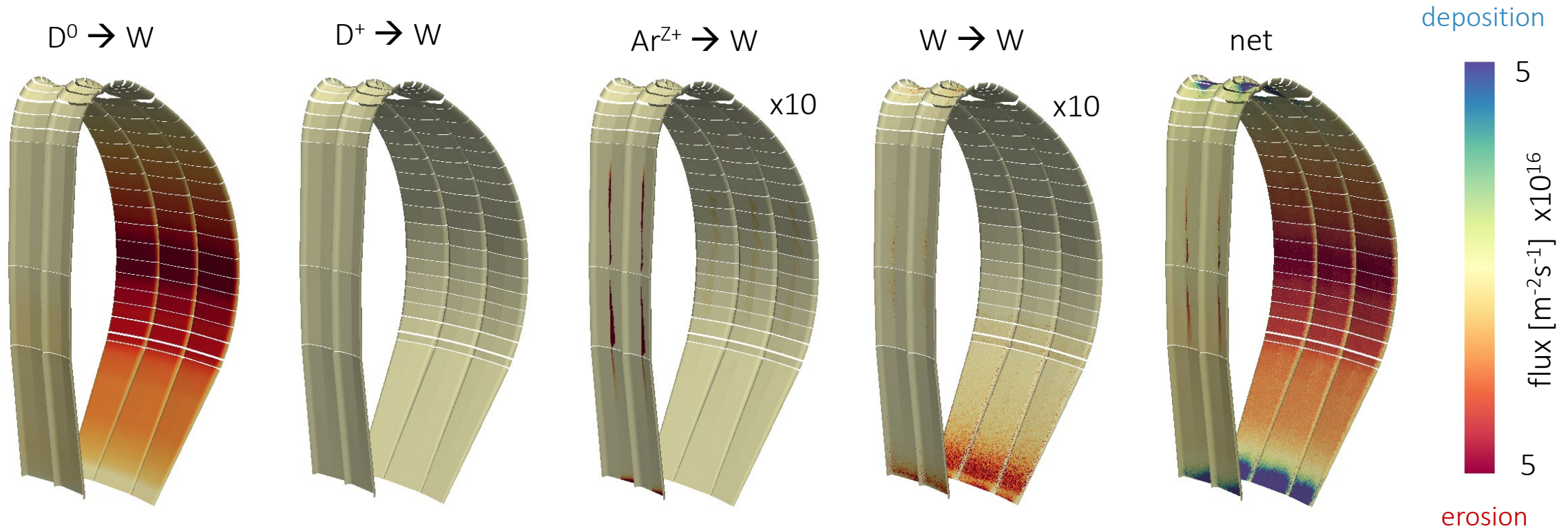
EDF approach:

- Reduction of main chamber gross erosion by factor 2-3 compared to the mean energy approach
- Additional wall area locations are subject to finite gross erosion



ERO2.0 modelling: erosion and deposition mapping

Erosion and re-deposition maps (T_e in far-SOL capped at 2 eV)



[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	0.0	57.8	28.9

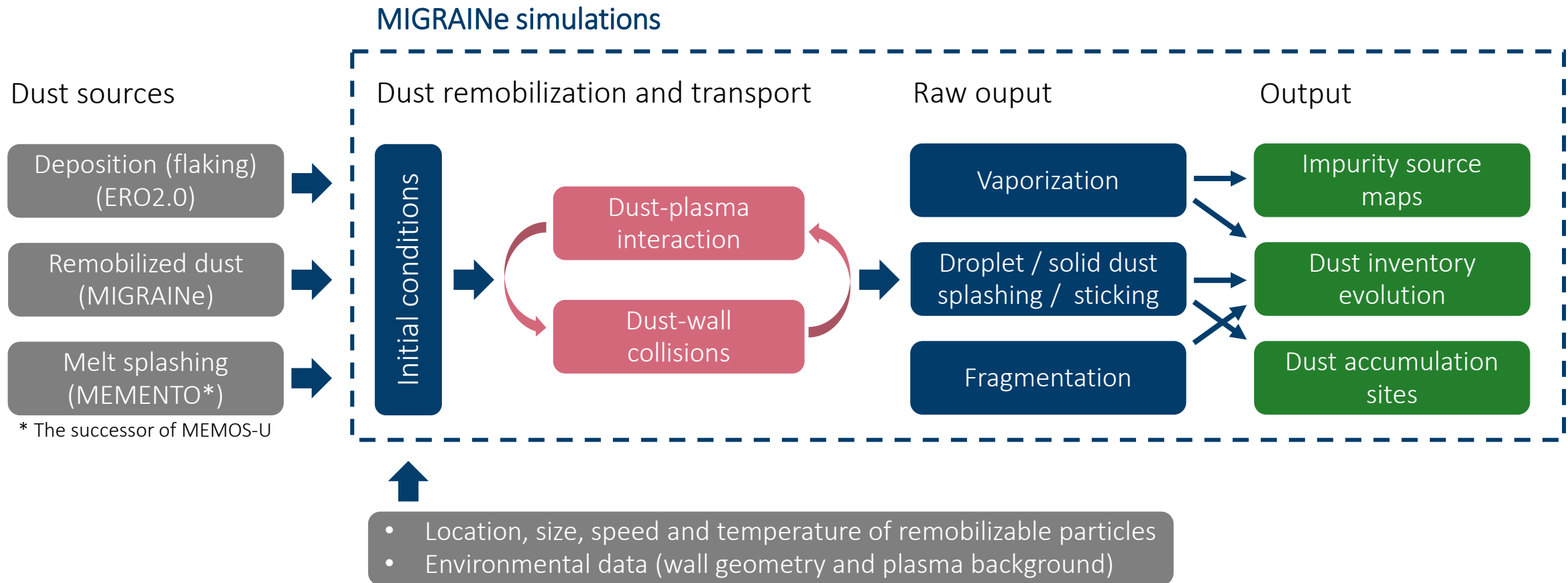
- Main chamber erosion dominated by CX neutrals
- Divertor erosion dominated by Ar ions and self-sputtering
- Strong transport from main chamber into the divertor (long ionization mean free path), no transport from the divertor
- Main deposition locations: inner and outer divertor, wall gap above outer divertor, top of the machine

Dust inventory evolution

Ratynskaia et al. Rev. Modern Plasma Phys. 6:20 (2022)



Metallic dust in fusion devices – safety and licensing issue (fuel retention, radioactivity, chemical reactivity)



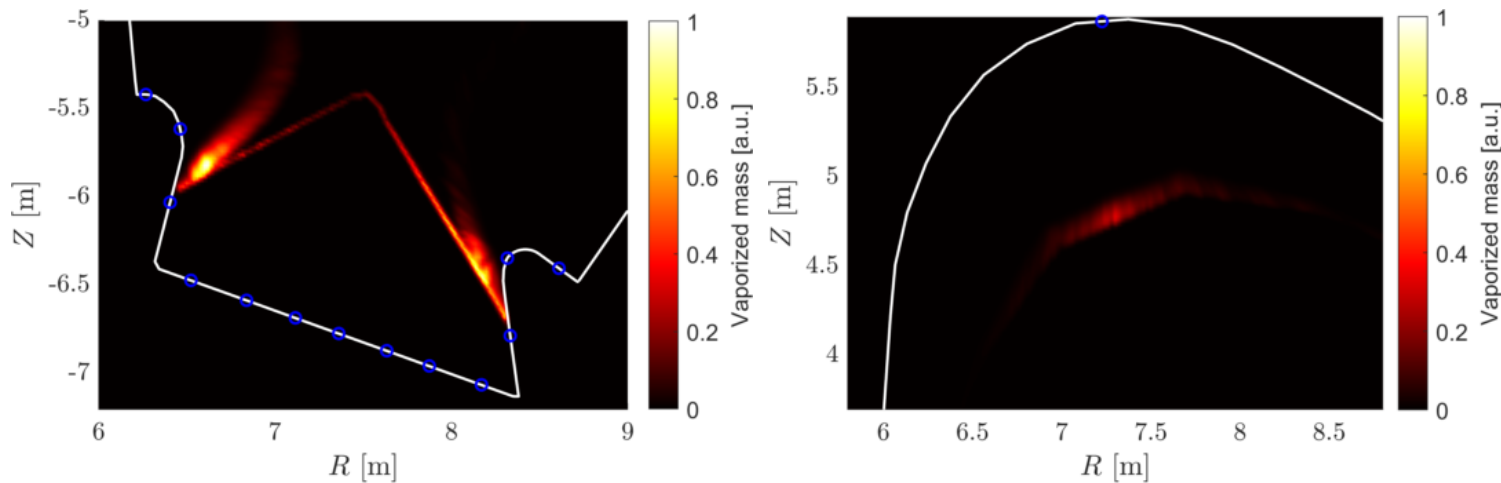


Dust inventory evolution

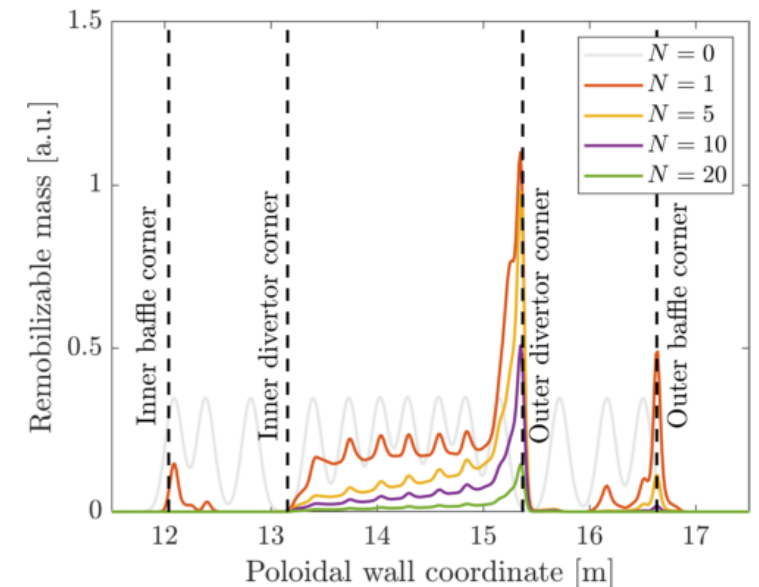
DEMO scenario and addressed questions © L. Vignitchouk

- Using baseline 2017 equilibrium with SOLPS-ITER plasma
- Tracing dust with pre-defined grain size distributions and speeds
- Injection sites in the divertor and at the top of machine (ERO2.0)
- Vaporization dominant for small grains (<25 μm) along separatrix
- Dust accumulates primarily in corner-like geometries

Maps for W vaporization (ion drag activated, $r = 10 \mu\text{m}$, $v_{\text{max}} = 10 \text{ m/s}$)



Evolution of dust spatial distribution in divertor (ion drag activated, $r = 40 \mu\text{m}$, $v_{\text{max}} = 50 \text{ m/s}$)



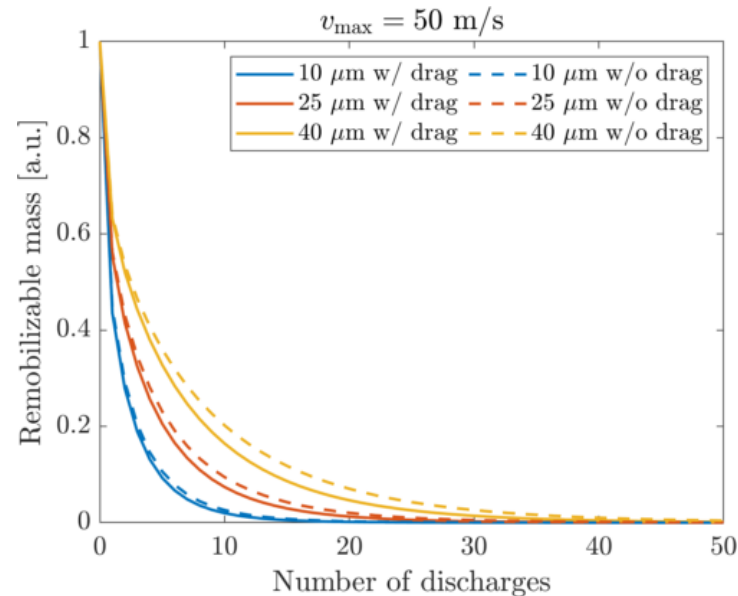
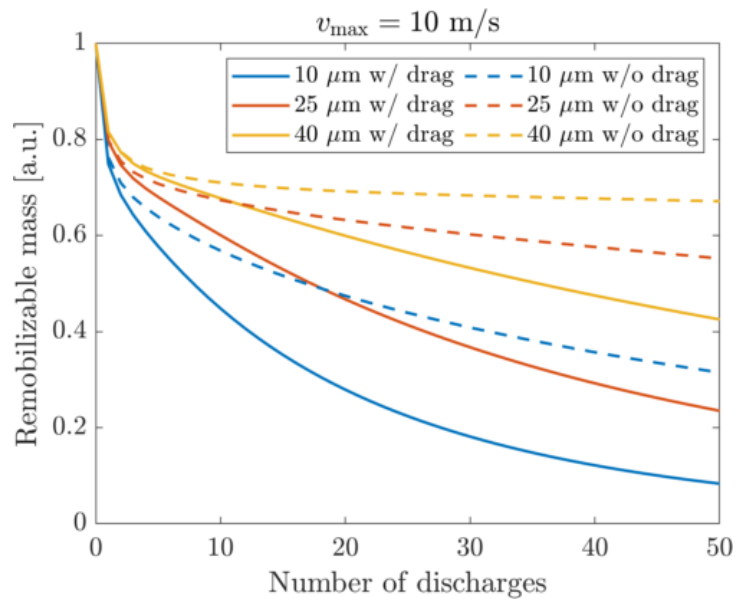


Dust inventory evolution

DEMO scenario and addressed questions © L. Vignitchouk

- Using baseline 2017 equilibrium with SOLPS-ITER plasma
- Tracing dust with pre-defined grain size distributions and speeds
- Injection sites in the divertor and at the top of machine (ERO2.0)
- Iteration of single-discharge results to predict long-term inventory
- Initial velocity has major impact on the survival of particles

Total in-vessel remobilizable dust mass evolution with and without ion drag for various initial dust size and velocity distributions





PFC response to transient events

MEMENTO (Metallic Melt Evolution in Next-step TOkamaks)

S. Ratynskaia et al. NME 52 (2022)

K. Paschalidis et al. NME (2023)

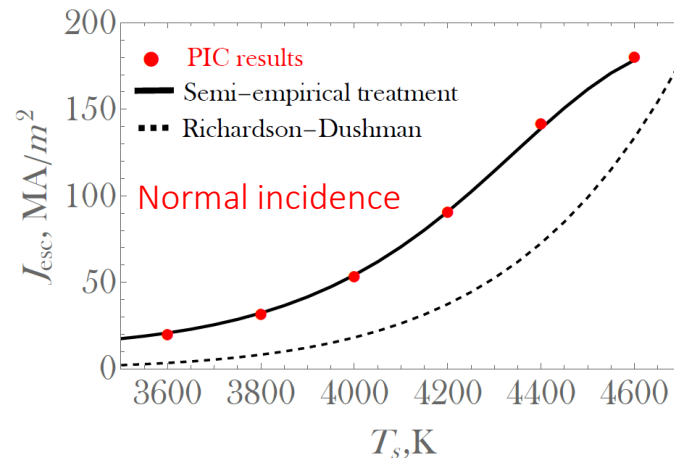
- Successor of MEMOS-U implemented using AMReX adaptive meshing framework (<https://amrex-codes.github.io/amrex/>)
- Coupled heat transfer, fluid dynamics and current propagation + physics updates (surface tension, dynamo term)
- Critical input:
 - heat loads and respective time scales (external input from WPDES & DCT)
 - description of escaping thermionic emission (multi-emissive* sheath treatment by SPICE2)

SPICE2 – a 2D3V PIC code (multi-emissive sheaths)

(*relevant for ITER/DEMO)

- Simulations of field-assisted thermionic emission (TE) with secondary electron emission (SEE) and electron backscattering (EBS) confirm the validity of the earlier developed semi-empirical scaling models [M. Komm et al. NF 60 \(2020\)](#)

[P. Tolias et al. NF 63 \(2023\)](#)



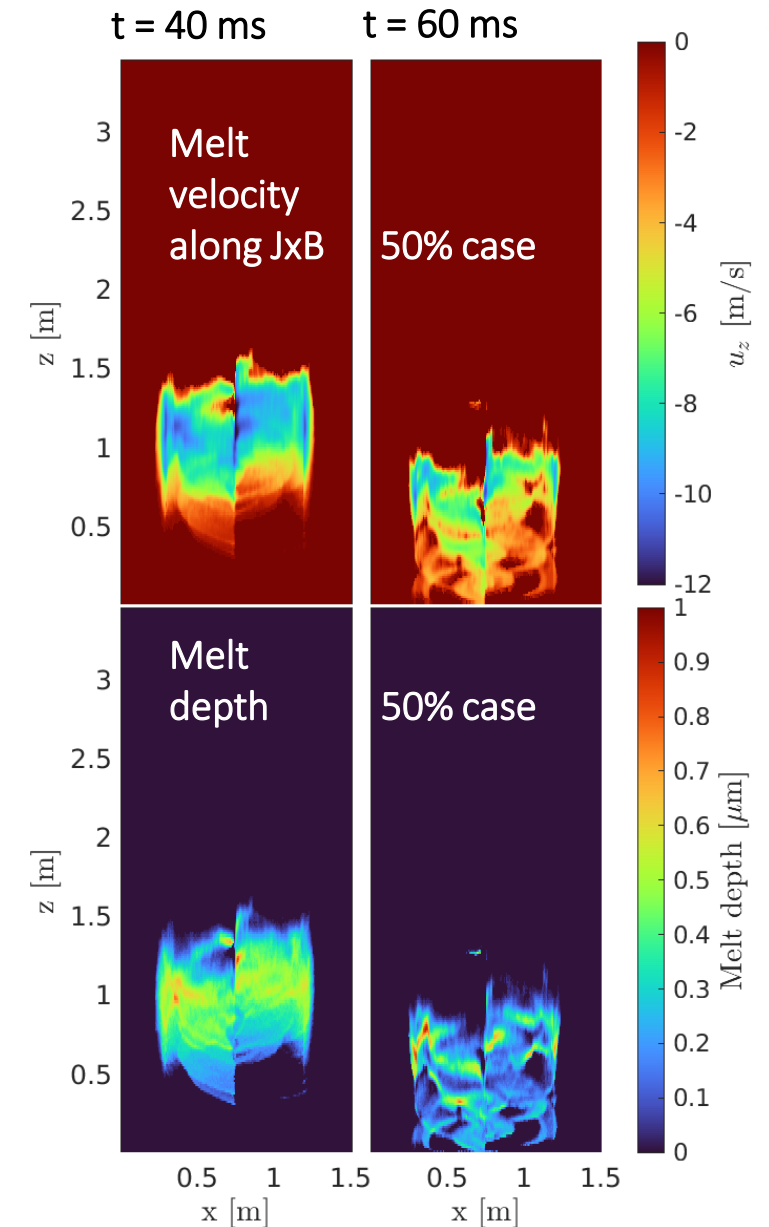
MEMENTO uses respective scalings deduced from PIC simulations

PFC response to transient events



Simulations of transient melting with MEMENTO

- Thermionic emission scaling laws provided by dedicated PIC simulations
- Addressing upper limiter damage under current quench with updated heat loads input accounting for time-dependent loading patterns
- Compared to 2023 PFCFlux input, ~ 10 times higher max heat flux values, up to 28 GW/m^2 (for 50% conversion from all poloidal magnetic energy)
- 10% conversion is judged as realistic, 50% as a worse case scenario
- No vapor shielding – melting is robust, but erosion damage is not
- Escaping thermionic emission is within ~ 2 to 3 MA/m^2 in both 10% and 50% scenarios, dominating over the halo current (Lorentz force)
- Instantaneous melt pools up to 0.3 - 0.5 mm depth
→ prone to splashing

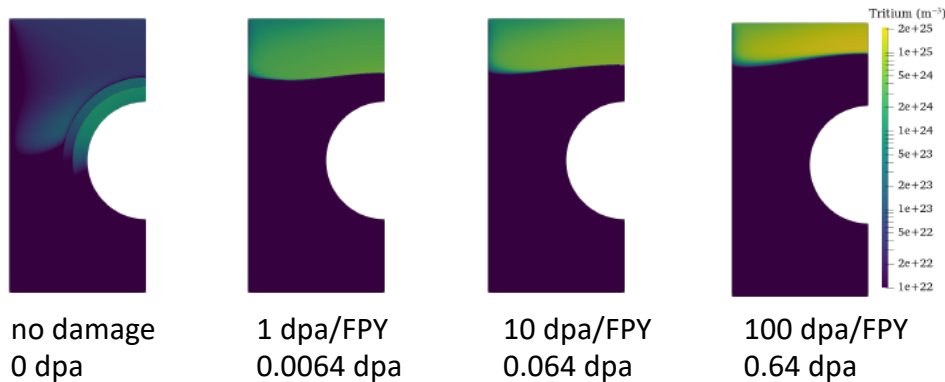




Fuel retention and permeation

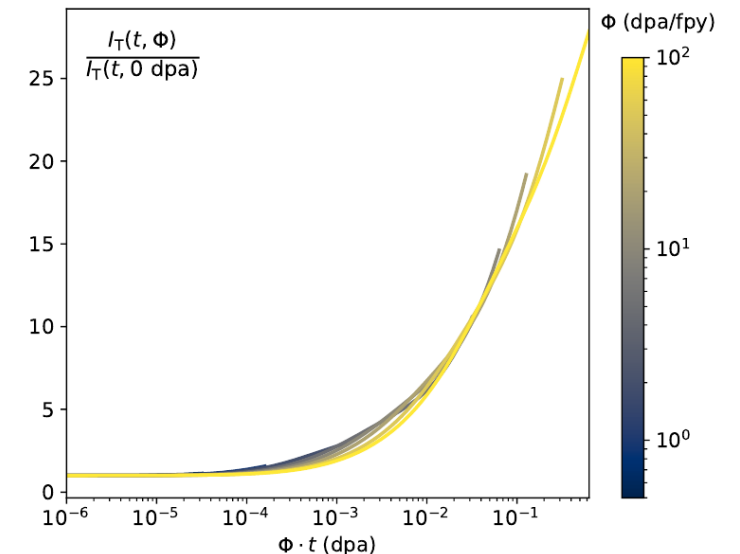
Tritium retention and permeation with TESSIM and FESTIM

- First wall retention and permeation, in particular in view of tritium self-sufficiency (TESSIM-X):
[K. Schmid et al, Nucl. Fusion 64 \(2024\) 076056](#)
- Implementation of the Soret effect: reduces T inventory and time to steady-state retention
- 3D effects (monoblocks): [R. Delaporte et al, Nucl. Fusion 64 \(2024\) 026003](#)
 - Outgassing at sides reduces retention (stronger for thin monoblocks)
 - Surface limited recombination reduces the efficiency of baking
- Neutron-induced traps: [J. Dark et al, Nucl. Fusion 64 \(2024\) 086026](#)
 - Increase retention / reduce permeation by orders of magnitude



T retention field
after 200,000 s
of plasma exposure
for different neutron fluxes
using FESTIM code
with neutron damage model

Ratio of T inventory with and without
n-damage using FESTIM code





ACH support

- ERO2.0: optimization of hybrid parallelization performance and GPU enabling (ACH BSC)
- SPICE2: parallelization of Poisson solver in 2D (ACH BSC)
- MIGRAINE: HPC enabling via MPI parallelization (ACH VTT)
- RAVETIME: HPC optimization (ACH VTT)
- MEMENTO: HPC optimization (ACH VTT)
- IMASification: ERO2.0, MIGRAIN (ACH PSNC)

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- ACH PSNC: Dmytro Yadykin, Grzegorz Pelka, Natalia Grzybicka



Outlook and perspectives

Capitalize on dedicated experiments under WPTE: focused validation effort

✓ to advance through collaboration with WPTE

- Validation of steady state erosion in full W device with relevant divertor geometry and impurity seeding: ERO2.0 in AUG (approved)
- Validation of dust evaporation and impurity deposition: MIGRAINE + ERO2.0 in AUG (possible within AUG internal program)
- Validation of thermo-mechanical response of W PFCs under runaway electrons (REs): GEANT4 + MEMENTO in AUG (approved)

Address the frontier problem of PFCs damage by REs created during disruptions

✓ to advance through collaboration with TSVV9

- High sensitivity of PFCs response to REs impact characteristics – can be obtained from nonlinear MHD codes such as JOREK
- Explosive W PFCs response under REs: GEANT4 (energy deposition) + MEMENTO (heat transfer) + LSDYNA (flow, fragmentation)

Expand the codes with reactor-relevant physics beyond the initial project scope

✓ to advance through collaboration with WPPWIE

- Effect of multiple isotopes on erosion and fuel retention/permeation for predictive simulations of reactor start-up and T clean-up
- Elaborating the neutron damage model from phenomenology to physics
- ERO2.0 coupling to core transport codes; edge turbulent transport effects on PWI

✓ to advance through collaboration with TSVV4&6

Towards DEMO and beyond

✓ to advance through collaboration with WP-DES (plasma backgrounds with AI)

- Framework test applications (VNS, DTT, BEST, ...) and development of surrogate models for iterative design-cycle applications



Thank you for your attention!