

“THEORY, SIMULATION, VERIFICATION AND VALIDATION”

TSVV TASK 7: PLASMA-WALL INTERACTION IN DEMO

EUROfusion Science Meeting - TSVV Final Reports (2021-2025) | 28.01.2026

D. Matveev on behalf of TSVV-7 team



Acknowledgements



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DEMO Central Team: Sven Wiesen, Fabio Subba, Jonathan Gerardin, Francesco Maviglia

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

Project overview papers

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

+ Presented at IAEA FEC 2025, Chengdu, China

Design-specific geometry, plasma background, transient loads

Global PWI *
in steady-state
wall erosion, impurity
transport & deposition,
dust inventory evolution

Fuel retention
and permeation
implantation,
neutron damage,
co-deposition

Local PWI **
in transients
melting,
melt motion,
droplet splashing

DEMO-relevant material erosion and plasma sheath physics








Framework optimization and integration for advanced computing

* incl. complementary projects on improvement of DEMO-relevant PWI data, divertor sheath physics and related code capabilities

** incl. dedicated PIC studies regarding thermionic emission



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

OUTLINE

- Modelling of W erosion, transport and re-deposition
 - DEMO-relevant sheath physics and PWI data
 - Wall erosion sources
 - Dust transport and inventory evolution
 - Dust ablation sources
- Fuel retention analysis
- PFC Response to transient events
 - Scaling laws for thermionic emission currents
 - Melting simulations under VDE loads
- Summary & Outlook

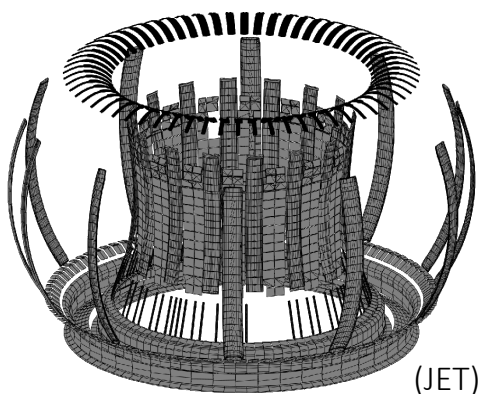
OUTLINE

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INPUT DATA FOR PWI MODELLING WITH ERO2.0

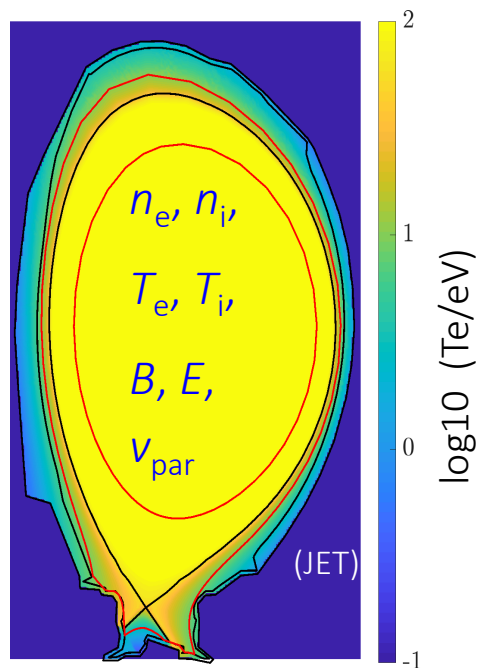
device & scenario specific

wall geometry
and materials



from technical drawings

plasma and neutrals
background

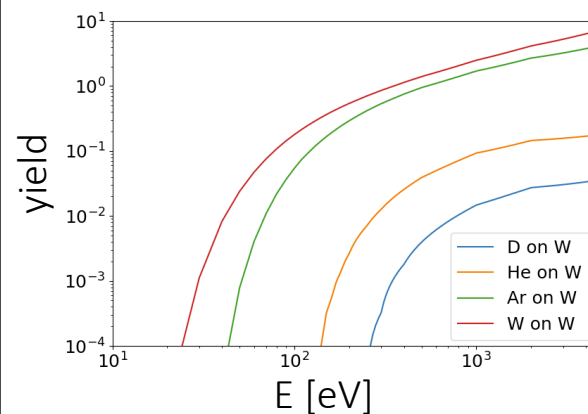


SOLPS, EMC3-EIRENE,
SOLEDGE-EIRENE, OEDGE

- + magnetic equilibrium / shadowing
- + energy / angular resolved fluxes

fundamental

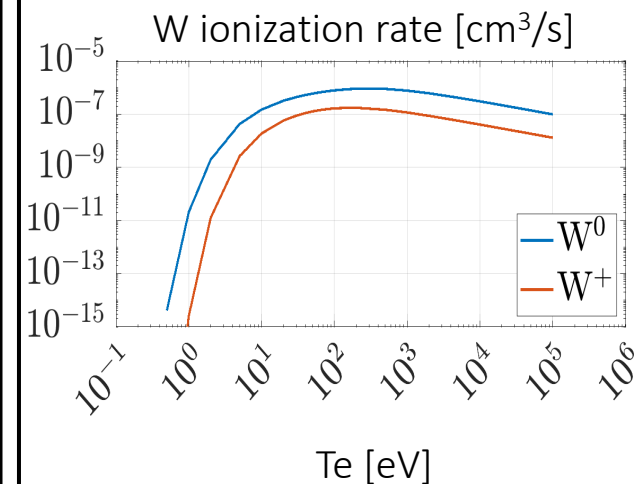
sputtering yields
reflection coefficients



SDTrimSP, Molecular Dynamics

ideally, with known surface
composition dependencies

atomic & molecular data



ADAS, GKU, ATOM

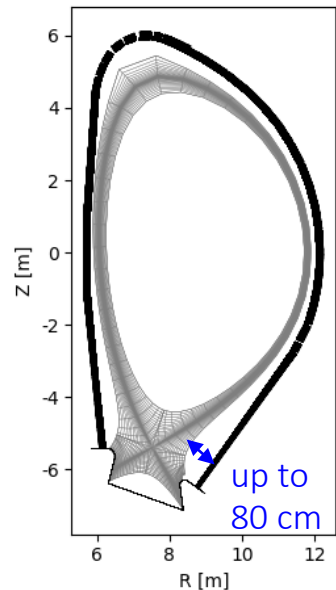
ERO2.0 MODELLING OF W EROSION, TRANSPORT AND RE-DEPOSITION



Addressing challenges of PWI modeling for DEMO

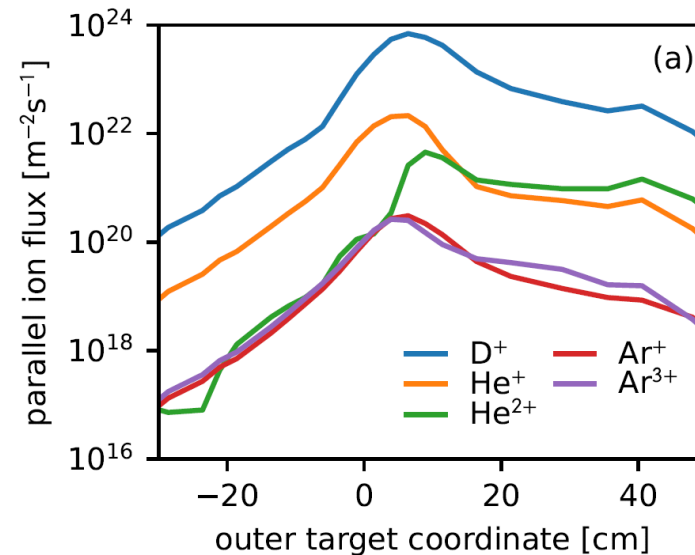
SOLPS-ITER solution:
F. Subba NF 61 (2021) 106013

Large plasma-wall gap
(narrow-grid SOLPS)



(baseline 2017)

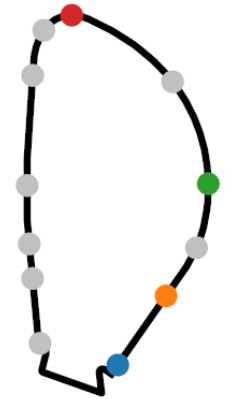
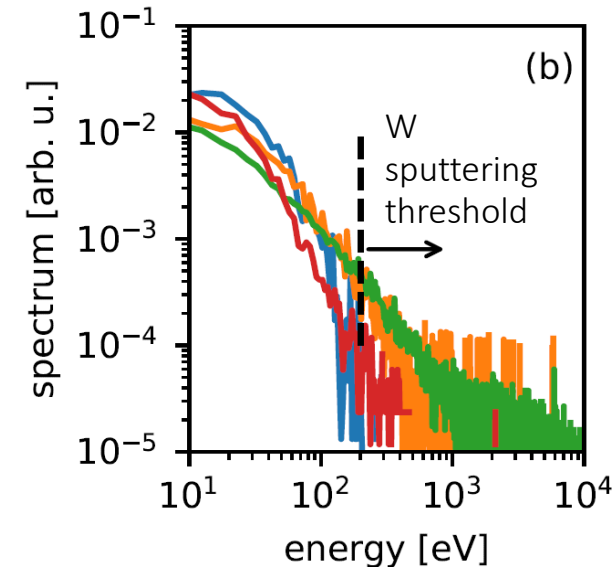
Charge-state resolved
impurity fluxes to the wall



consistent extrapolation in
pre-processing pipeline,
change to field-aligned grid

common ion sound speed for all
background species, in agreement
with SOLPS-ITER modelling

Energy and angular resolved
fluxes of charge-exchange neutrals (CXN)



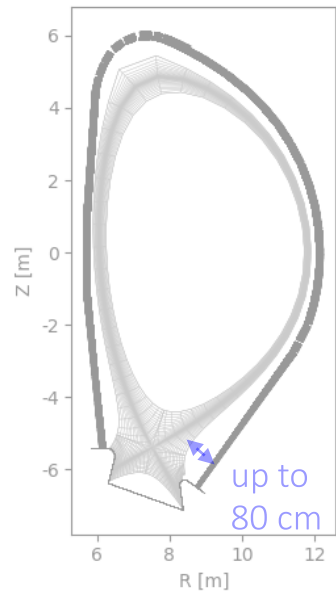
bivariate distributions from additional
standalone EIRENE simulations with
extended output

ERO2.0 MODELLING OF W EROSION, TRANSPORT AND RE-DEPOSITION

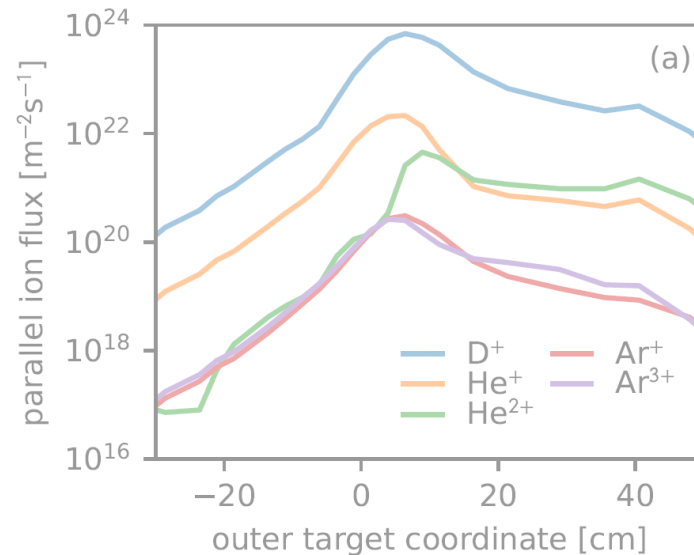


Addressing challenges of PWI modeling for DEMO

Large plasma
extrapolation volume

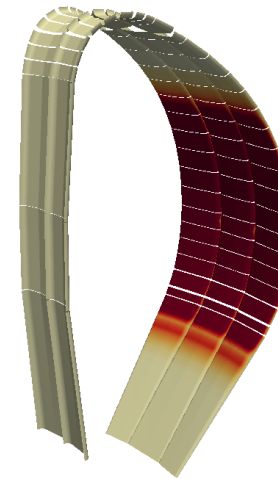


Charge-state resolved
impurity fluxes to the wall

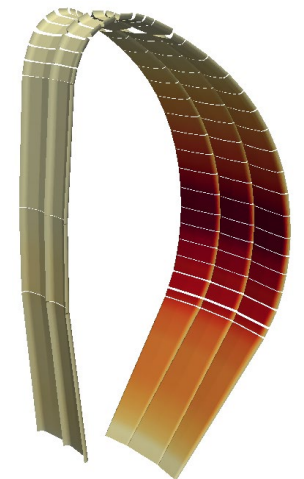


Energy and angular resolved
fluxes of charge-exchange neutrals (CXN)

mean energy



energy distribution



consistent extrapolation in
pre-processing pipeline,
change to field-aligned grid

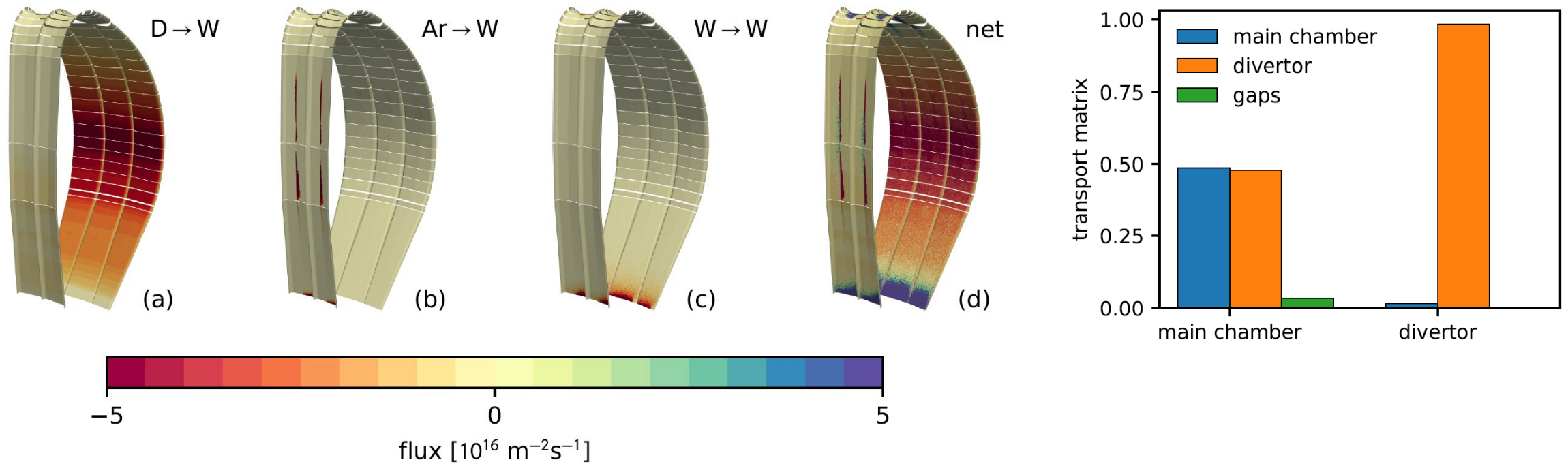
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ERO2.0 MODELLING OF W EROSION, TRANSPORT AND RE-DEPOSITION

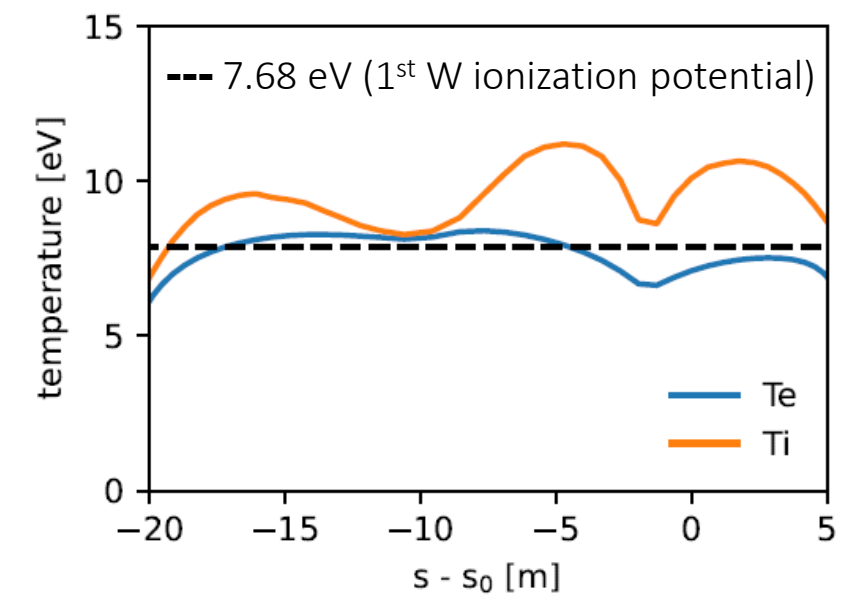


Example of resulting erosion-deposition maps by species (for T_e cut-off at 2 eV in the far-SOL)





Role of far-SOL extrapolation assumptions (T_e cut-off: 2 eV / 5 eV / last plasma grid value)



2 eV

5 eV

const

[10 ¹⁸ atoms/s]	net	gross	D → W	Ar → W	W → W
main chamber	-12.85	31.43	27.58	2.01	1.84
divertor	11.69	318.56	-	248.59	69.96

[10 ¹⁸ atoms/s]	net	gross	D → W	Ar → W	W → W
main chamber	-24.70	63.17	27.58	25.64	9.96
divertor	21.13	341.21	-	253.93	87.27

[10 ¹⁸ atoms/s]	net	gross	D → W	Ar → W	W → W
main chamber	-43.44	122.64	27.58	65.84	29.22
divertor	36.41	382.22	-	263.76	118.45

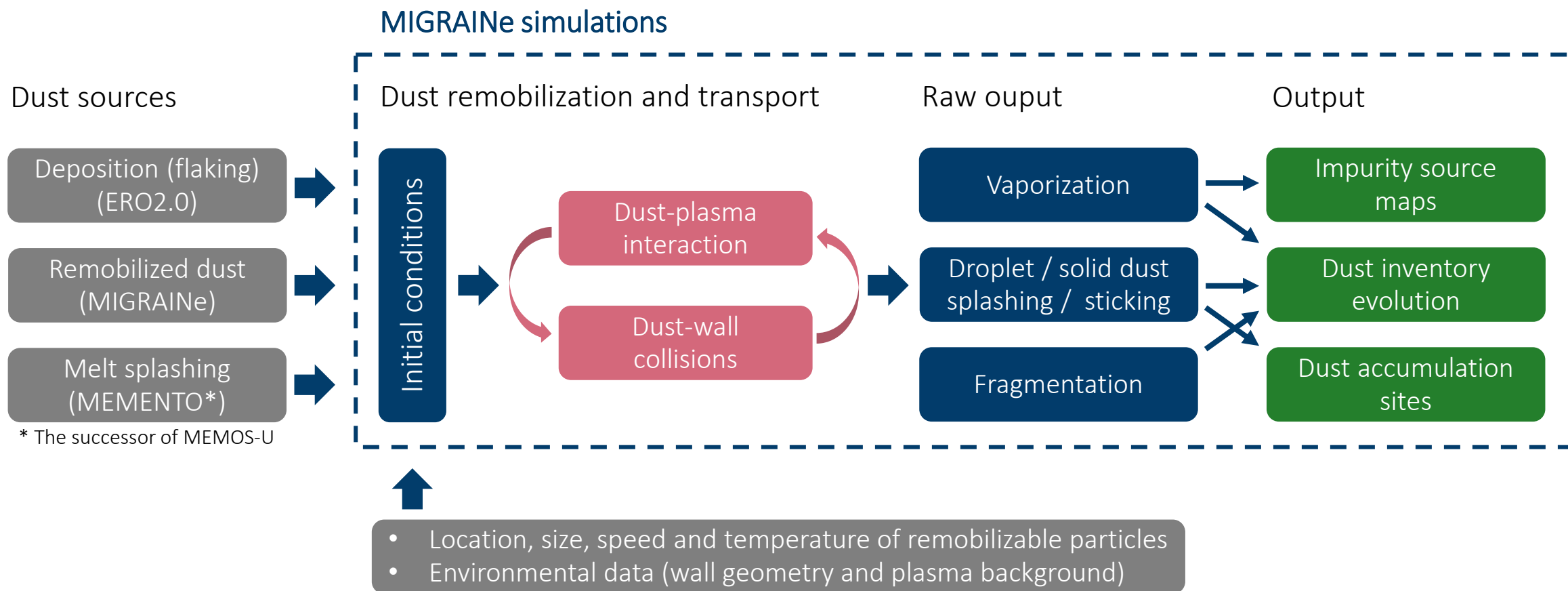
Increase of erosion by ions in the main chamber and re-deposition in the divertor

MIGRAINE MODELLING OF DUST TRANSPORT AND INVENTORY EVOLUTION



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

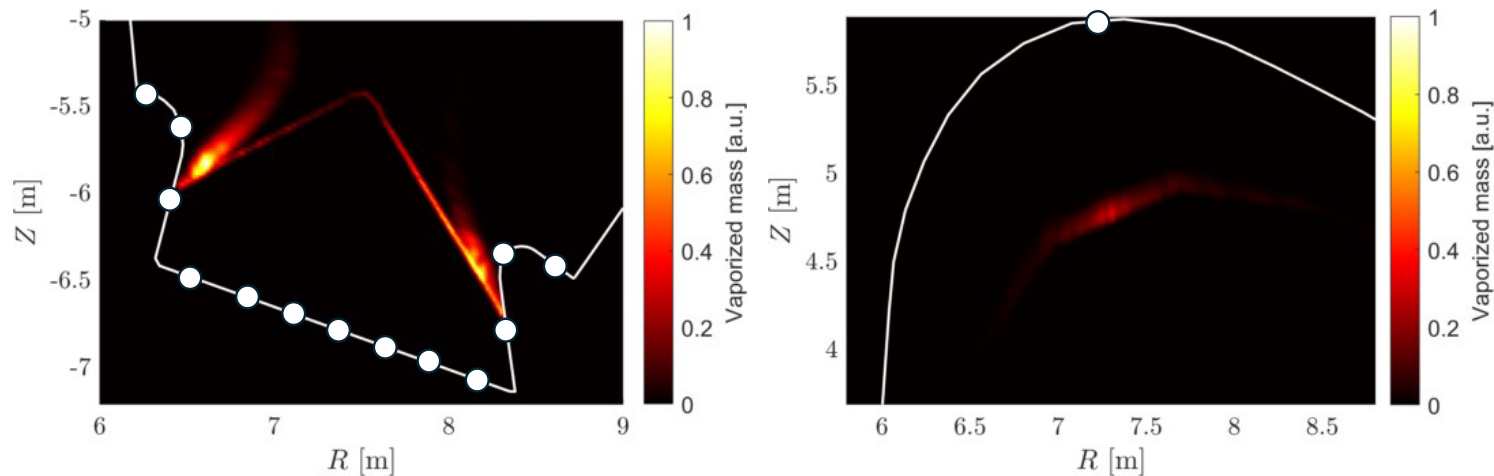
Metallic dust in fusion devices – safety and licensing issue (fuel retention, radioactivity, chemical reactivity)



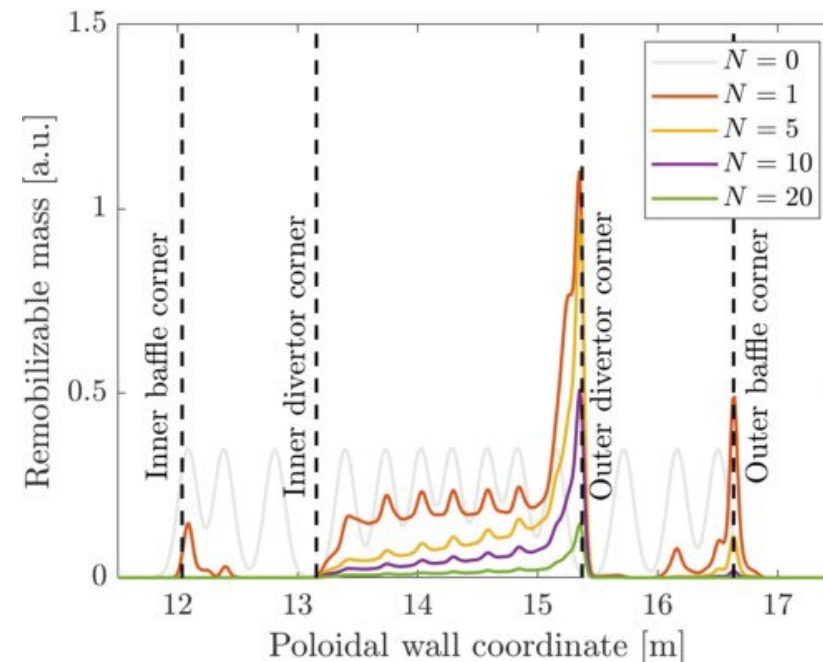
MIGRAINE MODELLING OF DUST TRANSPORT AND INVENTORY EVOLUTION



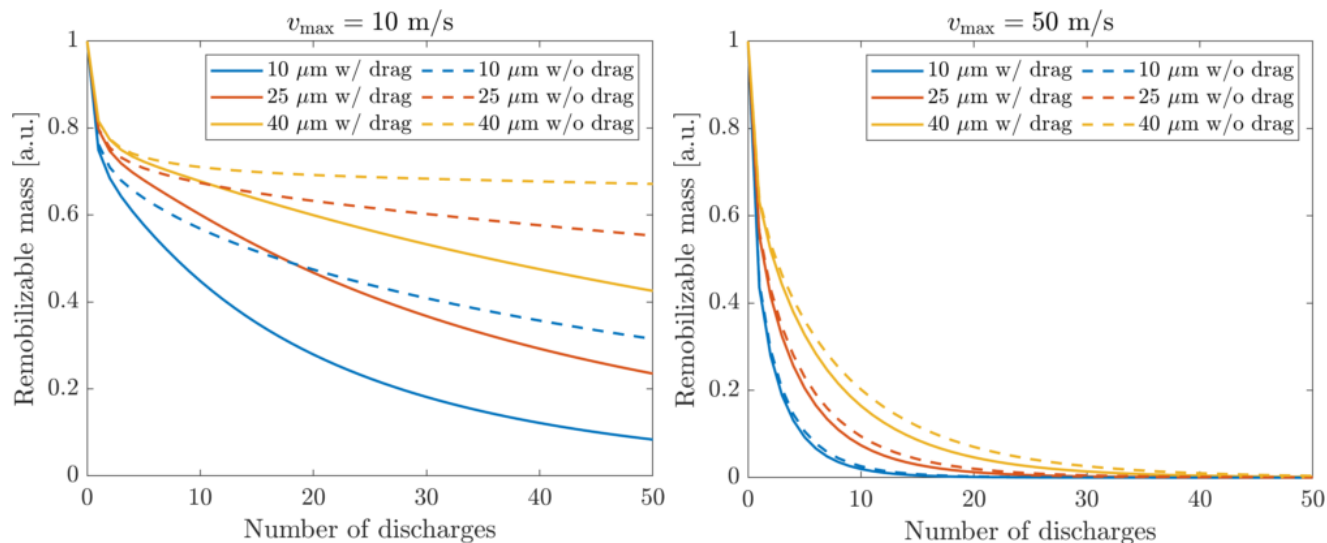
Dust starting locations and evaporation maps



Dust redistribution



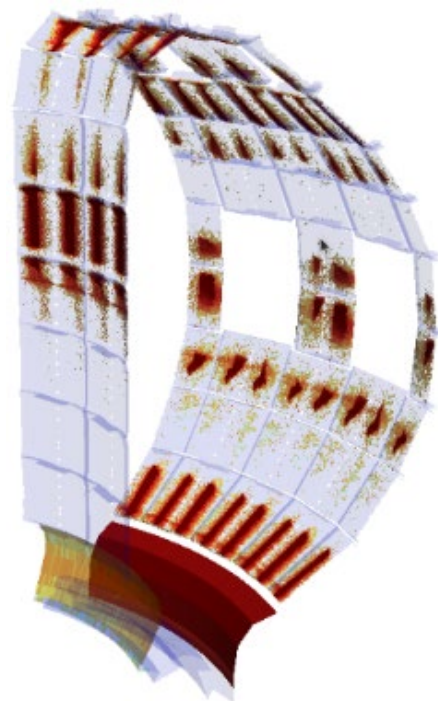
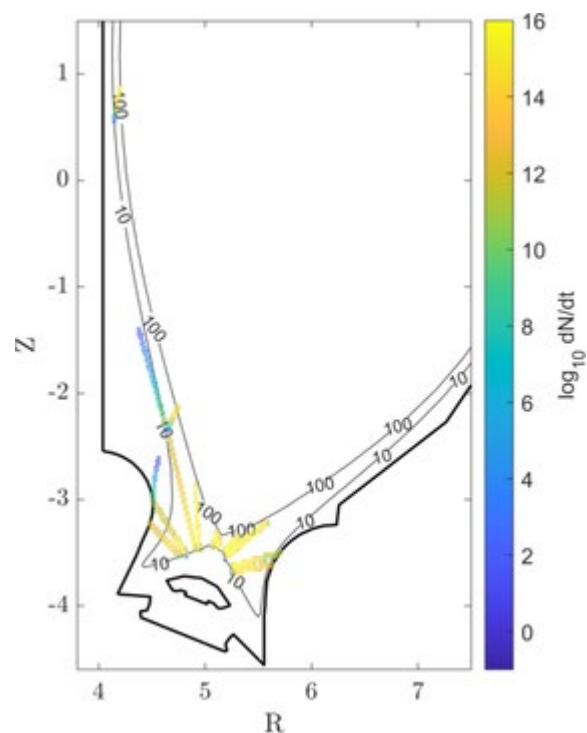
Dust inventory evolution



MIGRAINE to ERO2.0 DATA EXCHANGE FRAMEWORK



Dust evaporation maps via IMAS – ITER as setup for testing (same geometry and plasma solution via IMAS)



Wall source



Dust source



Gross tungsten deposition fluxes in full-W ITER for wall erosion source (left) dust ablation source (right) shown for a 40-degree sector centred around the dust injection location (from the divertor)

W dust re-mobilization source in the divertor → atomic W source due to dust ablation
→ impurity tracing in plasma → gross deposition (the shown case does not account for reflection and re-erosion)

EXTRA: DEMO-RELEVANT PLASMA SHEATH PHYSICS



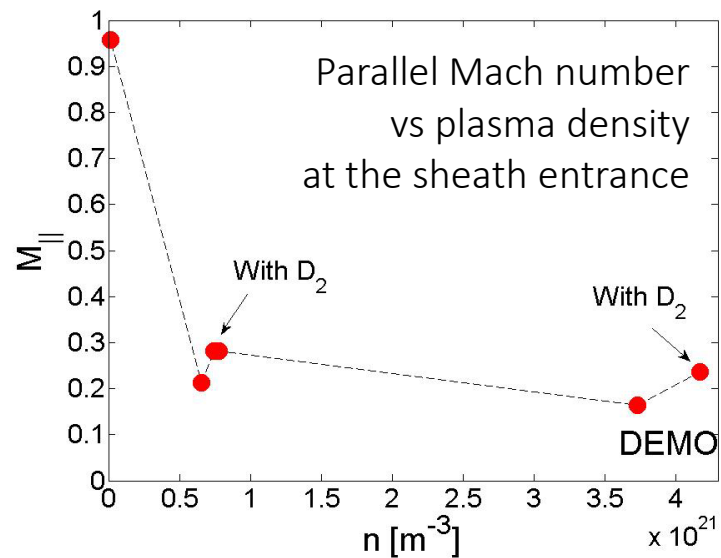
High density divertor sheath physics addressed by PIC modelling with BIT1 (collisionality, A&M processes)

D. Tskhakaya,
EPS 2021

	Divertor sheath	
	n_{\max} [10^{20} m^{-3}]	T_{\min} [eV]
COMPASS	0.3	10
ASDEX-U	2	1
JET	5	1
ITER	50	0.3
EU DEMO	~100	0.2 (?)

- Redistribution of heat loads to neutrals, modification of ion and neutral distribution functions \rightarrow energies and angles of wall impact
- Parallel Mach number at sheath entrance can be incompatible with standard boundary conditions of edge plasma simulations, e.g. SOLPS
- W prompt re-deposition is reduced \rightarrow D⁺-W CX need and multi-step ionization need to be included for accurate estimates

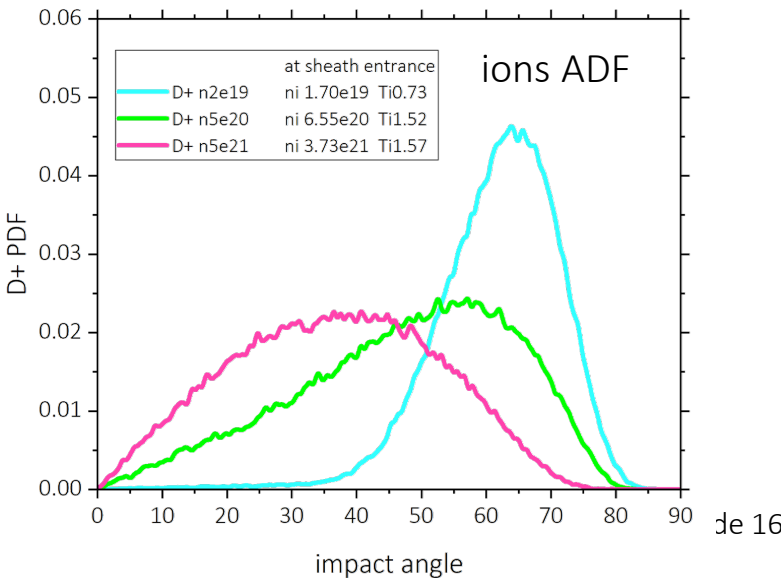
D. Tskhakaya, PSI-26, Marceille 2024



← boundary conditions
for edge plasma simulations
($M_{||} < 1$)

angular distributions of ions
acquire the shape similar
to that of neutrals \rightarrow

Exemplary characteristics of high density divertor sheath, such as ion and neutral EDF and ADF are available for utilization in ERO2.0



EXTRA: DEMO-RELEVANT PLASMA SHEATH PHYSICS

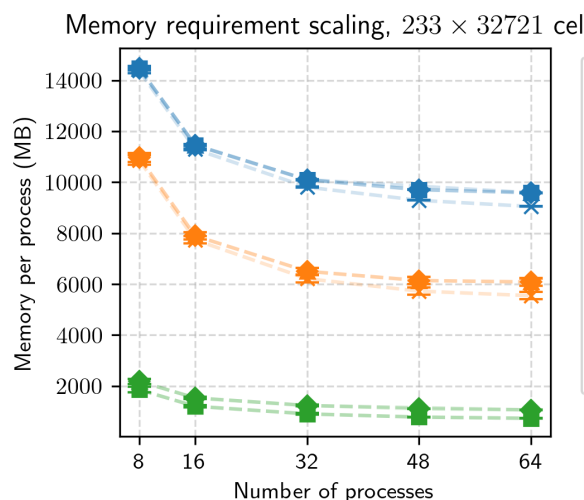


2D Particle-in-Cell simulations (e.g. castellated tiles)

2024: SPICE2 nonuniform injection scheme (2D PIC) routinely applicable;
memory optimization was found to be **extremely important** for DEMO-scale

Code updates finalized

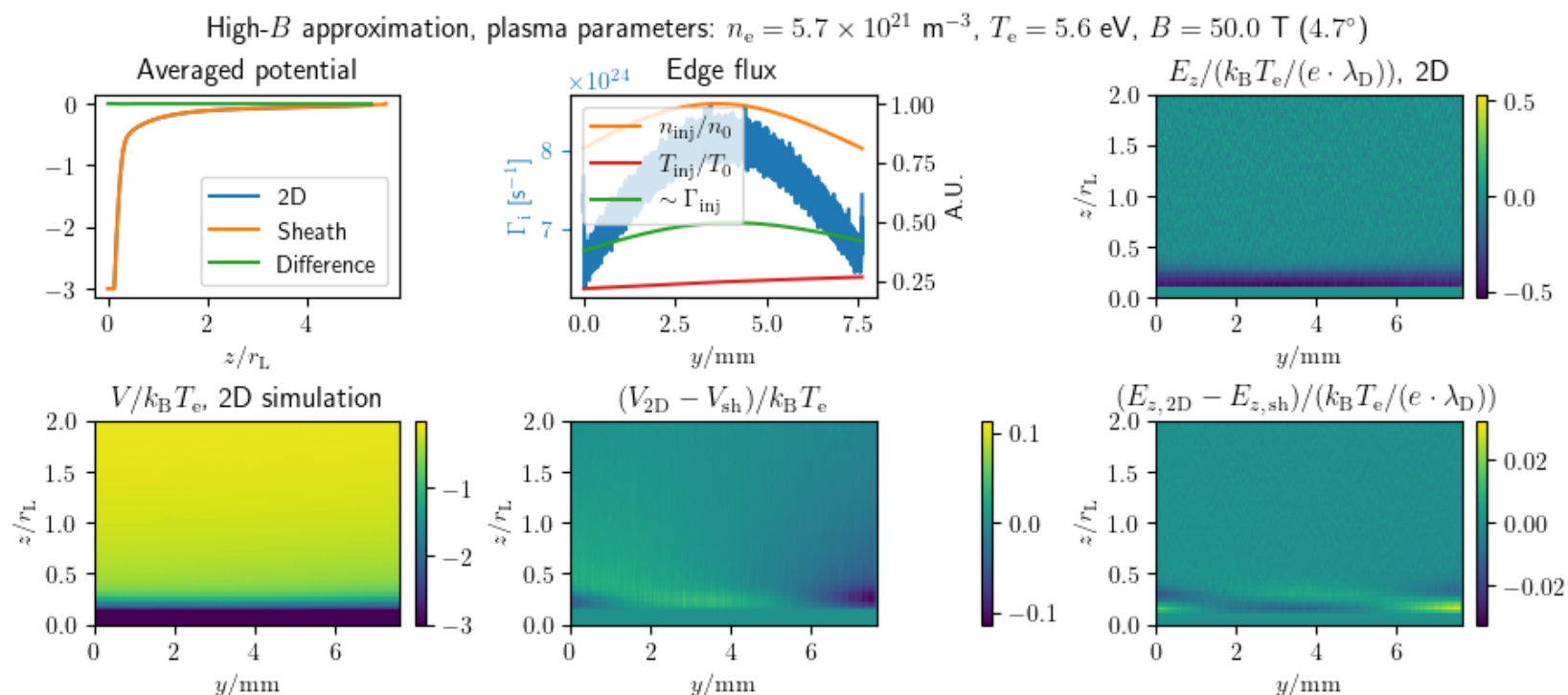
Memory footprint reduction $\sim 10\times$
(new, before update, intermediate)



Summary: Scalability substantially improved, reducing time req. 2-5x.
Down to \sim month per simulation.

Simulations performed with strikepoint-like plasma

Increased electric field at the strike-point location observed



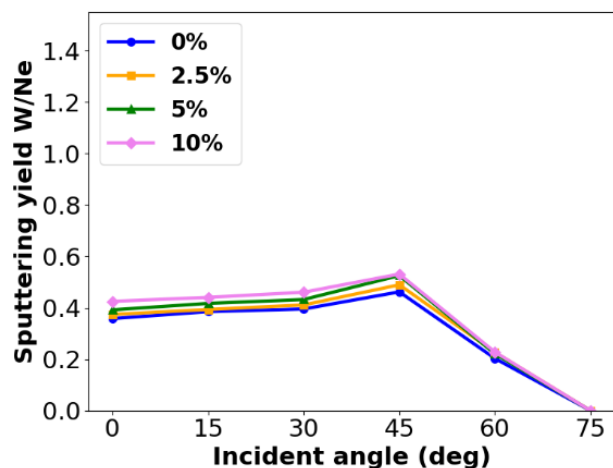
EXTRA: DEMO-RELEVANT PWI DATA



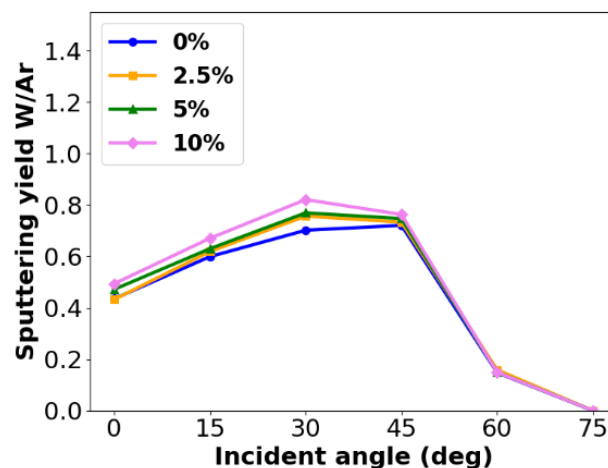
Sputtering of D-decorated W surfaces

F. Kporha, JNM 613 (2025) 155856

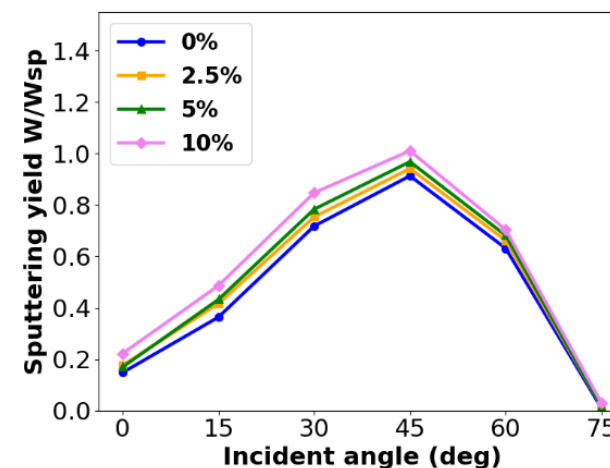
Example: 200 eV impact on W(100) surface



(a) Ne



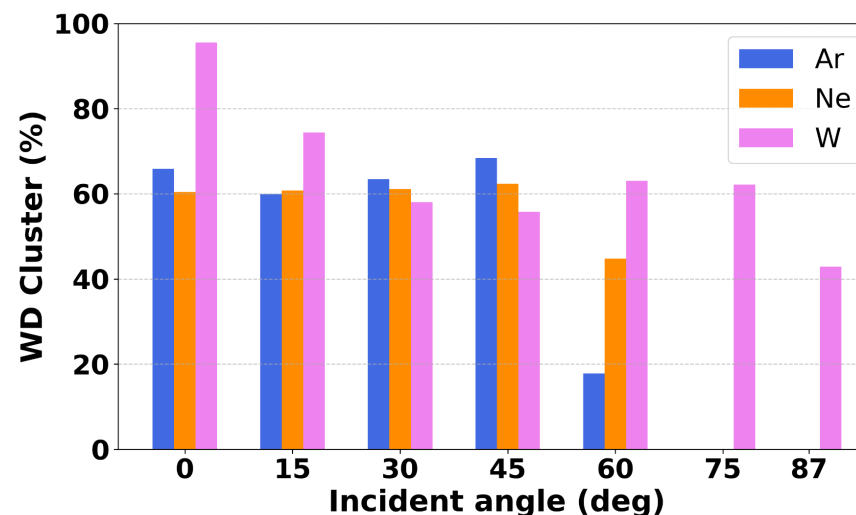
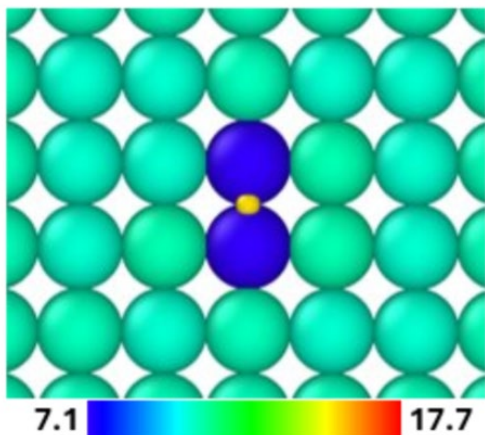
(b) Ar



(c) W_{sp}

+ developed interatomic potential for W-O-H system

Energy required for sputtering (eV)



Average percentage of WD clusters relative to the total number of W leaving the surface for 10at-% D and 100 eV impact (average over 4 surface orientations)

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FUEL RETENTION ANALYSIS



Questions and codes

- First wall retention and permeation in view of tritium self-sufficiency (TESSIM-X)
- Retention in divertor monoblocks and permeation to coolant (MHIMS, FESTIM)
- High throughput simulations, physically informed NN, UQ (RAVETIME)

Highlights of code development and verification

- Soret effect implemented in TESSIM-X and FESTIM
- Material interface model implemented and validated in FESTIM
- Empirical n-damage creation/annealing model implemented in FESTIM
- He retention model (He bubbles) using FenicsX framework
- Capabilities of 2D and 3D simulations (monoblock geometry)

R. Delaporte et al, Nucl. Fusion 61 (2021) 126001

E. Hodille et al, Nucl. Fusion 61 (2021) 126003

R. Delaporte et al, Nucl. Fusion 64 (2024) 026003

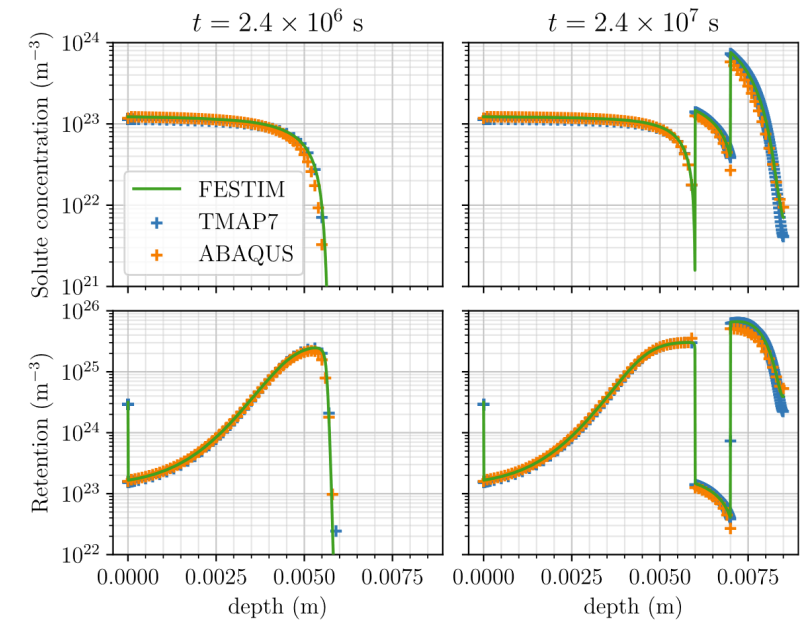
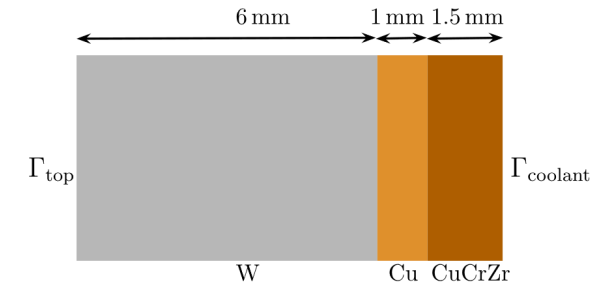
J. Dark et al, Nucl. Fusion 64 (2024) 086026

K. Schmid et al, Nucl. Fusion 64 (2024) 076056

K. Schmid et al, Nucl. Fusion 65 (2025) 026039

E. Hodille et al, Int.J. H Energy 205 (2026) 153245

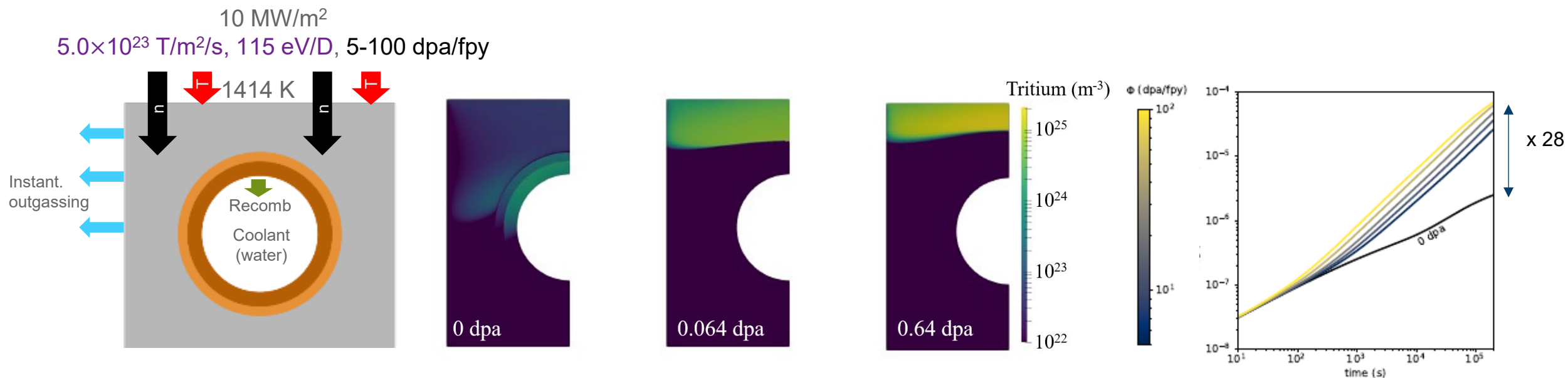
T self-sufficiency assessment



FUEL RETENTION ANALYSIS WITH FESTIM



2D modelling of n-damaged divertor monoblock



Includes trap creation/annealing model by J. Dark et al, NF 64 (2024)

Tritium retention field after 200,000 s of plasma exposure for different neutron fluxes (damage rates) compared to undamaged case (0 dpa): resulting damage up to 0.064 dpa (10 dpa/EFY), and 0.64 dpa (100 dpa/EFY)

Ratio of T inventory with and without n-damage

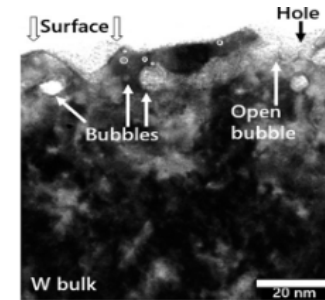
FUEL RETENTION ANALYSIS WITH FESTIM/FENICS



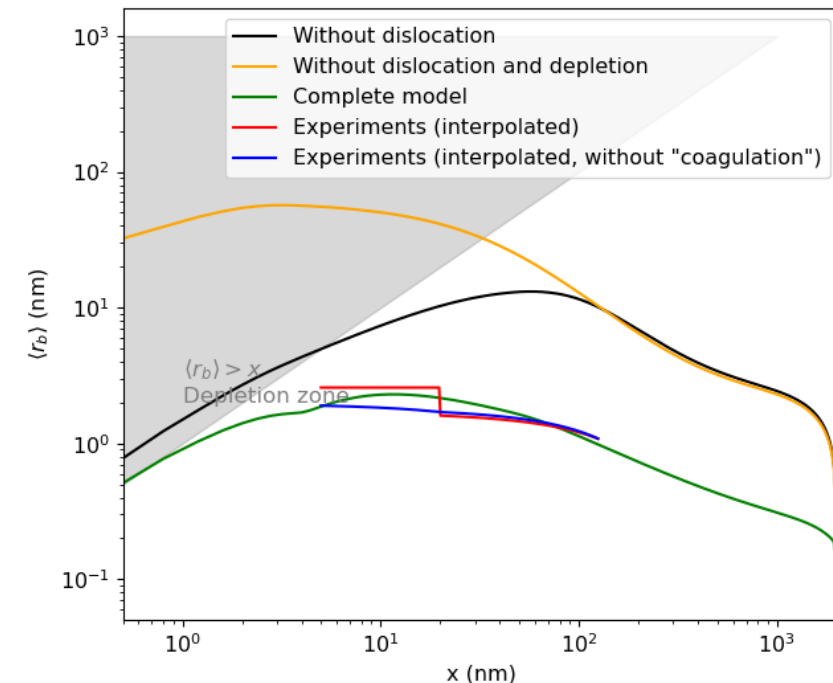
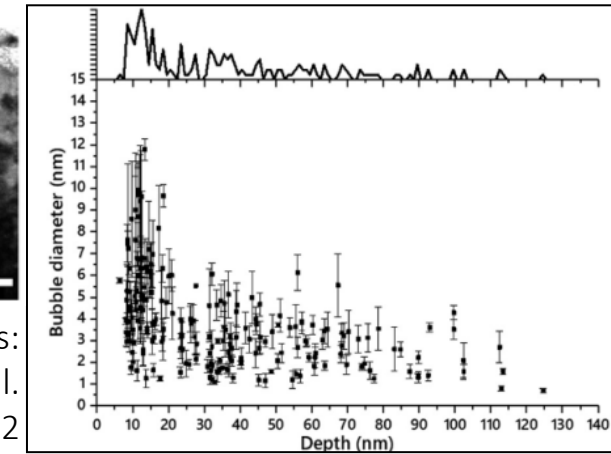
He clustering model including dislocations

Simulations done with an extended model from Delaporte-Mathurin, Scientific Reports 11 (2021) and solved with FenicsX

- Model includes now dislocations and pre-existing vacancies as source of trapping and nucleation of He bubbles
- Coagulation and bubble migration are being developed
- Paper submitted to Journal of Physics D: Applied Physics comparison to experimental data including the temporal evolution of porosity



Experiments:
Ialovega et al.
NF 62 (2022) 126022



TRAP EQUATIONS WITH PHYSICS-INFORMED NEURAL NETWORKS (PINNS)

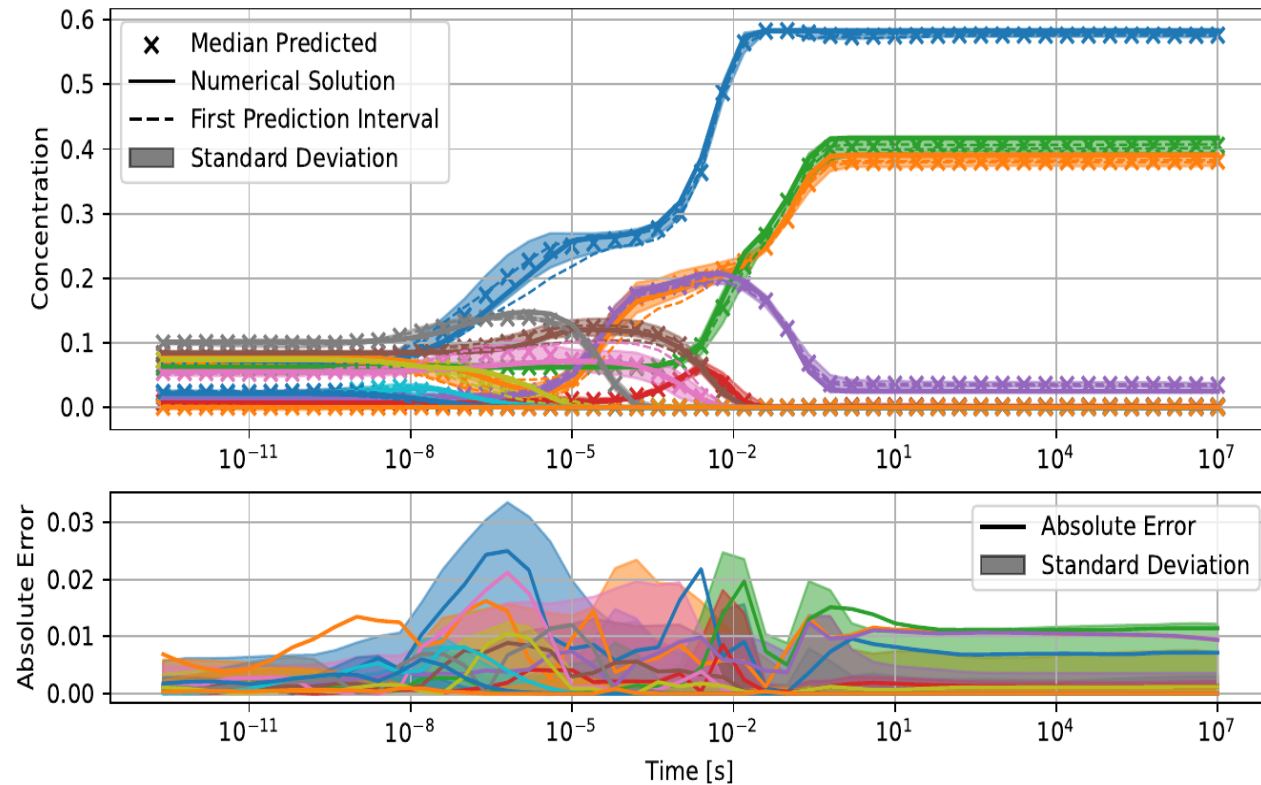


Training data from RAVETIME-Code :

3-D Advection-Diffusion-Reaction Solver for hydrogen (finite volume) transport in matter

$$\frac{d\vec{c}}{dt} = \mathbf{E} \left[\sum_{i=1}^I \gamma_i \mathbf{A}_i \vec{c} + \sum_{i=1}^I (\mathbf{H}_i \vec{c} \circ \mathbf{M}_i \vec{c}) \right]$$

Vector-Riccati-Equation
Generalisation to 'fill-level' dependent traps and multiple isotopes



Proof of principle successful

- so far only reaction terms
- still on the scale of single volume element
- less suited for evolving scenarios
- to be assessed for joint reaction-diffusion

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MEMENTO (Metallic Melt Evolution in Next-step TOkamaks)

S. Ratynskaia et al. NME 52 (2022)

K. Paschalidis et al. FED 206 (2024) 114603

- 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)

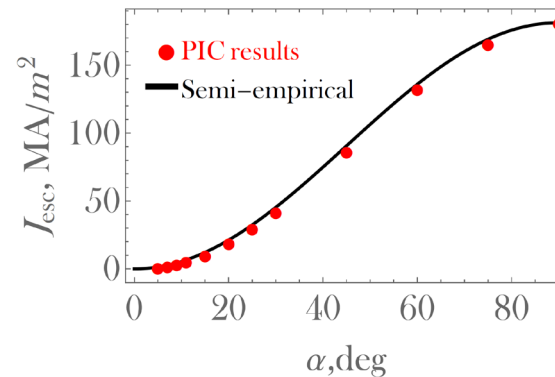
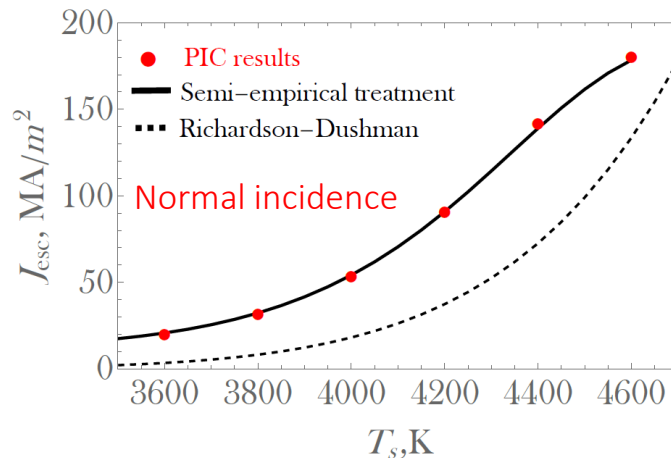
SPICE2 – a 2D3V PIC code (multi-emissive sheaths)

(*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)



At oblique magnetic field inclination angles:

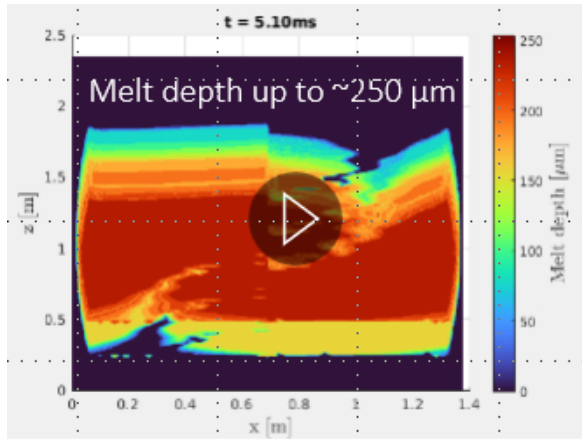
- For space charge limited regime, an accurate semi-empirical expression proven valid
- For the monotonic potential profile regime, escaping current $\sim 80\%$ of scaling prediction

MEMENTO uses respective scalings deduced from PIC simulations

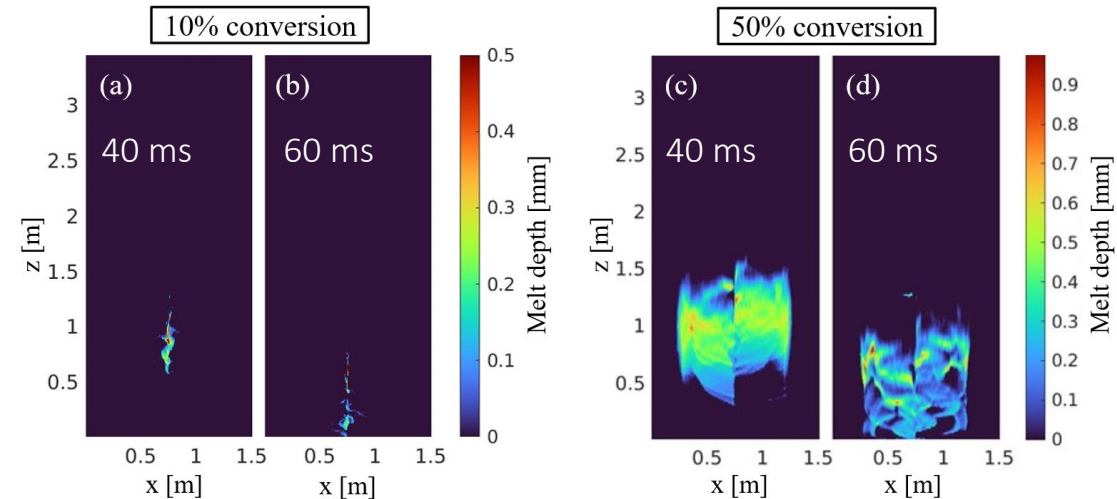
PFC RESPONSE TO TRANSIENT EVENTS – MELTING WITH MEMENTO



- Thermionic emission scaling laws provided by dedicated PIC simulations
- Addressing upper limiter damage under vertical displacement event (VDE)
- No vapor shielding in the model – mockup by capping the heat flux from previous experience and exp. data
- Thermal quench up to $63 \text{ GW/m}^2 \sim 10 \text{ ms}$
- Current quench up to 5.6 GW/m^2 (10%) or 28 GW/m^2 (50%) $\sim 100 \text{ ms}$



- Melt velocity $\sim 0.5 \text{ m/s}$, pool lifetime $\sim 5 \text{ ms}$
→ expected small displacements
compared to characteristic scales of the limiter
- At the edge, $60 \mu\text{m}$ melt depth and 1 cm/s velocity,
Weber number $\sim 5 \times 10^{-5}$ → melt should remain attached



- Instantaneous melt pools up to 0.3 - 0.5 mm depth
Weber number ~ 10 → prone to splashing

SUMMARY



I. Advanced capabilities in addressing PWI reactor-relevant conditions

- Consistent narrow-grid plasma extrapolation, field-aligned grid (essential for plasma flux resolution in divertor), charge-state resolved ion fluxes along wall surfaces, energy and angular resolved poloidally resolved CXN fluxes, consistent physics assumptions in line with SOLPS-ITER (e.g. ion sound speed), inclusion of thermal force and electric fields, radially resolved transport coefficients, etc
- Implementation of impurity tracing for dust ablation sources
- Addressing high density divertor sheath conditions and D supersaturated W surfaces under high flux conditions
- Kinetic simulations for efficient description of non-uniform plasma ion and heat loads on W monoblocks (divertor)

II. Advanced capabilities of reaction-diffusion codes

- Soret effects, complex 3D geometries, multi-material systems, n-damage defect creation and annealing, He bubble clustering and burst model, physically informed neutral network model

III. Predictive simulations perform and design and safety relevant information provided

- W erosion and deposition rates in steady-state, locations of preferable re-deposition, dust inventory evolution associated with destabilization of deposited layers, fuel retention estimates for divertor monoblock geometries including n-damage effects, tritium self-sufficiency analysis accounting for n-damage, melting and likelihood of melt splashing under VDE conditions

IV. Codes' performance optimization, GPU enabling and IMAS integration (ERO2.0 & MIGRAINE I/O) with help of ACHs

V. Several experiments in AUG pending or under analysis for validation of ERO2.0 predictions and MIGRAINE data (TE/PWIE)



2026-2027 outlook – TSVV-D: Summary of scientific tasks

Steady-state PWI with ERO2.0

- Surrogate models for PWI
- W to core, field-aligned grid
- Time-dependent dust evaporation sources
- Validation in AUG
- Predictive modelling and comparison (TSVV-E)

Dust transport

- Improved electron collection model
- Remobilization by plasma-induced forces
- Time-dependent dust evaporation sources
- Validation in AUG
- Predictive modelling

Fuel retention

- Physics-informed defect annealing model
- Optimization of numerical convergence (large eq. sys.)
- Scenario-resolved retention & outgassing (reactor scale)
- Validation in AUG
- Predictive modelling

Transient events → RE

- Surrogate models for RE energy deposition and secondary products
- Full thermo-mechanical response model with explosive fragmentation
- Validation in AUG
- Predictive modelling

Thank you for your attention!