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“THEORY, SIMULATION, VERIFICATION AND VALIDATION”

TSVV TASK 7: PLASMA-WALL INTERACTION IN DEMO

WP PWIE Meeting | 08.02.2023

D. Matveev on behalf of TSVV-7 team

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TSVV-07 PLASMA-WALL INTERACTION IN DEMO

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

TSVV-07 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 rates)
- Assessment of W erosion rates for locations affected by transients
- Assessment of tritium in-vessel inventory (co-deposition, bulk retention with He-induced and neutron damage)

PWI in DEMO

Team codes & contributions

FZJ	ERO2.0, CRDS	Impurity transport and PWI: erosion-deposition mapping. Fuel retention.
IPP Garching	SDTrimSP, TESSIM, RAVETIME	PWI data. Fuel retention. Uncertainty quantification.
KTH	MEMENTO, MIGRAINE	Material response to transient heat loads. 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.
VTT/Helsinki	MD, potential development	Interatomic potentials, MD modelling for PWI.

TSVV-07 PLASMA-WALL INTERACTION IN DEMO

Team members

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KTH:	S. Ratynskaia, L. Vignitchouk, P. Tolias, E. Thoren, P. Konstantinos
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CEA:	R. Delaporte-Mathurin, E. Hodille, C. Grisolia, F. Montupet-leblond,
IPP:	U. Von Toussaint, K. Schmid
Helsinki:	F. Granberg, F. Kporha
JSI:	J. Kovačič, S. Costea

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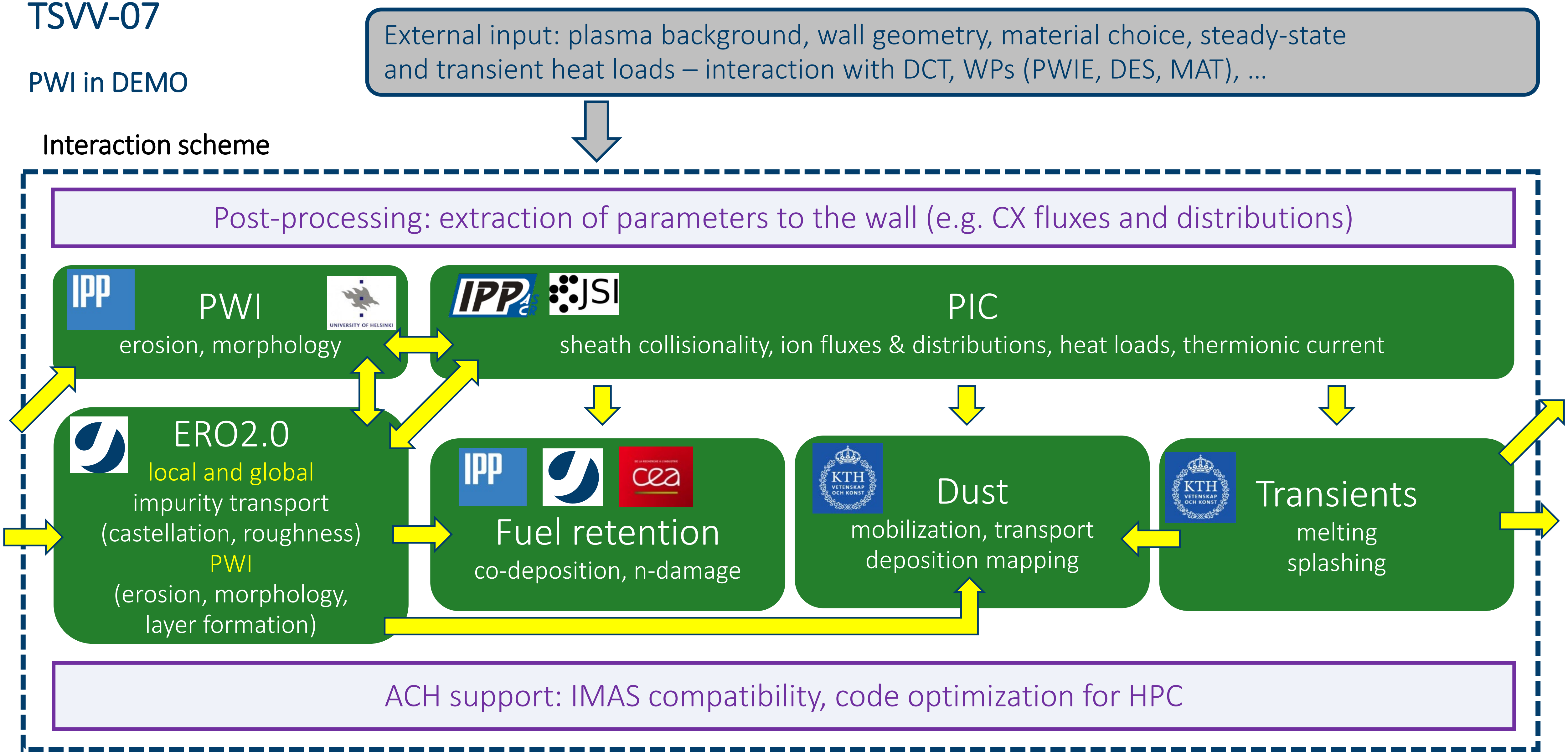
PWI in DEMO

Interaction scheme



TSVV-07 Timeline

	2021	2022	2023	2024	2025
Plasma	ITER bg proc.	DEMO bg proc.		Updates from DEMO team:	
		VDE, LOC values	VDE, LOC profiles	geometry, materials, plasma profiles	
PIC	Sheath ion distrib.		Gaps		
	Thermionic & SEE			BIT3 vs BIT1	
PWI 1	W erosion under D/T supersaturation			W-O-H potential	
			W-O potential		
PWI2		Gyromotion	SDTrimSP-3D	UQ interface	UQ studies
ERO2.0	Preps (geom., bg)			Deposition in gaps	
	Simulations ITER-like		SDTrimSP-1D coupling		
		Simulations DEMO		SDTrimSP-3D data and coupling	
Fuel retention	Thermomigration	Simulations DEMO	Simulations DEMO	He (H diffusion)	He (W mechanical)
	Interface model	w/o n-damage	with n-damage		
	Test cases			UQ interface	UQ studies
Transient melting		Preps			
		Melting, splashing			
Dust	Scoping studies	Simulations DEMO steady			
	Simulations ITER-like		Simulations DEMO transients		

Report DEMO CDR (end of 2023)

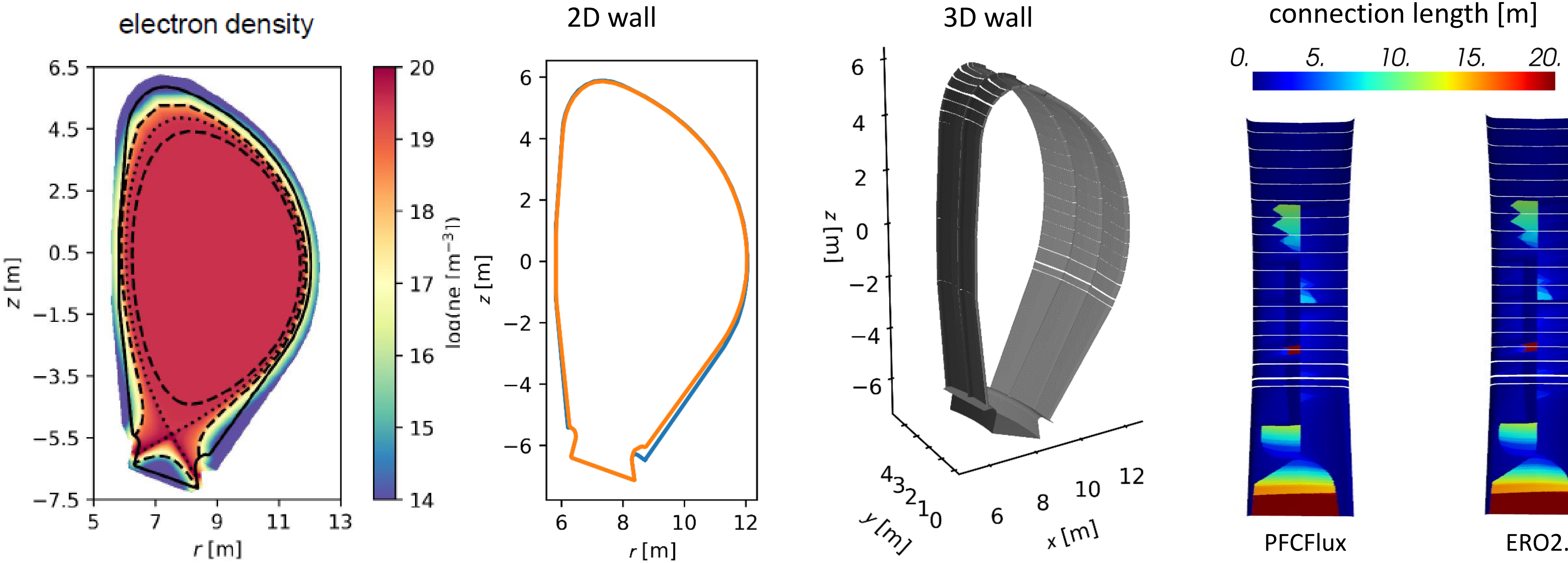
Final report (end of 2025)

TSVV-07 PROGRESS

Tasks 2022

Full 3D ERO2.0 simulations using existing PWI databases, sheath models and the plasma solution

Wall geometry, plasma equilibrium (baseline 2017), SOLPS-ITER plasma solution [F. Subba et al 2021 Nucl. Fusion 61 106013], neutral fluxes (not yet angular and energy resolved), magnetic shadowing and extrapolation to the wall implemented in ERO2.0



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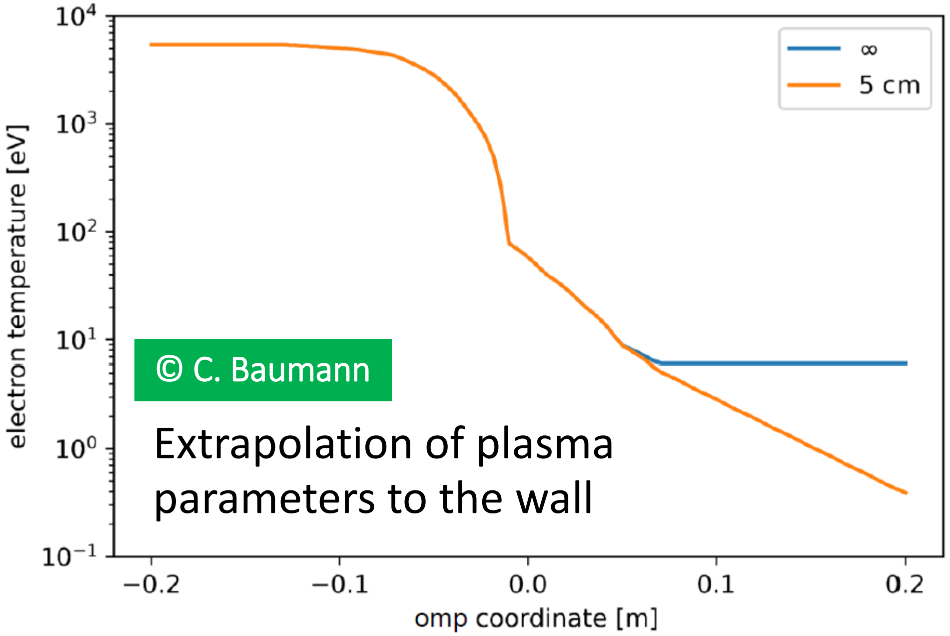
Tasks 2022

Full 3D ERO2.0 simulations using existing PWI databases, sheath models and the plasma solution

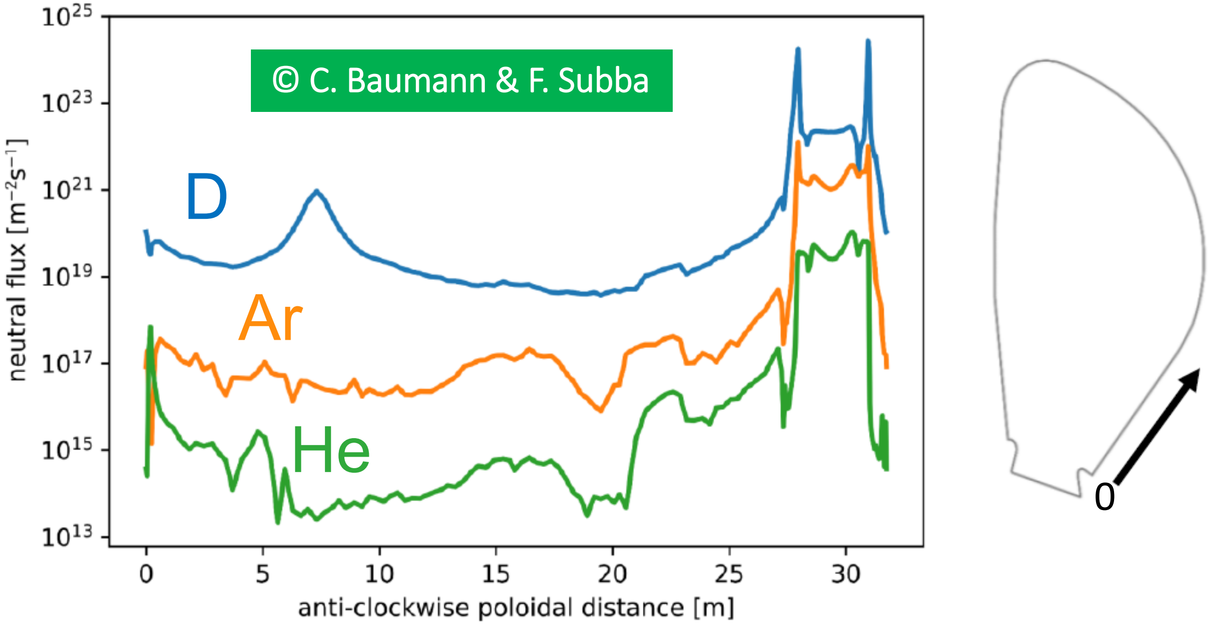
Wall geometry, plasma equilibrium (baseline 2017), SOLPS-ITER plasma solution [F. Subba et al 2021 Nucl. Fusion 61 106013], neutral fluxes (not yet angular and energy resolved), magnetic shadowing and extrapolation to the wall implemented in ERO2.0

outer mid-plane



Extrapolation of plasma parameters to the wall

Neutral fluxes



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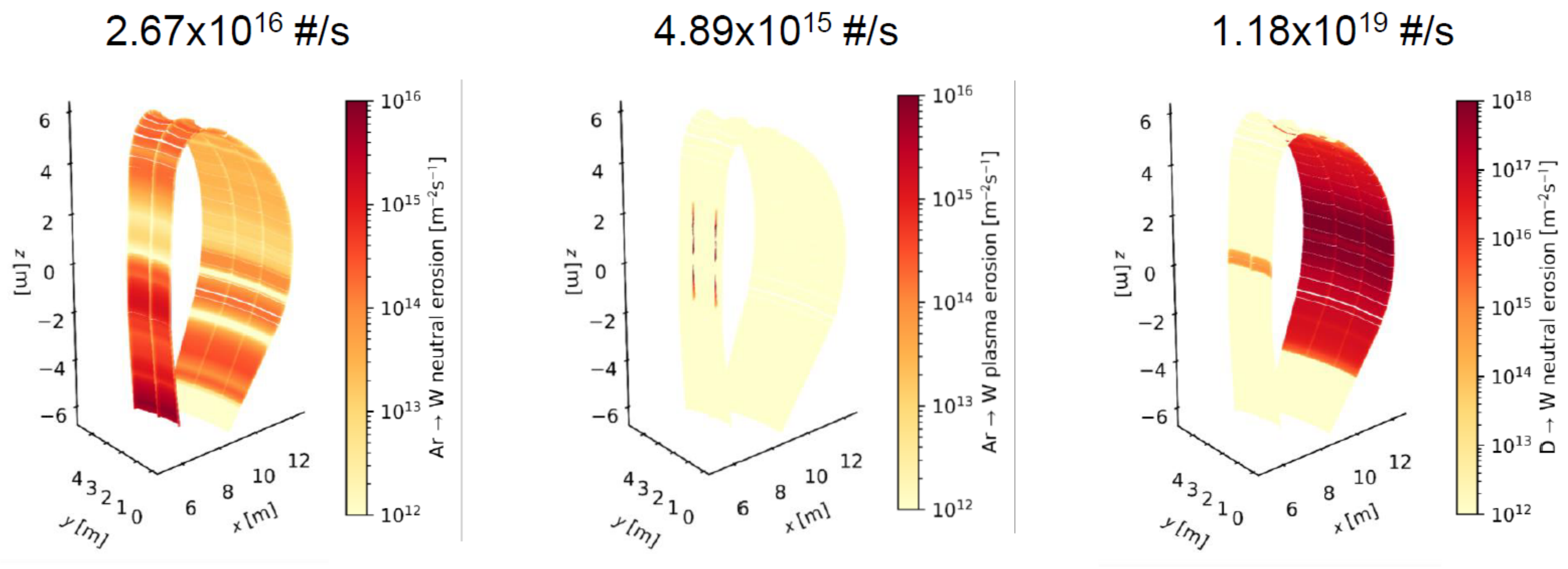
Tasks 2022

Full 3D ERO2.0 simulations using existing PWI databases, sheath models and the plasma solution

First preliminary simulations of W erosion



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Here: globally constant ion impurity concentrations based on integrated volumetric SOLPS data

- D^+ ~ 0.855
- He^{2+} ~ 0.134
- He^+ ~ 0.008
- Ar^{13+} ~ 0.003

(mean charge state of Ar)

Zero erosion by D^+, He^0, He^{Z+} !

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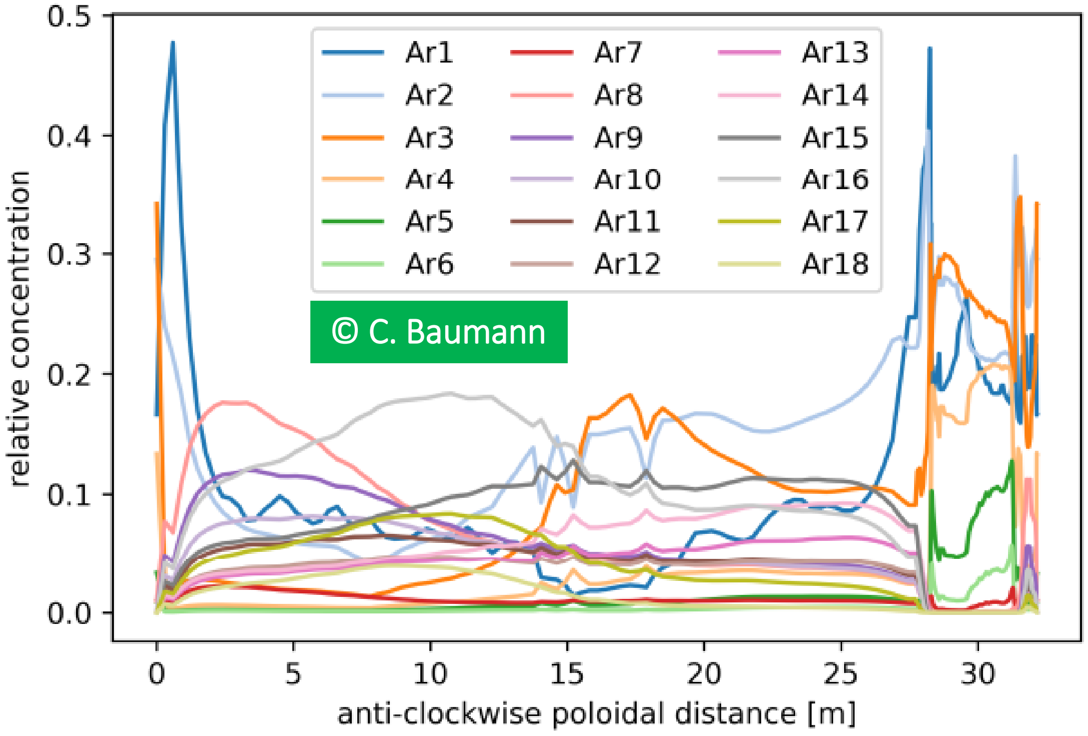
Ongoing work

Full 3D ERO2.0 simulations using existing PWI databases, sheath models and the plasma solution

Accounting for charge state resolved impurity concentrations and fluxes



! Recent ERO2.0 update has introduced fully charge state resolved impurity concentrations and respective PWI, so that new erosion results are coming soon

! SOLPS-ITER solution with extended grid will be very important – is pending (DCT)

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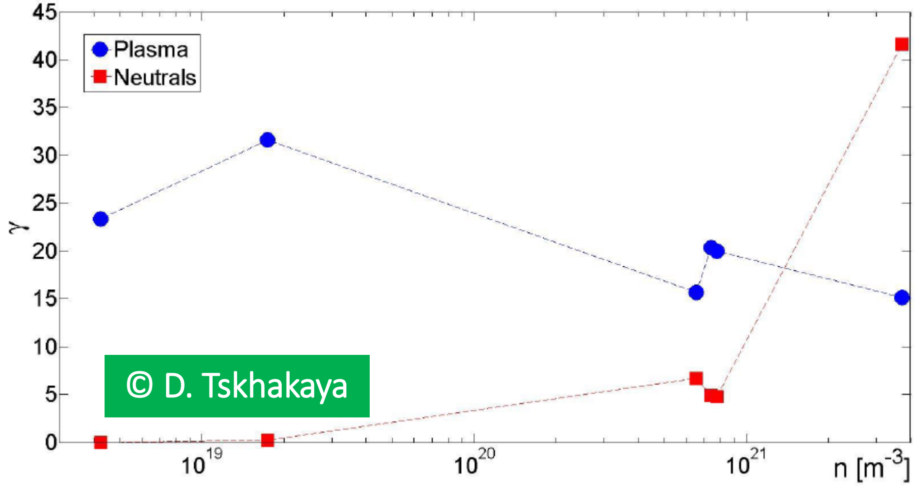
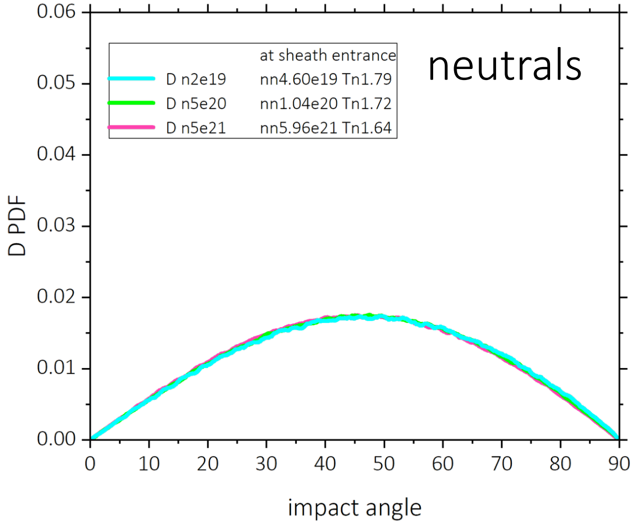
Tasks 2022

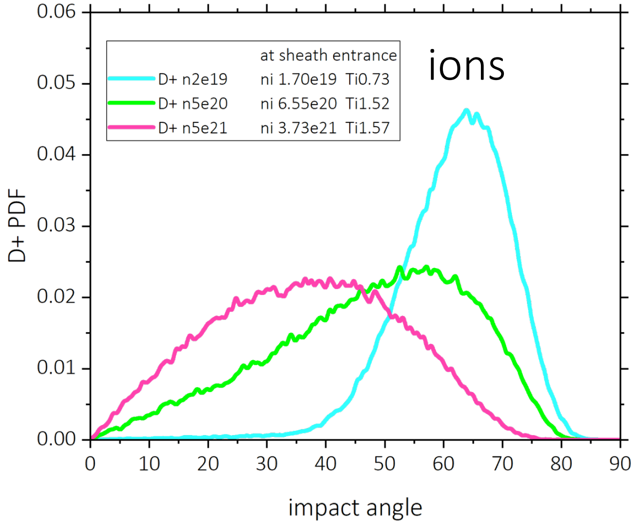
Dedicated PIC studies with BIT-1 for DEMO-relevant high-density divertor sheath as relevant input for erosion, dust transport and transient melting simulations

Simulations for DEMO relevant divertor sheath with densities up to $5x10^{21}$ m^{-3} indicate that neutrals dominate heat loads



The angular distributions of impacting ions are strongly affected in the collisional sheath and acquire the shape similar to the distribution of neutrals for the highest density cases





Characteristics of the high density divertor sheath, such as plasma parameters and impact energies and angles of ions and neutrals are available for implementation in ERO2.0 for simulations of divertor erosion

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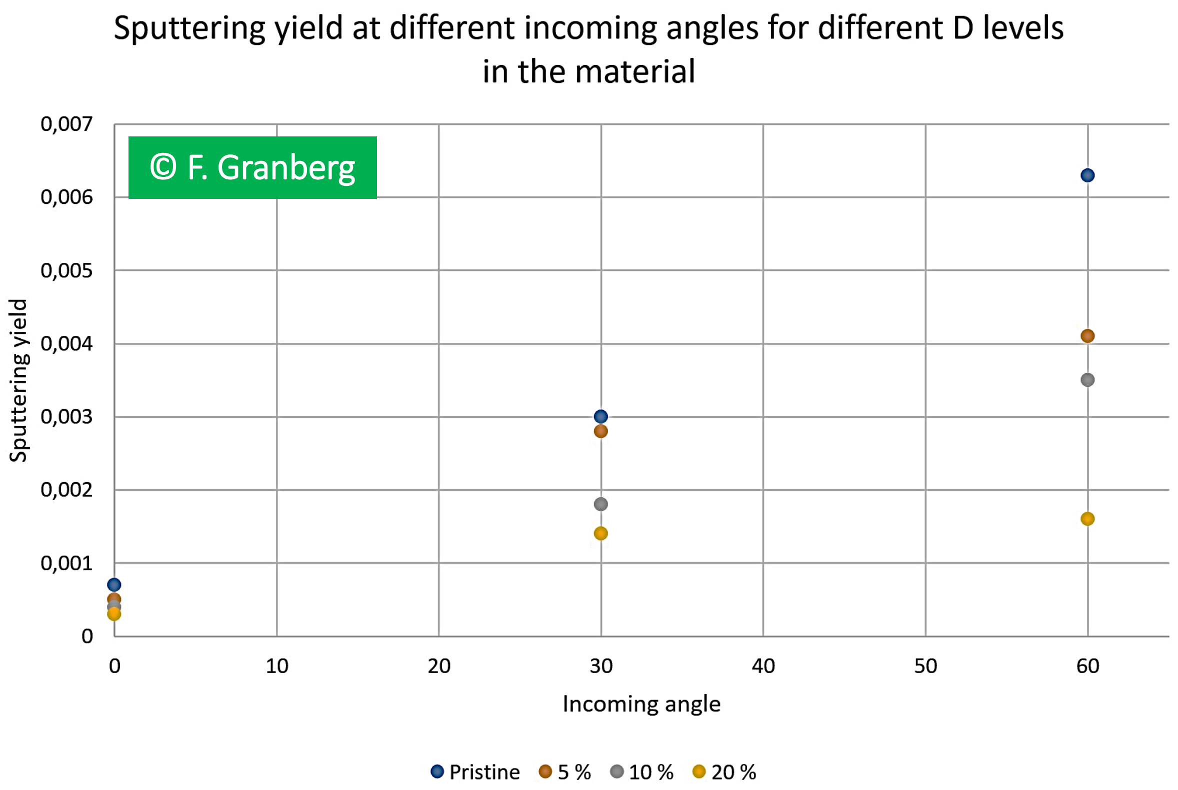
Tasks 2022

MD simulations utilizing available W-H interatomic potentials to simulate supersaturated W surfaces under ion irradiation

- Yet static only simulations due to forced usage of slow Tersoff-type interatomic potential
- Studied pure and supersaturated W irradiated by D and D_2 ions → no difference due to molecules
- 5%atD, 10%atD, 20%atD
- 0º, 30º, 60º angles of incidence
- Supersaturation decreases the sputtering yield that seems to be not due to dilution, neither enhanced reflection, work in progress



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Tasks 2022

Dedicated dust transport simulations with MIGRAINe (aiming at net deposition locations provided by ERO2.0 simulations)

Based on 2021 MIGRAINe simulations using ITER geometries and low-power plasma profiles, estimates of long-term W dust inventory evolution in 12 remobilization scenarios were refined [Vignitchouk 2022]

Simple Markov chain fit models improved to sub-percent errors

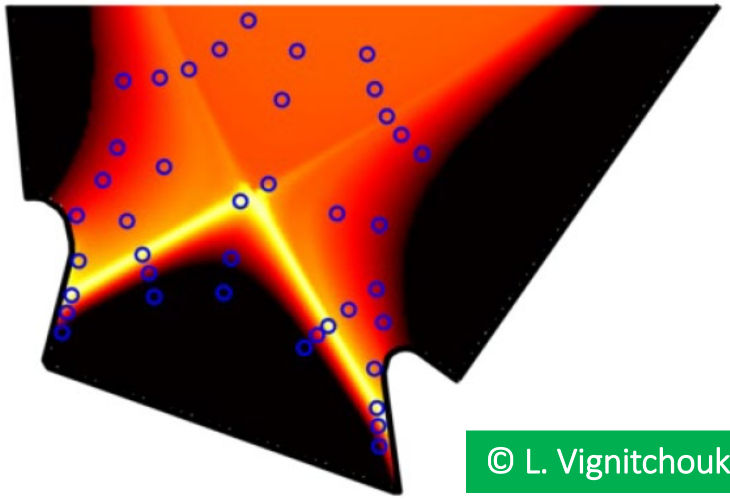
Dust distributions shift to larger sizes as time evolves (small dust does not survive in plasma due likely vaporization)

Sampled DEMO plasma profiles are similar to ITER high recycling conditions considered for the dust survival studies

Work in progress: MIGRAINe modifications to allow multiple impurity species and ion charge states are in progress

Simulations for ERO2.0 deposition location maps expected in 2023

Sampling of plasma conditions from DEMO plasma profiles (Te)



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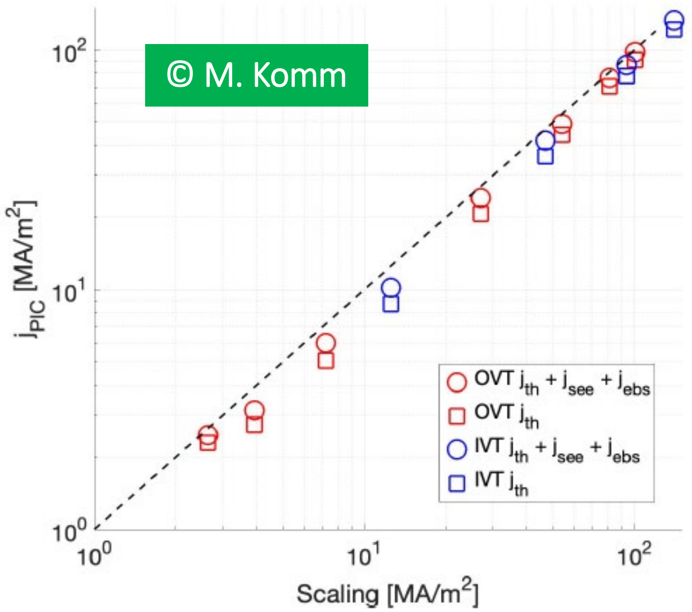
Tasks 2022

PIC simulations with SPICE to identify whether the escaping current scales with electron thermal velocity or on ion sound speed

Simulations of thermionic emission (TE) with secondary electron emission (SEE) and electron backscattering (EBS) confirm the validity of the earlier developed semi-empirical scaling model [Komm 2020, Tolias 2023]

In the case of high density emissive sheath and normal magnetic field inclination that is relevant for exposed leading edges, the transition to the space-charge limited regime will not take place before W melting, thus implying that the monotonic potential profile regime is most relevant for melt motion applications



Implementation of representative values of surface heat fluxes and halo current densities for transient melting simulations with ~~MEMOS-U~~ MEMENTO

The MEMOS-U model was re-implemented in a new code using the open-source AMReX adaptive meshing framework

For current DEMO design, the thermal and the current quench of VDEs are considered relevant for melting (WPDES, late 2022) – assessment of melt layer stability in these conditions is pending

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Tasks 2022

Retention and permeation studies for DEMO main chamber and divertor with TESSIM-X, MHIMS, FESTIM, RAVETIME

Highlights: implementation of Soret effect, introduction of source terms for n-induced defects, work on mobile dislocations, H-He interaction, simulations of the role of interface conditions and 3D effects for ITER-like W monoblocks

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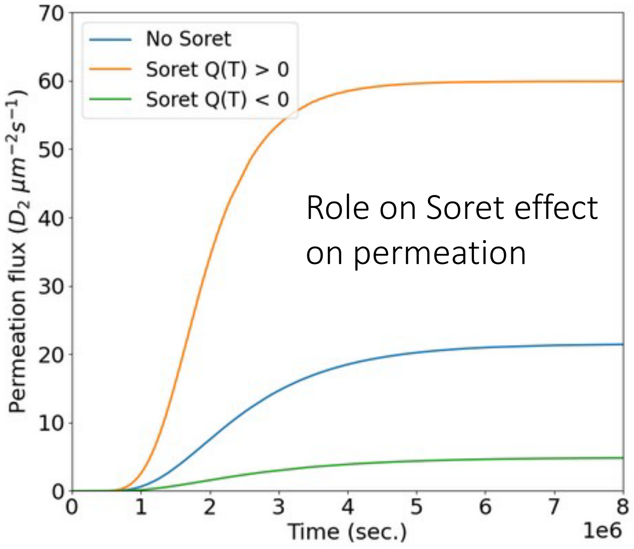
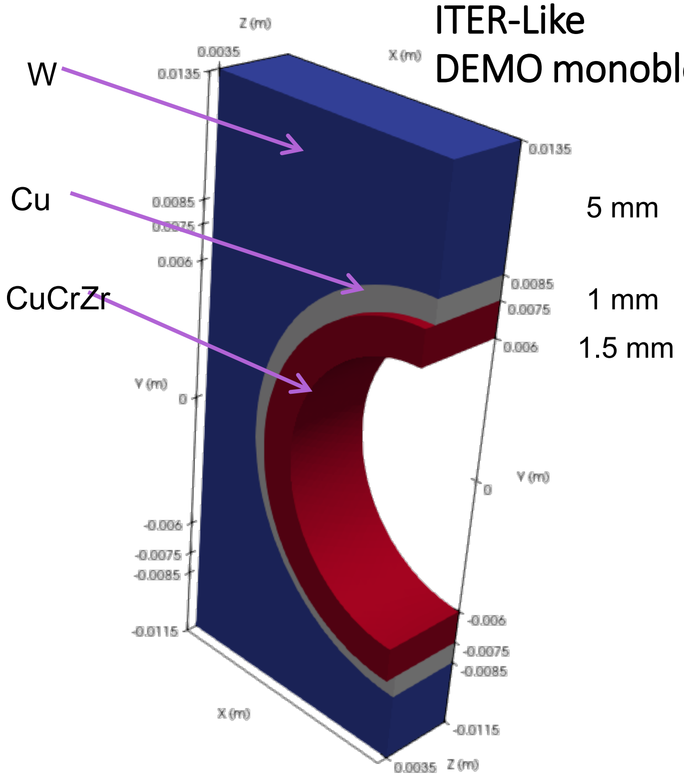


ITER-Like DEMO monoblock



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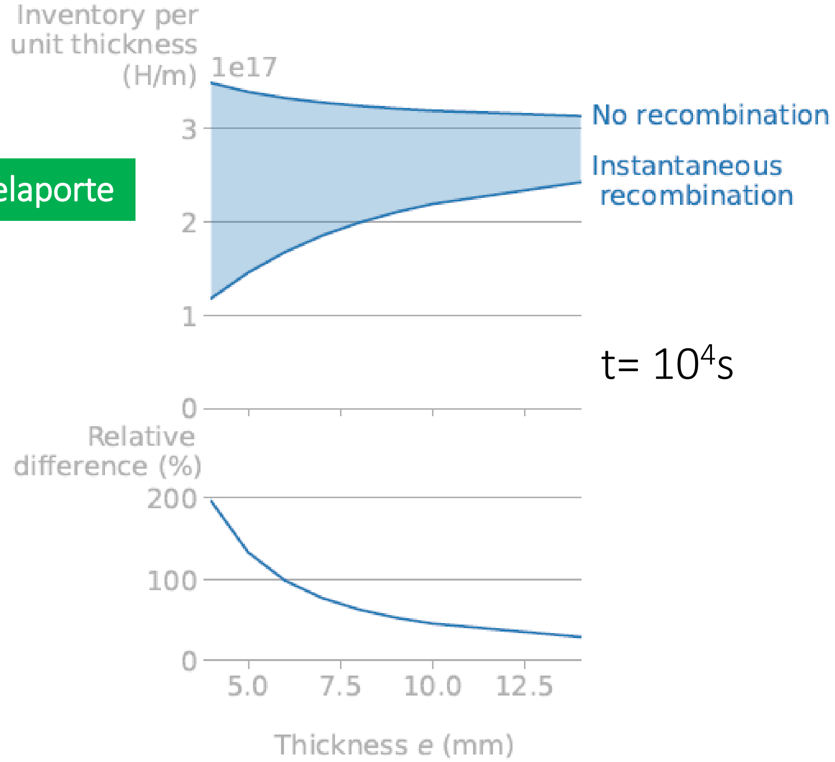

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Tasks 2022

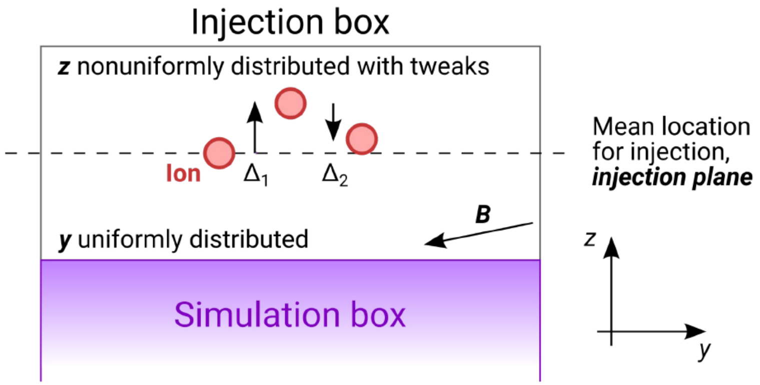
Implementation of the gyro-motion module in SDTrimSP-3D

Gyro-module implemented, optimization and implementation of crystalline lattice capabilities are on the way / validation

Future work: cross-check with ERO2.0, evaluation of sample exposures in AUG, cross-validation with MARLOWE and MD

Implementation of non-uniform injection schemes in SPICE

For the cases of non-uniform plasma density, temperature



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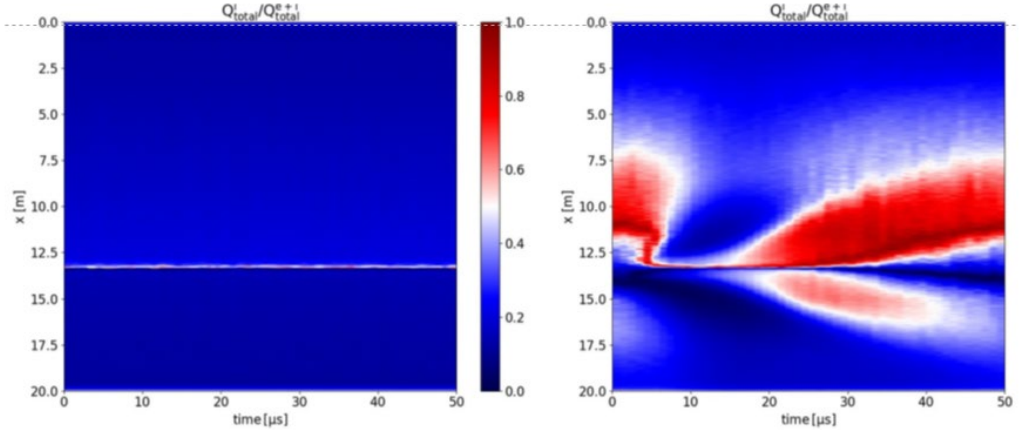
Implementation of non-steady-state sources in BIT1 (blobs)

Steady-state vs Blob-filament

(total power flux)



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Tasks 2023 (1/2)

1. Implement the MD erosion data under D/T supersaturation into ERO2.0.
2. Implement the PIC-inferred sheath characteristics into the ERO2.0 code.
3. Perform full 3D ERO2.0 simulations using updated databases and sheath models. New plasma?
4. Provide erosion-deposition maps and wall lifetime for the main chamber and divertor of DEMO.
5. Perform MEMENTO simulations of PFC response under VDEs. Assess macroscopic surface modifications in form of melting, melt re-solidification and possibly splashing. In case of splashing, analyze the size and velocity distributions of droplets.
6. Perform dedicated dust transport simulations with MIGRAINe for net deposition locations provided by ERO2.0 simulations.

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Tasks 2023 (2/2)

7. Perform SDTrimSP-3D simulations for rough surfaces of specific morphology and in particular that of re-solidified melt resulting from MEMENTO to obtain effective erosion yields.
8. Perform PIC simulations with SPICE codes to obtain heat loads and ion penetration into gaps of divertor and limiter monoblocks under DEMO sheath conditions.
9. Perform TESSIM-X and FESTIM simulations of fuel accumulation in DEMO PFC with relevant material structure and fuel permeation to coolant, accounting for neutral damage. Cross-validate the results of both codes.
10. Develop with help of ML approach an interatomic potential for W-O.
11. Prepare an extensive integrated report for the DEMO conceptual design review regarding the DEMO wall lifetime in steady-state and transients and regarding fuel uptake, retention and permeation.

TSVV-07 Timeline