EUROfusion

“THEORY, SIMULATION, VERIFICATION AND VALIDATION”

TSVV TASK 7: PLASMA-WALL INTERACTION IN DEMO

Dmitry Matveev on behalf of TSVV-07 team

EUROfusion Science Meeting on Status of TSVV projects | 11-12.09.2023

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TSVV-07 PLASMA-WALL INTERACTION IN DEMO

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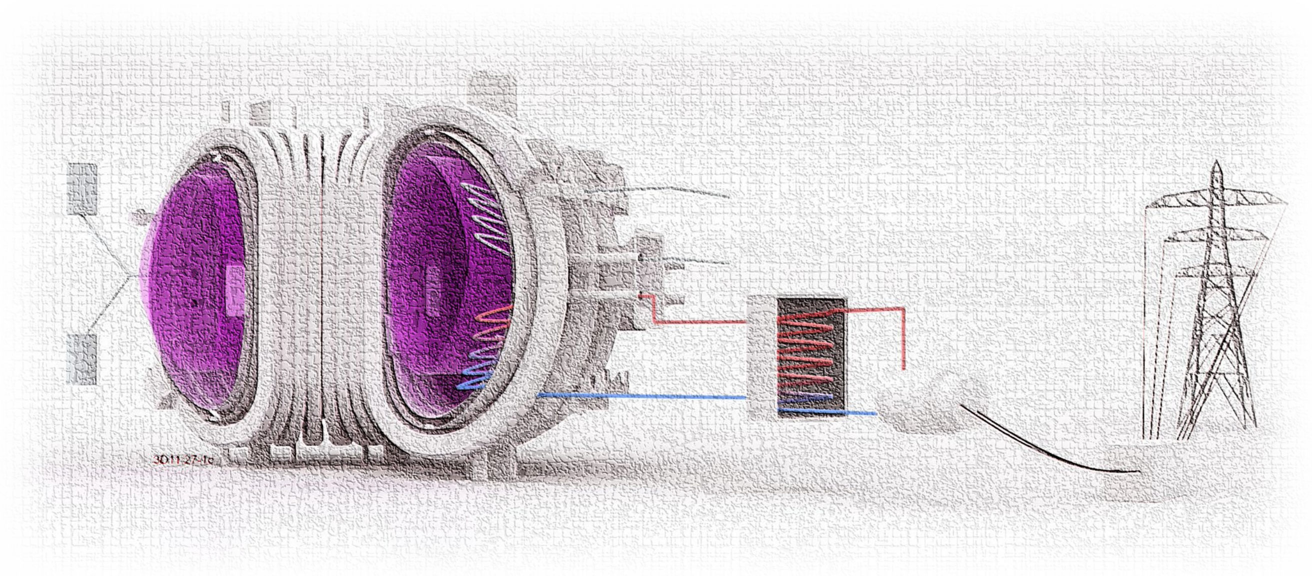
TSVV-07 PLASMA-WALL INTERACTION IN DEMO

Outline

- Aims and objectives
- Teams, codes and competences
- Project structure & workflows
- Key achievements to date
- ACH support
- Open questions and future plans
- Backup: status of deliverables/milestones



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)
- 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)

TSVV-07 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

TSVV-07 PLASMA-WALL INTERACTION IN DEMO

Structure & workflows

External input: plasma background, wall geometry, material choice, steady-state and transient heat loads – interaction with DCT & WPs (PWIE, DES, MAT), ...

Post-processing / extraction of parameters (e.g. CX fluxes and distributions – link to TSVV-05)

PWI
erosion, morphology

PIC
sheath collisionality, ion fluxes & distributions, heat loads, thermionic current

ents
elting
shing
-dust

ERO2.0
local and global
impurity transport
(castellation, roughness)
PWI
(erosion, morphology,
layer formation)

Fuel
retention
co-deposition
n-damage

Dust
mobilization
transport
deposition

Transients
melting
splashing
droplet-to-dust

ACH support: IMAS compatibility, code optimization for HPC

KEY ACHIEVEMENTS, PART 1:

EROSION-DEPOSITION MAPPING

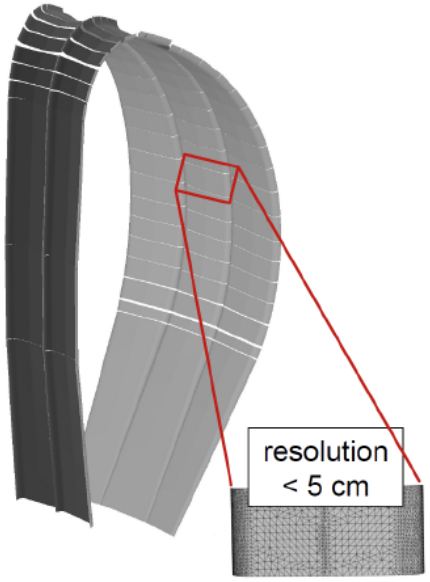
ERO2.0 modelling: erosion and deposition mapping

Critical input data

Full-W ITER simulations:
Eksaeva et al. Phys. Scr. 97 (2022)

Wall geometry

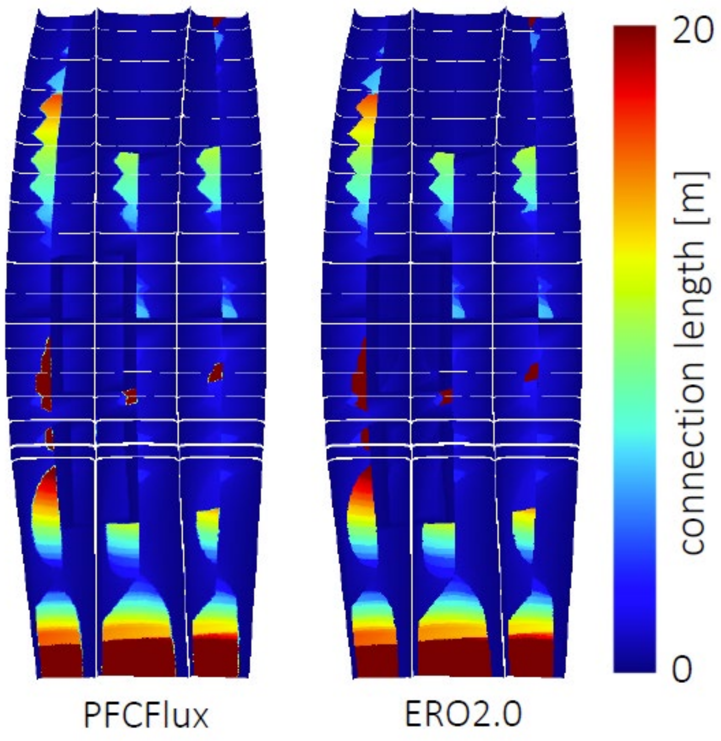
(baseline 2017)



EU-DEMO main chamber geometry as polygon mesh ($\sim 10^5$ polygons)

Magnetic equilibrium

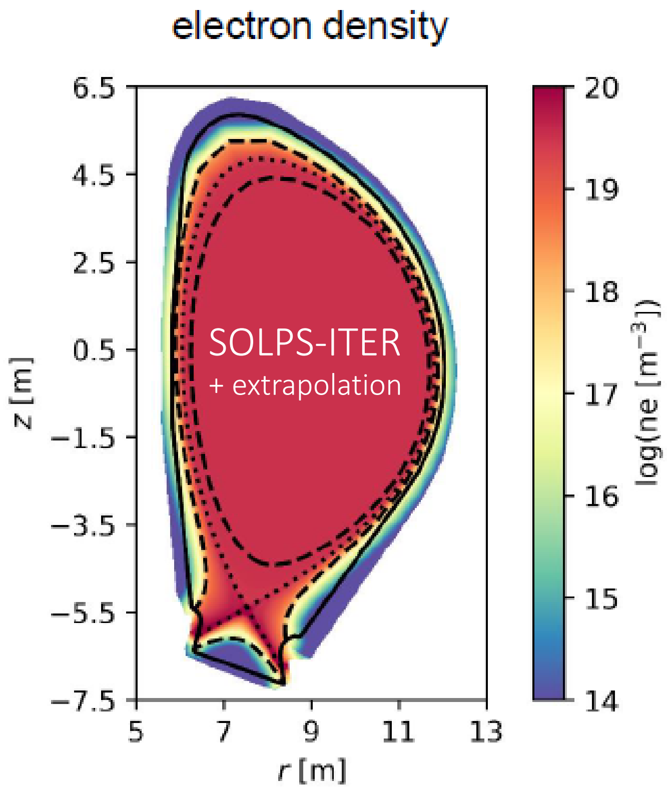
(baseline 2017)



ERO2.0 magnetic shadowing validated

Plasma solution

F. Subba et al 2021
Nucl. Fusion 61 106013



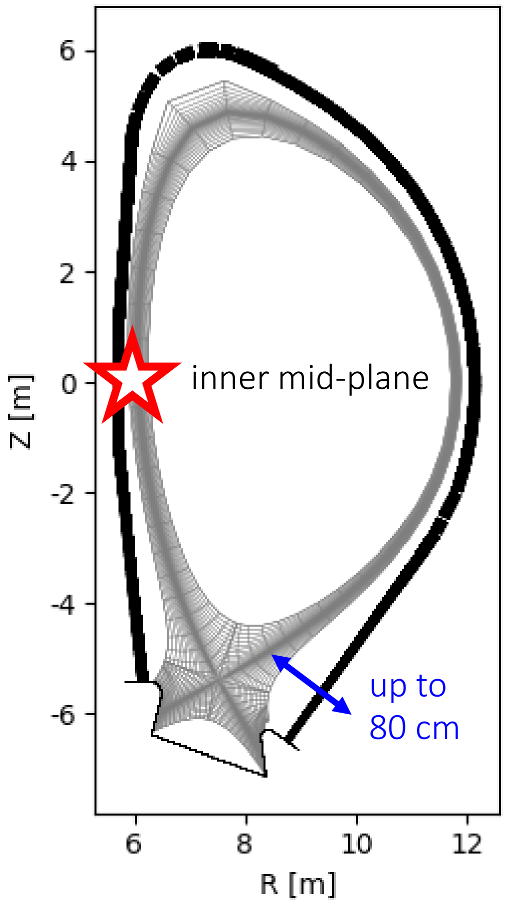
ERO2.0 modelling: erosion and deposition mapping

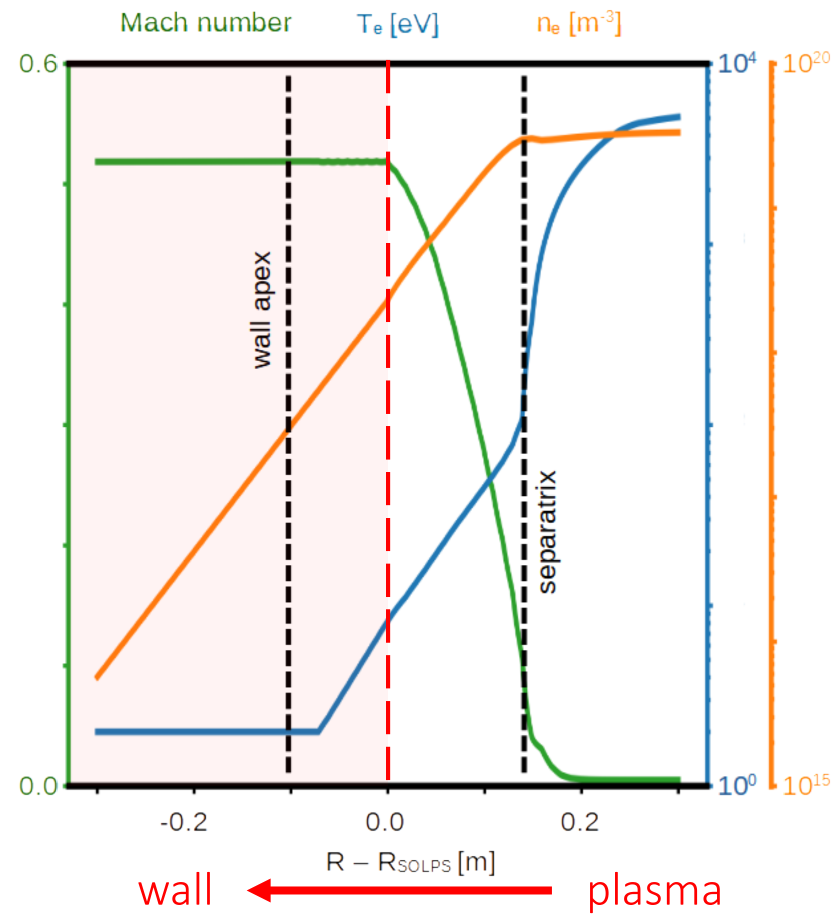
DEMO: unprecedentedly large volume for extrapolation of plasma solution to the wall

Large extrapolation volume introduces large modelling uncertainties

Following assumptions used so far:

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





ERO2.0 modelling: erosion and deposition mapping

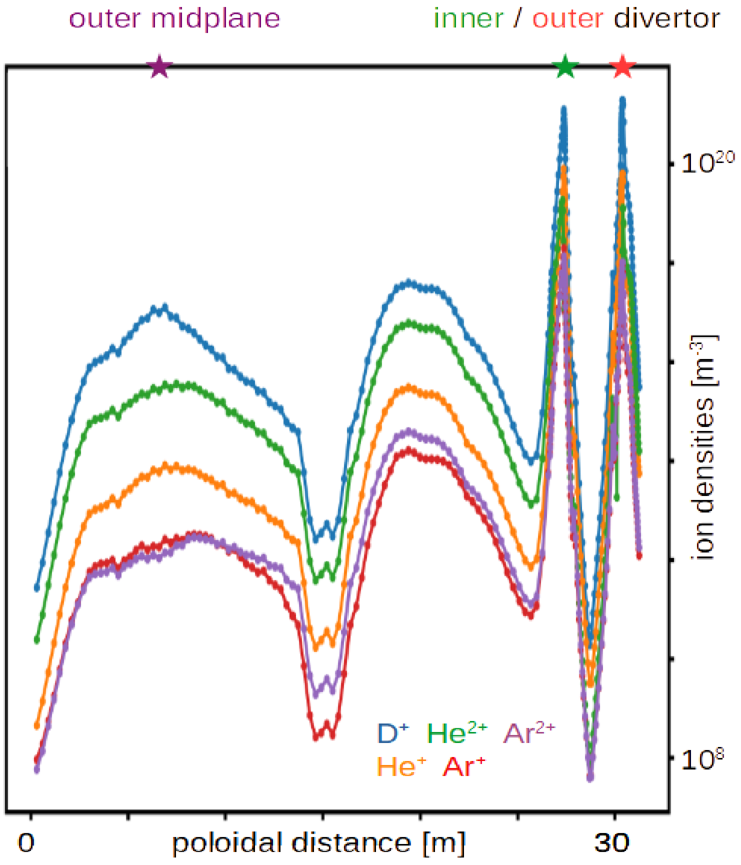
DEMO: critical role of charge-resolved spatially non-uniform impurity ion fluxes (He, Ar)

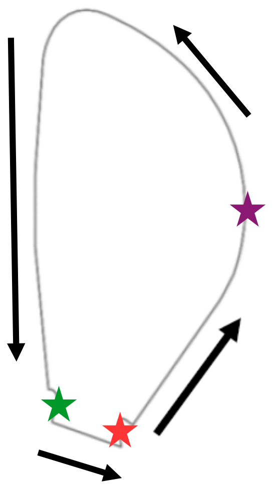
Accounting for charge state resolved impurity concentrations and fluxes is essential for proper calculation of sputtering yields

Formerly, only the total flux variation with mean volumentric charge state was used in ERO2.0 – overestimation of gross erosion

New capability of charged resolved spatially varying fluxes is now implemented in ERO2.0

This leads to significant reduction of divertor gross erosion rates by impurities (He, Ar)





ERO2.0 modelling: erosion and deposition mapping

DEMO: dominating role of charge-exchange (CX) fluxes on erosion in the main chamber

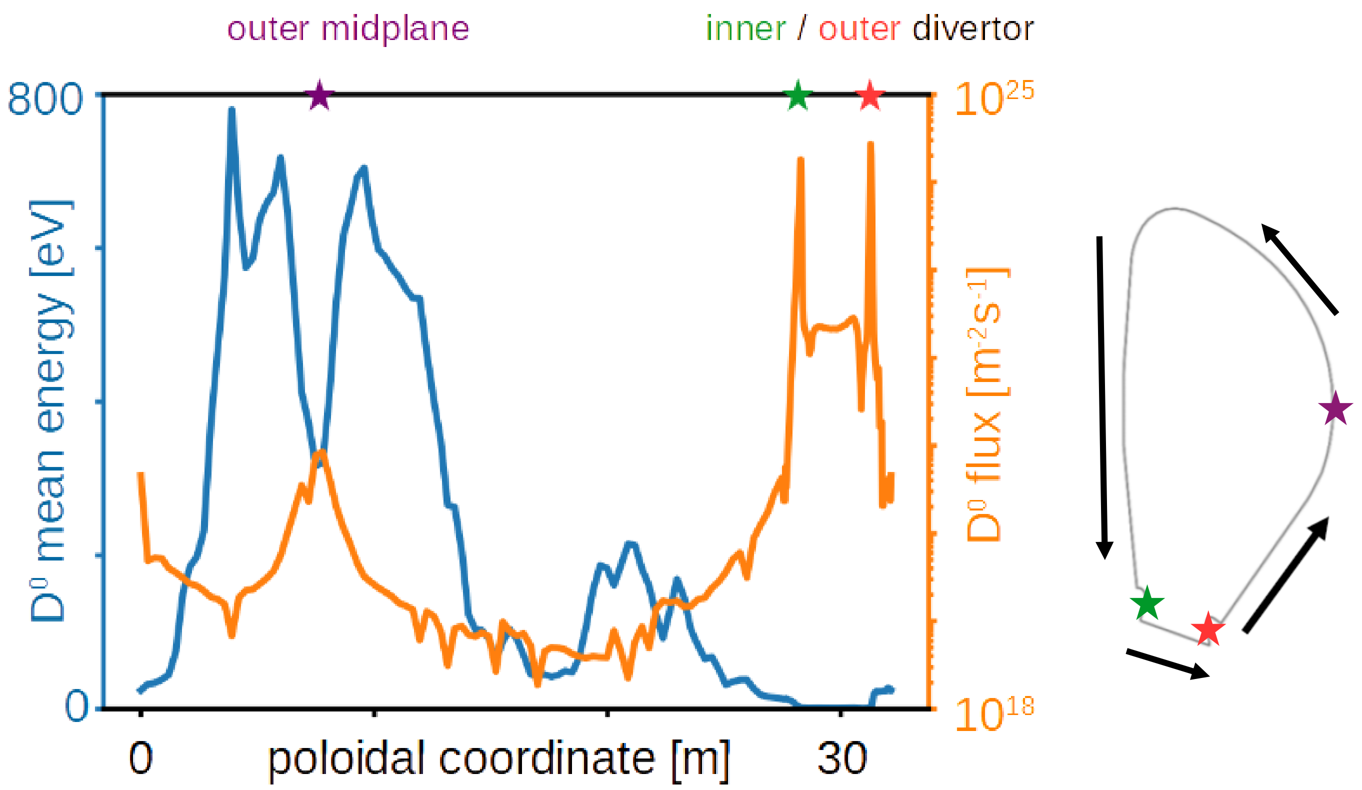
So far only poloidal profiles and mean energies available from SOLPS-ITER

Current assumptions for sputtering:

- Using the mean energy with the total flux proportionally reduced to represent only the contribution of atoms with $E > E_{th}^{D\text{->}W}$

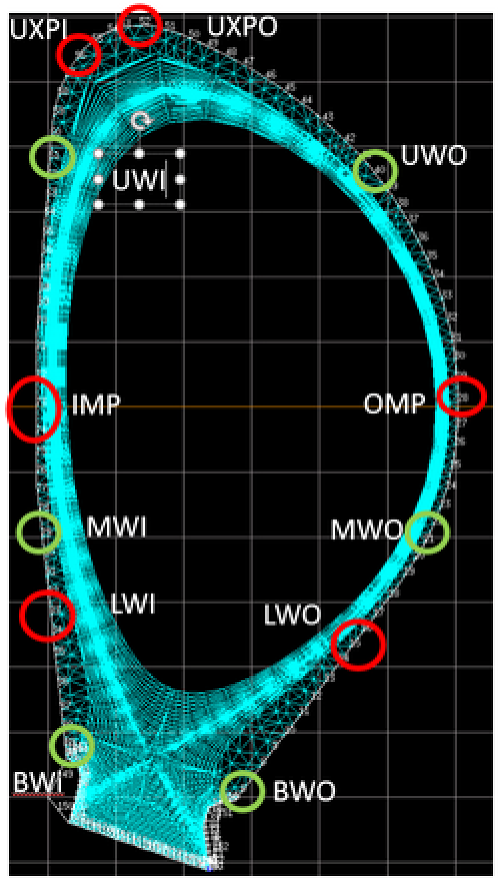
Ongoing work (DCT, TSVV-05):

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

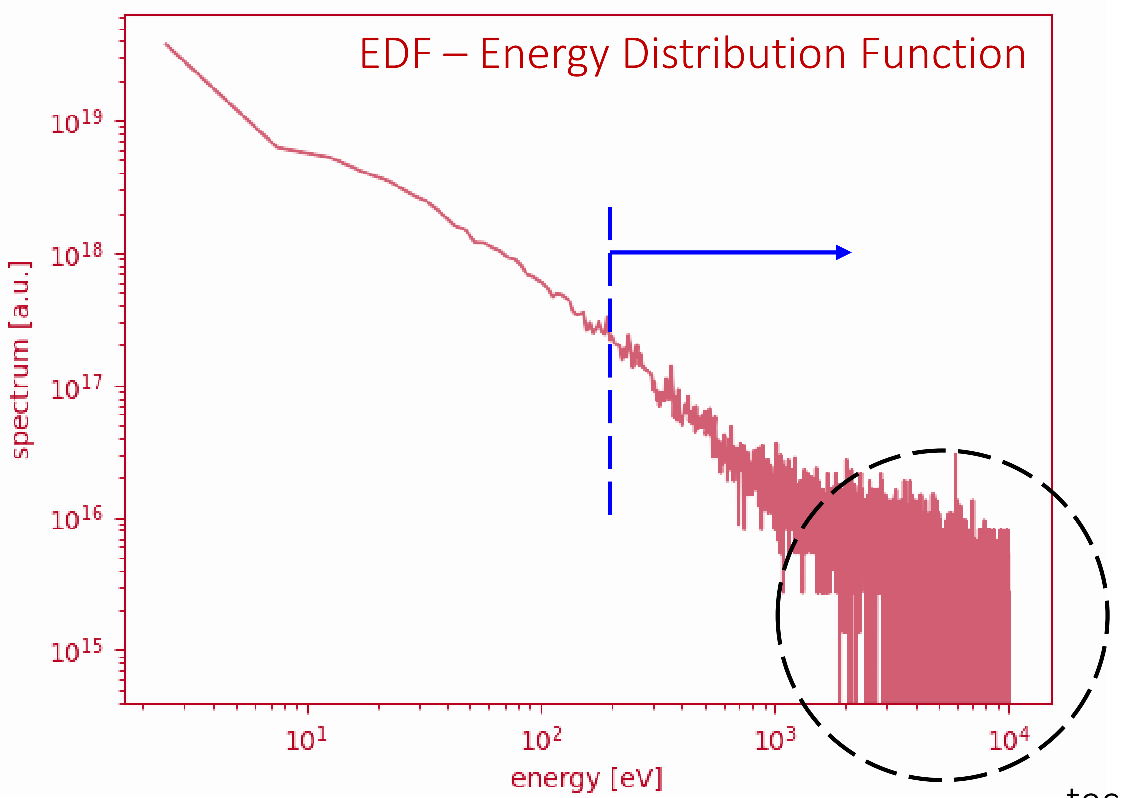


ERO2.0 modelling: erosion and deposition mapping

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



Test case example: energy spectrum at outer mid-plane (OMP)



Expected gross erosion rate at OMP (toroidially integrated) …

- Using mean energy and reduced flux (factor 10 from ITER case)

  3.5×10^{17} atoms/s

- Using the DEMO EDF

  1.4×10^{18} atoms/s

Large difference underlines importance of resolvd data

Data for impact angles (ADF) still lacking

technical aspects:
energy cut-off and numerical statistics

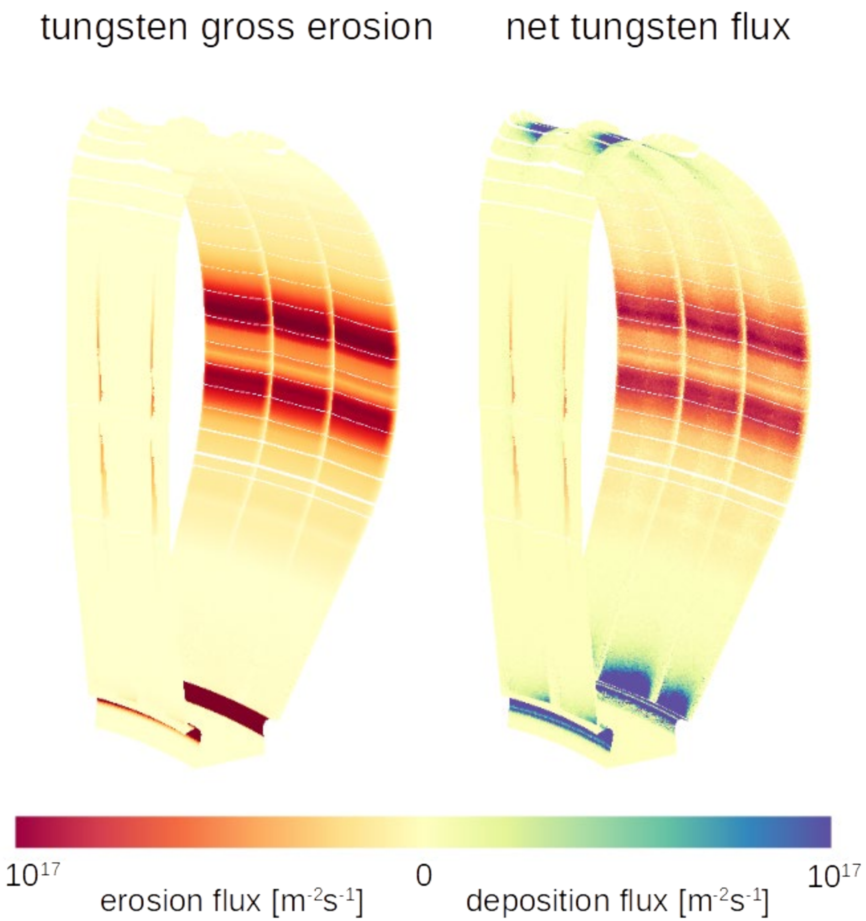
ERO2.0 modelling: erosion and deposition mapping

Erosion rates: (-) net erosion, (+) net deposition

[10^{18} atoms/s]	net rate	gross rate	... by Ar^{Z+}	... by D^0 (CX)	... by W^{Z+}
main chamber	(-) 10.8	23.7	0.3	23.2	0.2
divertor	(+) 9.6	73.4	57.8	-	15.5

(these are full machine integrated rates)

- Main chamber erosion dominated by neutrals (mostly ~mid-plane)
- Divertor erosion dominated by Ar ions 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)



ERO2.0 modelling: erosion and deposition mapping

Summary and further related ongoing work

Plasma background

- Major uncertainty for PWI modelling (non-optimal plasma scenario, large distance to the wall)
- DCT is working on the new baseline, as well as fluid neutrals and extended grid SOLPS solutions (other TSVVs?)

Improvement of erosion calculations

- Charge-state resolved wall fluxes → important mainly in the divertor
- Energy resolved CX neutrals → important mainly in the main chamber
- Angular resolved CX neutrals → pending, major effort with limited resources, link to TSVV-05

Further related studies

- Current ERO2.0 results suggest strong W accumulation in regions with low plasma density – under investigation
- Improvement of description of particular physics in ERO2.0 in view of DEMO – friction force, neutral collisions
- **PIC studies for high density divertor sheath beyond the classical model – input to SOLPS and ERO2.0**
- Improvement of PIC models for castellated surfaces – ion fluxes with non-uniform n_e, T_e injection profiles
- **Development of capabilities for erosion data on D supersaturated W and surfaces with developed morphology**

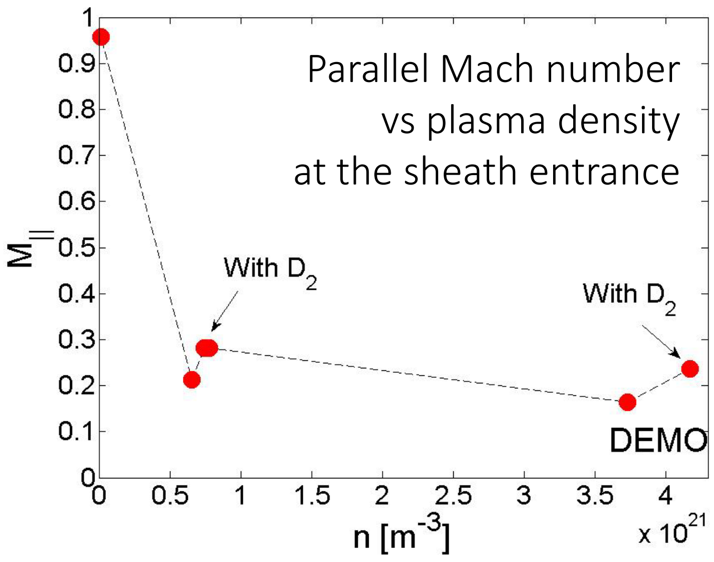
PIC modelling (BIT1): high density ($n_e > 5\cdot10^{21}$ m^{-3}) divertor sheath physics

Collisional sheath with a zoo of multi-step 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 (?)

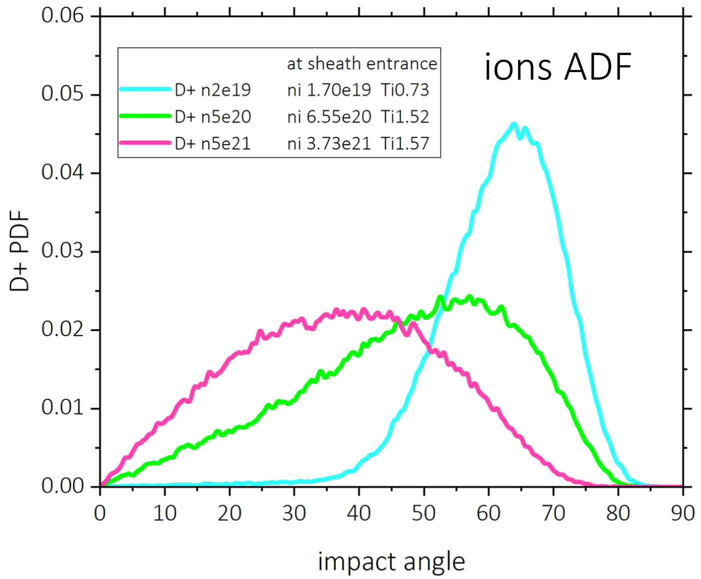
- Redistribution of heat loads to neutrals, modification of ion and neutral distribution functions (energies and angles of wall impact)
- Heavy calculations with up to 5M core-h call for code optimization and alternative A&M description (e.g. dressed cross-section method)
- W prompt re-deposition affected by $F_E > F_L$ and potential W-CX (simulations ongoing)



→ boundary conditions for edge plasma simulations (SOLPS)!

angular distributions of ions acquire the shape similar to that of neutrals ←

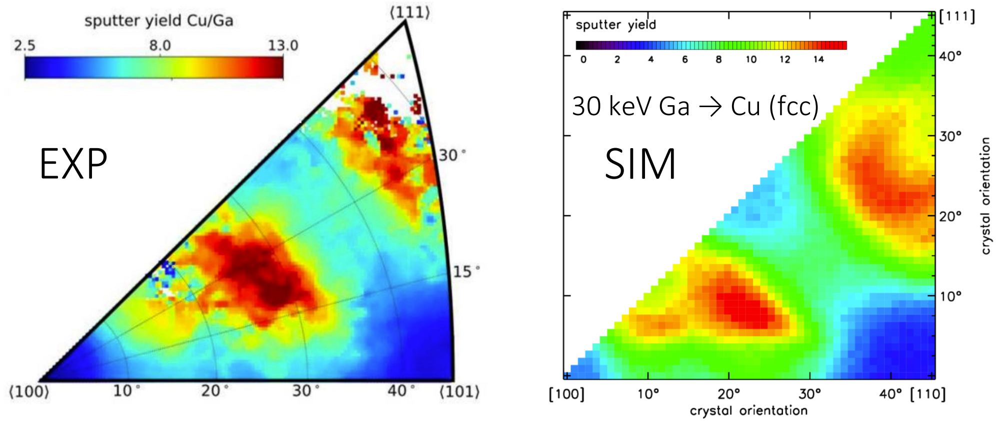
Exemplary characteristics of high density divertor sheath, such as ion and neutral EDF and ADF are available for implementation in ERO2.0 and will be compared to classical assumptions



PWI data and code capabilities improvement (in-brief)

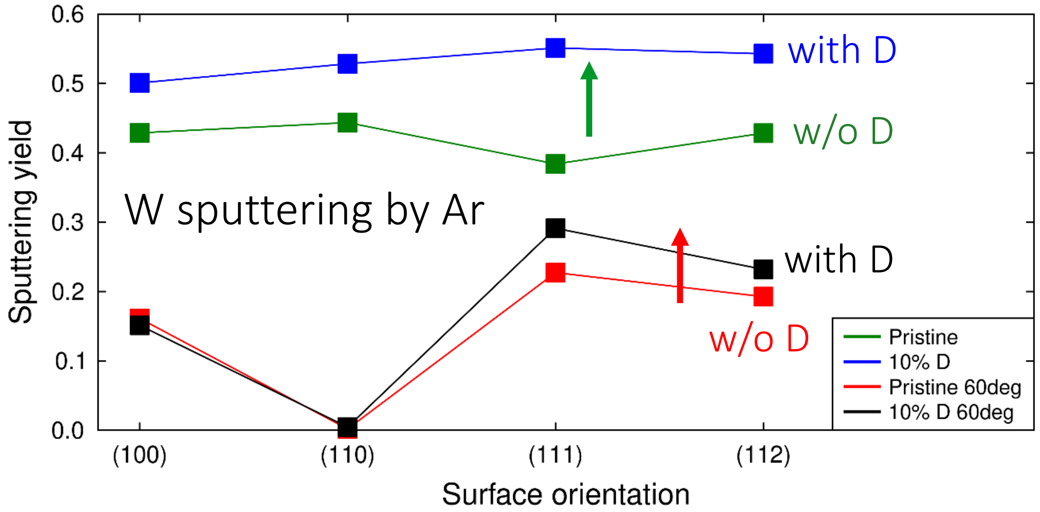
SDTrim-SP 3D

- **“Gyro-motion” extension:**
  - magnetic & electric field effects on impinging ions
  - implemented and verified against computations
  - current work: - performance optimization
    - validation against experiment
- **“Crystal” extension:**
  - static calculations validated (MD, Exp., MARLOWE)
  - current work: - pc samples & dynamic simulations



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

- Ar case studies accomplished: presence of D increases sputtering of W, strong grain orientation effect
- D and D_2 cases delayed by technical challenges (appropriate potential is slow, sputtering yield depends on the simulation cell depth, huge statistics required)
- Work on W-O started using ML-trained potential (tabGAP)



KEY ACHIEVEMENTS, PART 2:

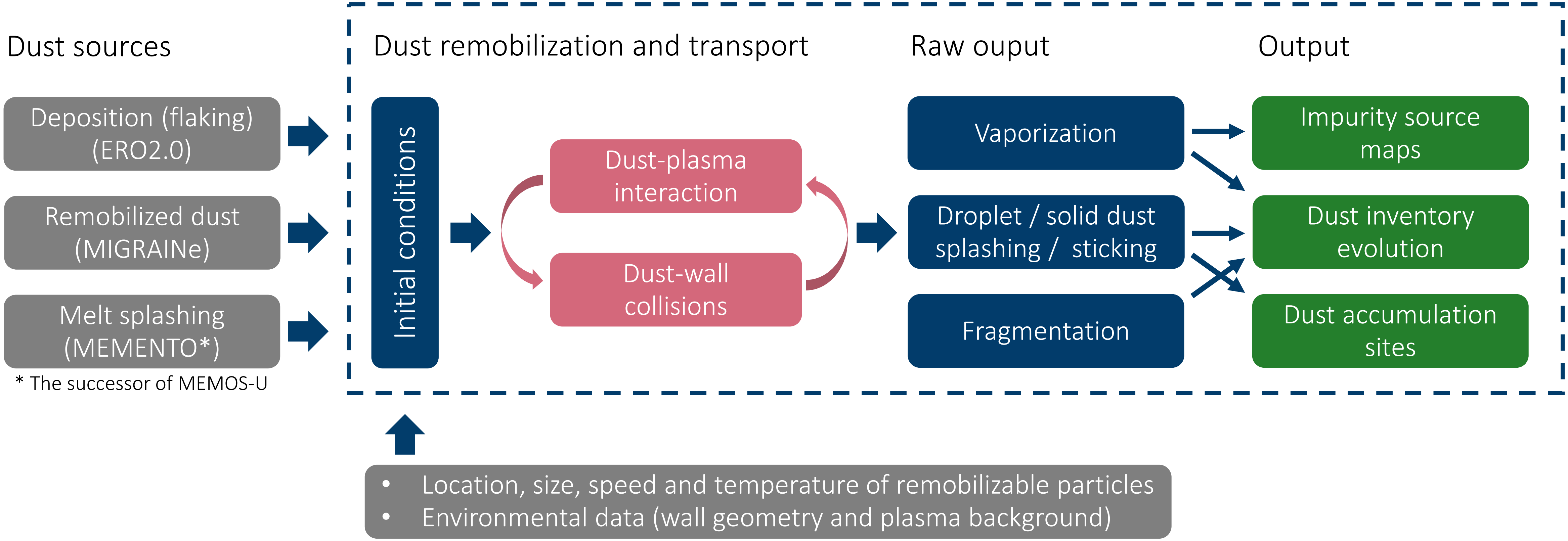
DUST TRANSPORT SIMULATIONS

Dust inventory evolution in fusion reactors

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 simulations

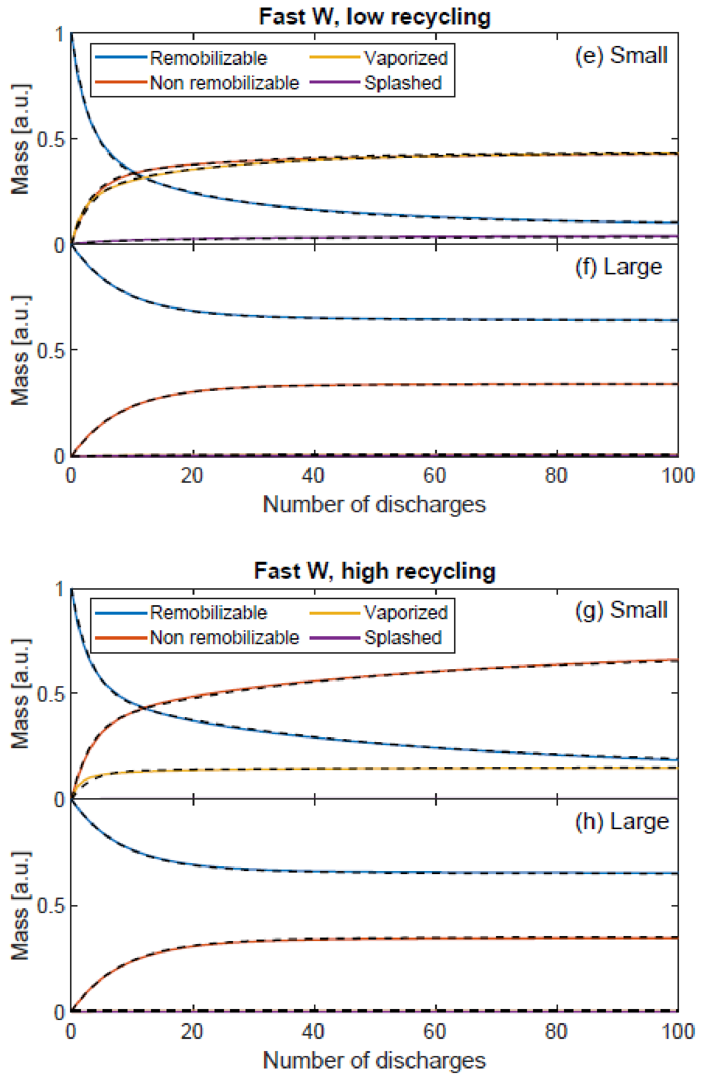


Dust inventory evolution in fusion reactors

Vignitchouk et al. PPCF 65 (2023)

Basic scenario and addressed questions

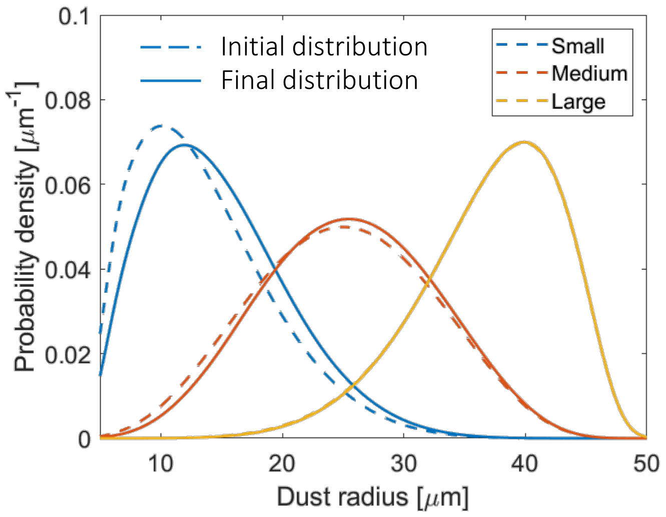
- Assume an initial dust size distribution (e.g. from past melt event)
- Particles are mobilized during discharge start-up
- Repeat identical discharges until dust inventory reaches steady-state
- Evaluate how many discharges it takes, what kind of particles are left and where in the vessel, map spatial profiles of vaporized impurities
- Initial simulations:
  - W dust in ITER-like discharges with 12 remobilization scenarios varying initial conditions (location, size distribution and speed)
  - Weighted statistical maps of atomic impurity source (vaporization)
  - Long-term in-vessel dust inventory evolution
  - Results fitted by sub-percent accuracy Markov chain models that can be integrated into more global plasma models
  - Small dust does not survive in plasma due to likely vaporization
  - Dust mobilization speed has the strongest influence on results

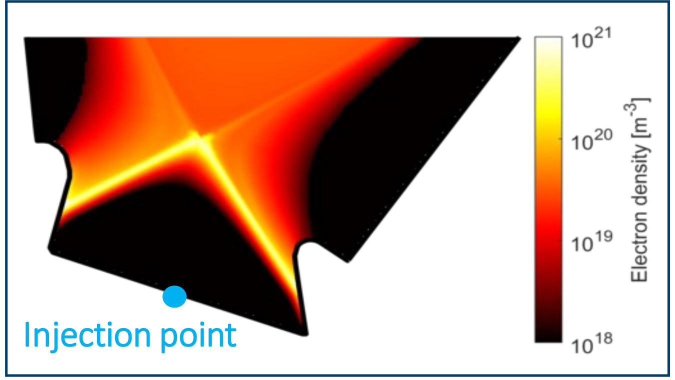


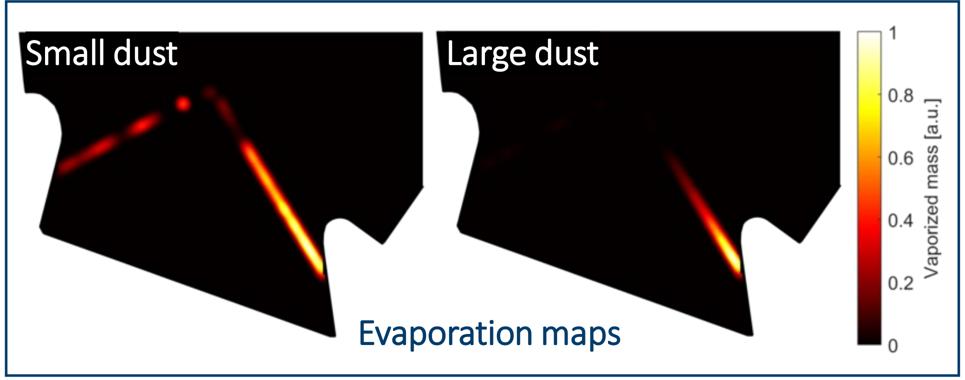
Dust inventory evolution in fusion reactors

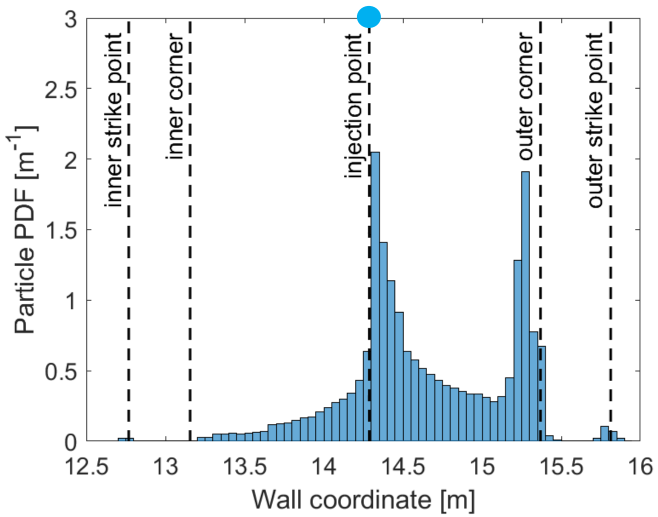
Preliminary simulations using DEMO plasma profiles (same as in ERO2.0)

- W dust injection from the middle of divertor floor
- Vaporization: significant for small particles, total mass similar to prev. study
- Impurity source echo the separatrix, outward shift for larger particles
- Outer divertor corner favored for re-deposition
- On-going: - further mobilization sites according to ERO2.0 deposition map
  - iterative simulations for long-term dust inventory evolution
  - incorporation of ion drag and multiple impurity species









KEY ACHIEVEMENTS, PART 3:

PFC RESPONSE TO TRANSIENT EVENTS

PFC response to transient events

MEMENTO (MEtallic Melt Evolution in Next-step TOkamaks)

Ratynskaia et al. NME **52** (2022)
Paschalidis et al. NME (2023) submitted

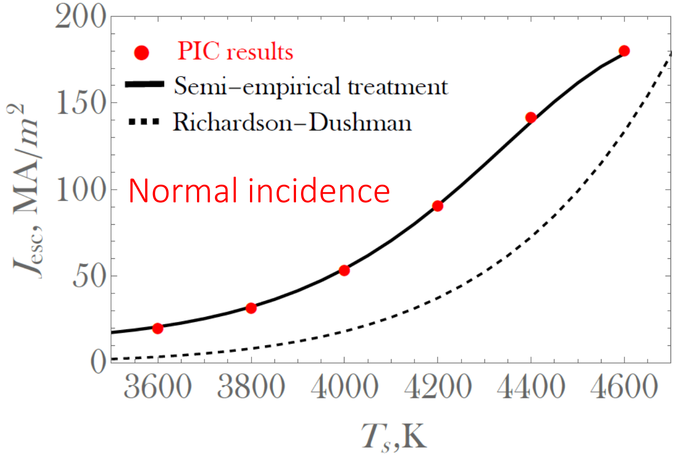
- Successor of MEMOS-U implemented using AMReX adaptive meshing framework (https://amrex-codes.github.io/amrex/)
- Coupled heat transfer, fluid dynamics and current propagation + physics updates (surface tension, dynamo term)
- Critical input: - heat loads and respective time scales (external input from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

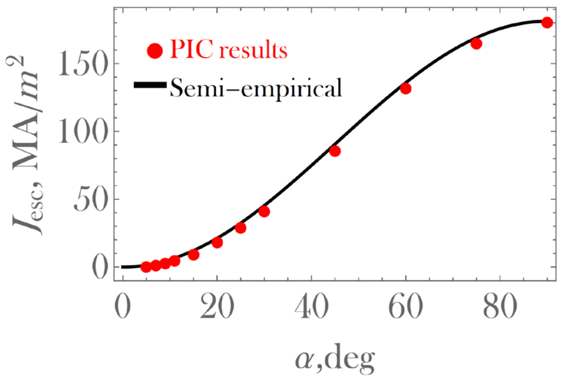
SPICE2 – a 2D3V PIC code (multi-emissive sheaths)

(*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

Komm et al. NF 60 (2020)
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 ~80% of scaling prediction

MEMENTO uses respective scalings deduced from PIC simulations

PFC response to transient events

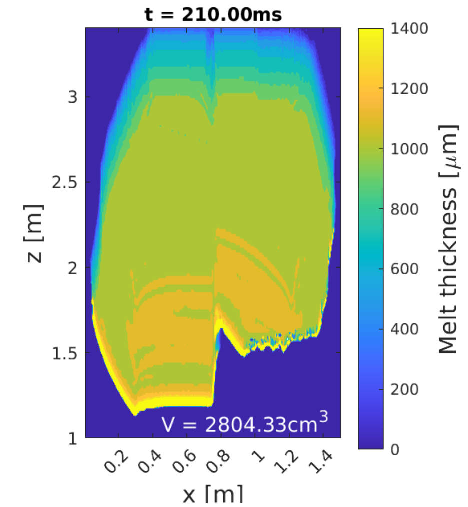
MEMENTO (MEtallic Melt Evolution in Next-step TOkamaks)

- For current DEMO design, the thermal (TQ) and the current quench (CQ) of VDEs are considered relevant for melting:
  - Downward VDE (D-VDE) TQ: max q = 4 GW/m^2 for 4 ms (lower limiter melting – negligible thickness & motion)
  - Upward VDE (U-VDE) TQ: max q = 65 GW/m for 4 ms (upper limiter melting)

  → Melt thickness reaches steady-state of < 200 µm in 4 ms for heat flux above 5 GW/m^2 (vapor shielding)

  → Modest melt thickness → appreciable viscous damping; weak TE at oblique B → modest displacement

  → Short life time of the pool due to re-solidification in few ms after termination of heat flux

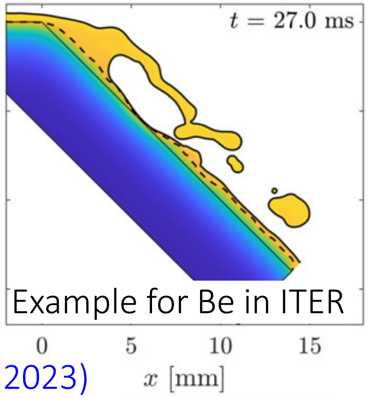


- DEMO-relevant CQ data missing: using ITER-like CQ with q = 300 MW/m^2 for 200 ms and overlapping TQ and CQ wetted areas: the absolute worst case! (halo current drives JxB)

  → Rayleigh-Taylor instability: for the estimated induced eddy current splashing within a few ms cannot be ruled out (link to WPPWIE SPD)

  → Kelvin-Helmholtz instability (due to near-wall plasma flow): unlikely

  → **W melt of 1 mm thickness and 3 m/s velocity** unstable when flowing across a sharp PFC edge → splashing is highly likely in such scenario



Vignitchouk et al. NF 63 (2023)

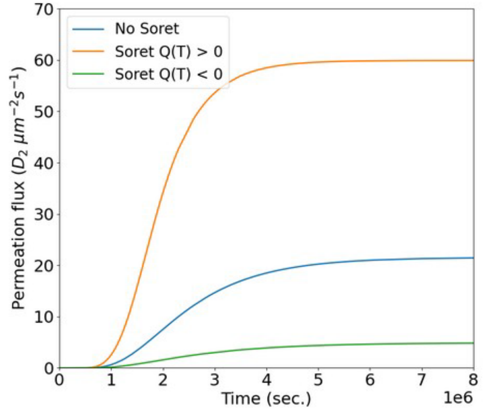
KEY ACHIEVEMENTS, PART 4:

FUEL RETENTION AND PERMEATION

Fuel retention and permeation

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 and uncertainty quantification (RAVETIME)



Highlights of code development and verification

- Soret effect implemented in TESSIM-X and FESTIM
- FESTIM interface model implemented and validated
- Simplified n-damage creation model implemented in FESTIM (ongoing)
- FESTIM He retention model under validation (He bubbles)

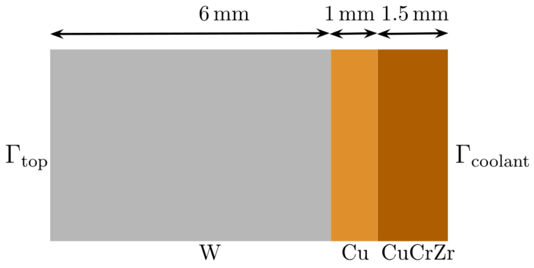
J. Dark et al. SOFT (2022)   E. Hodille et al. ISFNT-15

Creation from neutron damage − Destruction by annealing

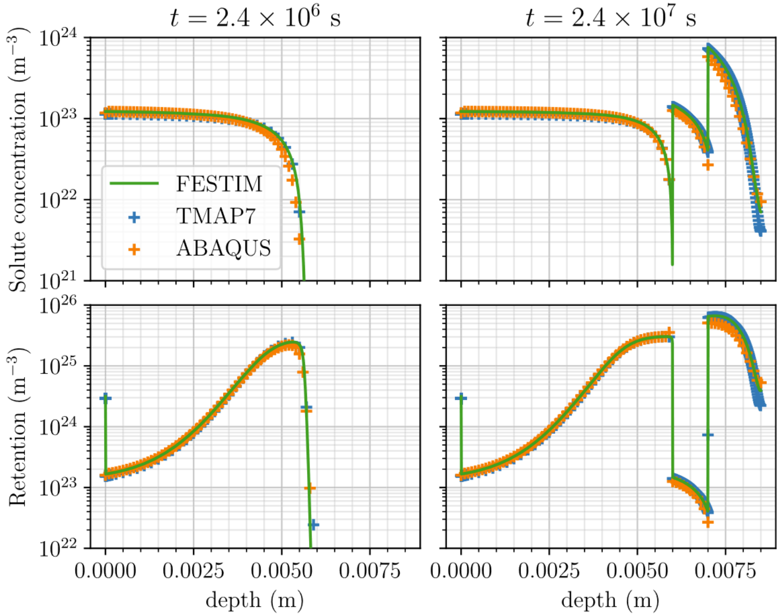
$$\frac{\partial n_t}{\partial t} = \phi \cdot K \left[1 - \frac{n_t}{n_{\max,\phi}}\right] - A_0 \cdot \exp\left(\frac{-E_A}{k_B T}\right) \cdot n_t$$

ϕ = damage rate [dpa s^{-1}]
K = trap creation factor [traps dpa^{-1}]
$n_{max,\phi}$ = maximum trap density [m^{-3}]

A_0 = trap annealing factor [s^{-1}]
E_A = annihilation activation energy [eV]
n_t = trap density [m^{-3}]



Delaporte-Mathurin et al. NF 61 (2021)

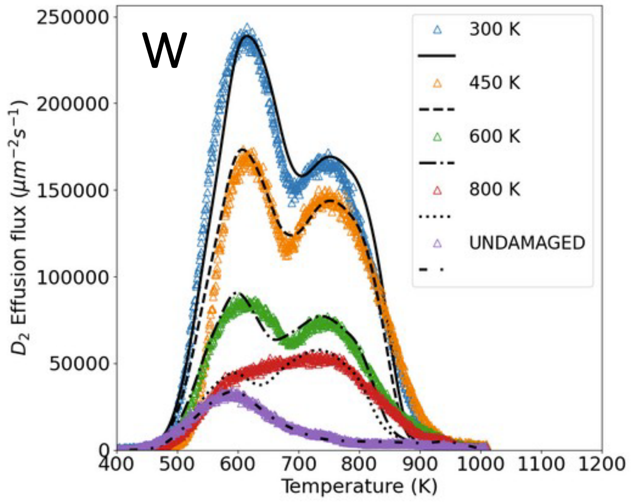


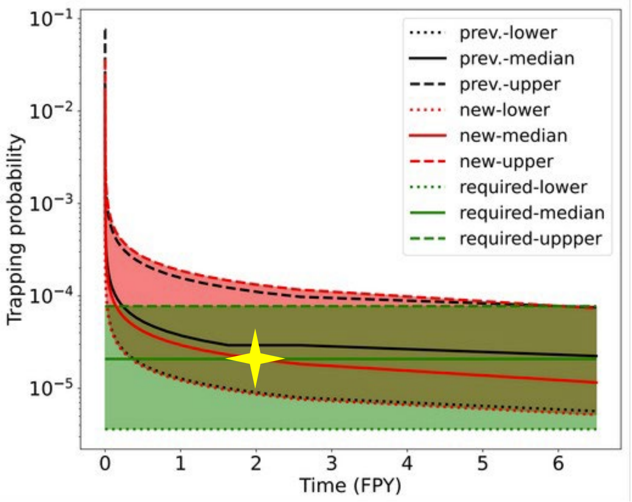
Fuel retention and permeation

DEMO first wall – refined calculations of trapping rates vs old data by R. Arredondo et al. NME 28 (2021)

- Wall approximation as W layer on EUROFER coolant structure, compare two coolant concepts (WCLL, HCPB)
- Trap energies in self-damaged W: re-fit data from M. Pečovnik et al NF 60 (2020)
- Trap energies in EUROFER: K. Schmid et al. NME 34 (2023) + new NME submission

  → displacement damage anneals at DEMO operating temperatures → only intrinsic remain
- 48 different cases considered (flux, coolant temperature and trap profiles, b.c.)
- Computing trapping probability, compare it to requirement for T self-sufficiency





- On average (for saturated n-damage):

  ~2 years for T.B.R. = 1.05

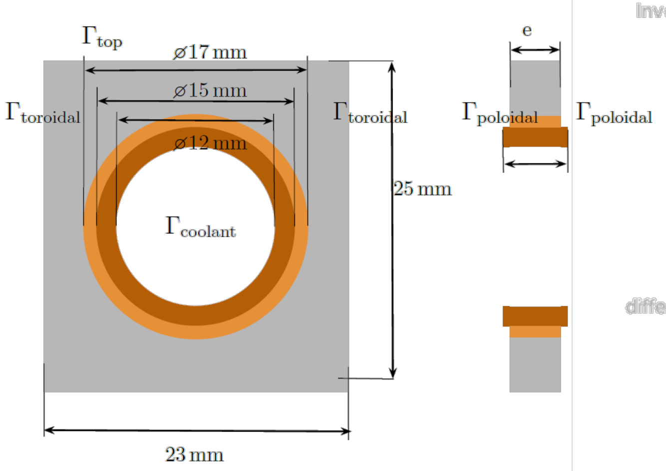
  ~1 year for T.B.R. = 1.10
- Reason: very high trap concentration by n-damage, very long time populate and thus to break through (onset of T permeation to coolant for T recovery)
- Use EUROFER armor? Does high temperature damage anneal? Increase of recycling by porous surfaces?

Fuel retention and permeation

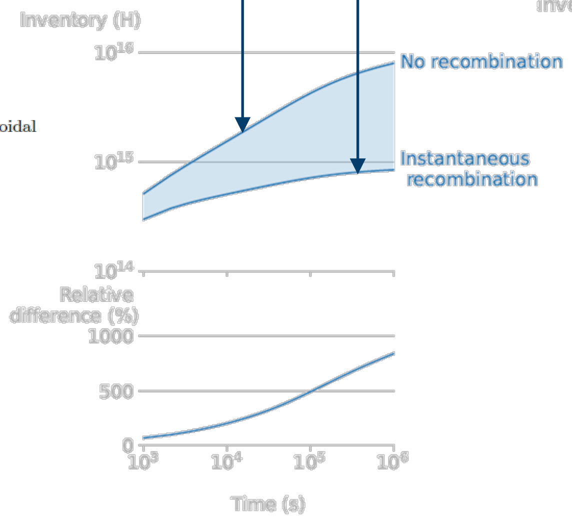
DEMO divertor

You et al. JNM 544 (2021)

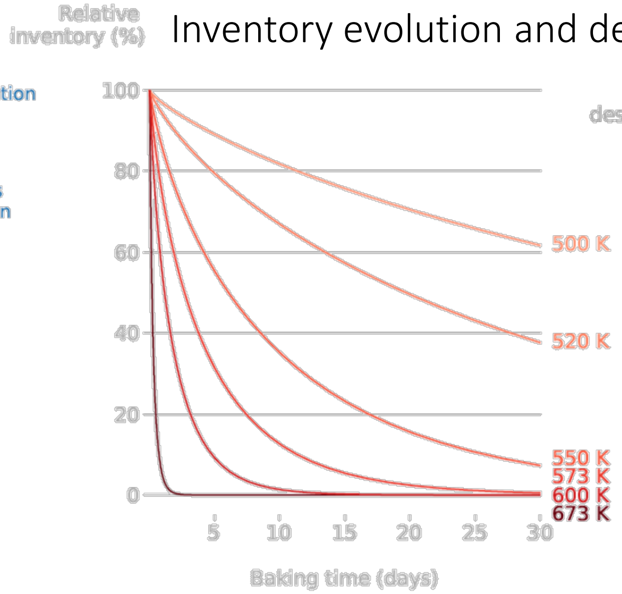
- FESTIM simulations for DEMO monoblock geometry varying monoblock thickness (e) and boundary conditions
- Addressing implantation and subsequent baking phase

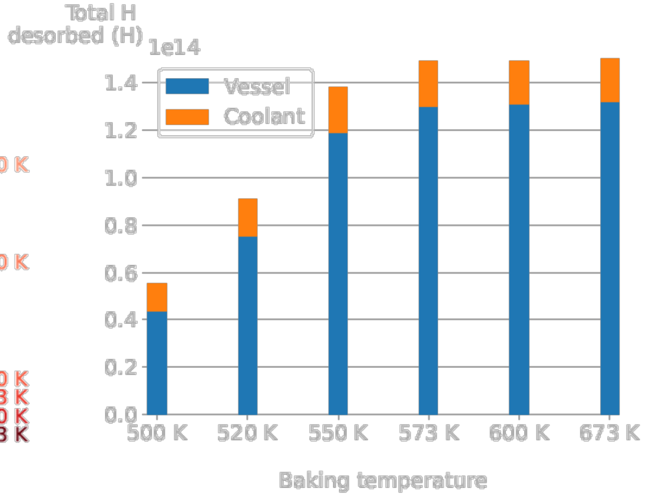


Inventory evolution during implantation
2D vs 3D



Inventory evolution and desorption/permeation during baking





Delaporte-Mathurin et al. NF submission

ACH support

- ERO2.0: optimization of hybrid parallelization performance and GPU enabling (ACH BSC – ongoing)
- SPICE2: parallelization of Poisson solver in 2D (ACH BSC – ongoing)
- MIGRAINE: HPC enabling via MPI parallelization (ACH VTT – accomplished)
- RAVETIME: HPC optimization (ACH VTT – accomplished)
- MEMENTO: HPC optimization (ACH VTT – just started)
- IMASification: ERO2.0 on the way, MIGRAIN and SPICE to follow (ACH PSNC)

Acknowledgements

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- ACH VTT: Fredric Granberg, Jan Åström, Laurent Chone
- ACH PSNC: Dmytro Yadykin, Piotr Chmielewski, Grzegorz Pelka

Open questions and future plans

Current status: most of milestones achieved, some delays and modifications (personnel, lack of DEMO specific input)

Critical for advancement:

- ERO2.0: plasma background with extended grid (new baseline) and angular resolved CX data (SOLPS, other codes?)
- MIGRAINe: transient plasma profiles for ramp-up and VDEs (via DCT, backup ENR arrangements)
- MEMENTO: better defined DEMO-specific heat loads for CQ (via DCT)

Next steps:

- ERO2.0 simulations with improved physics: CX, high density sheath, role of gaps, erosion data (incl. morphology)
- Detailed assessment of melt layer stability under VDEs: melt splashing and droplet-to-dust probabilities
- Finalized catalog of dust re-mobilization scenarios with corresponding dust inventory evolution & mapping
- Improved fuel inventory analysis with better parameterized n- and He-induced damage, uncertainty quantification
- IMAS compatibility (I/O) for ERO2.0, MIGRAINe and SPICE

- THANK YOU FOR YOUR ATTENTION -

TSVV-07 DELIVERABLES (BACKUP SLIDE)

Status: black – on a good way, in color – from 2024 on

D1. Steady state 3D-resolved W erosion rates at DEMO first wall and divertor
D2. Location mapping for net (co-)deposition and impurity sources from the wall
D3. Large-scale surface modifications due to melting / melt-motion induced by transients
D4. Assessment of surface roughness and lifetime of PFCs affected by transients
D5. Stability of melt layers during transients, droplet characteristics in case of splashing
D6. A catalog of representative cases for dust (re-)mobilization conditions
D7. Dust survival rates, inventory evolution, accumulation maps of re-solidified droplets
D8. Prediction of fuel inventory in multi-component PFCs accounting for thermal and mechanical effects, neutron and He damage, morphological changes
D9. Uptake of D/T in W and across interfaces to the coolant with UQ
D10. Fully kinetic sheath simulations in 1D/3D providing plasma profiles and boundary conditions at the plasma sheath based on the DEMO plasma solution
D11. Effective W erosion yields for rough surfaces and re-solidified melt layers with UQ
D12. W erosion yields under D/T supersaturation vs impact parameters and temperature
D13. W-O and W-O-H interatomic potentials for oxidized surfaces, e.g. after transients
D14. A suite of HPC optimized codes for DEMO PWI with IMAS-adapted data exchange

TSVV-07 MILESTONES (BACKUP SLIDE)

Year 1: ITER-like plasma case	
M1.1	SOLPS-ITER steady-state plasma background (ITER plasma) is adapted to DEMO, post-processed for ERO2.0 and MIGRAINe, relevant data are extracted for PIC
M1.2	Scoping PIC simulations are performed to assess the characteristics of the plasma sheath and resulting impact angles and energies in steady state
M1.3	Intermediate results on erosion of H supersaturated W from MD simulations are reported (with delay)
M1.4	MIGRAINe scoping dust transport simulations with ITER-like ramp-up and steady state plasma profiles are performed
M1.5	Thermo-migration is implemented in TESSIM-X and validated
M1.6	Validation of the interface model of FESTIM is completed
M1.7	Common test cases for retention modelling are identified (continuously ongoing)
M1.8	HPC optimization requirements for the codes are identified, the respective work initiated
Year 2: SOLPS DEMO solution	
M2.1	Preliminary ERO2.0 simulations with existing PWI database, sheath models & adapted ITER-like plasma background performed, first erosion-deposition maps provided
M2.2	MIGRAINe dust transport simulations are performed using ITER-like profiles and preferable net deposition locations provided by preliminary ERO2.0 runs
M2.3	DEMO plasma background obtained (external input from relevant work packages), post-processed to be used in ERO2.0 and MIGRAINe, relevant data for PIC extracted
M2.4	Scoping PIC simulations including combined thermionic emission and secondary electron emission performed, validity of existing scalings for MEMOS-U assessed
M2.5	Final results on erosion of D/T supersaturated W from MD simulations are reported
M2.6	Representative values of surface heat fluxes and halo current densities during DEMO VDEs obtained (external input) and processed for MEMOS-U simulations
M2.7	Gyromotion module is implemented in SDTrimSP-3D
M2.8	Neutron damage model with damage stabilization is implemented in FESTIM and TESSIM-X (validation not yet completed)
M2.9	TESSIM-X, MHIMS and FESTIM simulations of H retention under DEMO conditions (without n-damage) and relevant material structures are performed
M2.10	IMAS compatibility requirements for the codes are detailed and the work is initiated
Year 3: Conceptual design review	
M3.1	Erosion data under DEMO D/T supersaturation is implemented in ERO2.0
M3.2	Erosion-deposition maps from ERO2.0 with DEMO plasma solution are provided
M3.3	MEMOS-U simulations of PFC response under VDEs and loss of confinement are performed, macroscopic surface modifications and melt splashing are assessed
M3.4	MIGRAINe dust transport simulations are performed using DEMO steady state profiles and preferable net deposition locations provided by ERO2.0 (ongoing)
M3.5	SDTrimSP-3D simulations are performed to assess the role of rough surfaces and re-solidified melt morphology on effective erosion yields
M3.6	Role of gaps between divertor and limiter monoblocks is addressed by means of PIC simulations (heat loads and ion penetration)
M3.7	TESSIM-X and FESTIM simulations of H retention under DEMO conditions (with n-damage) and relevant material structures are performed and cross-validated
M3.8	Intermediate results on W-O potential development are reported
M3.9	Integrated results regarding W erosion (steady state and transients) and T retention for the DEMO conceptual design review are reported
M3.10	Intermediate results on IMAS interfaces implementation are reported
M3.11	Transient plasma profiles representative of VDEs and loss of confinement events in DEMO are obtained (external input) and implemented in MIGRAINe