WP PWIE: SP D reporting 2022 / SP D plans for 2023

SPL D: Andreas Kirschner

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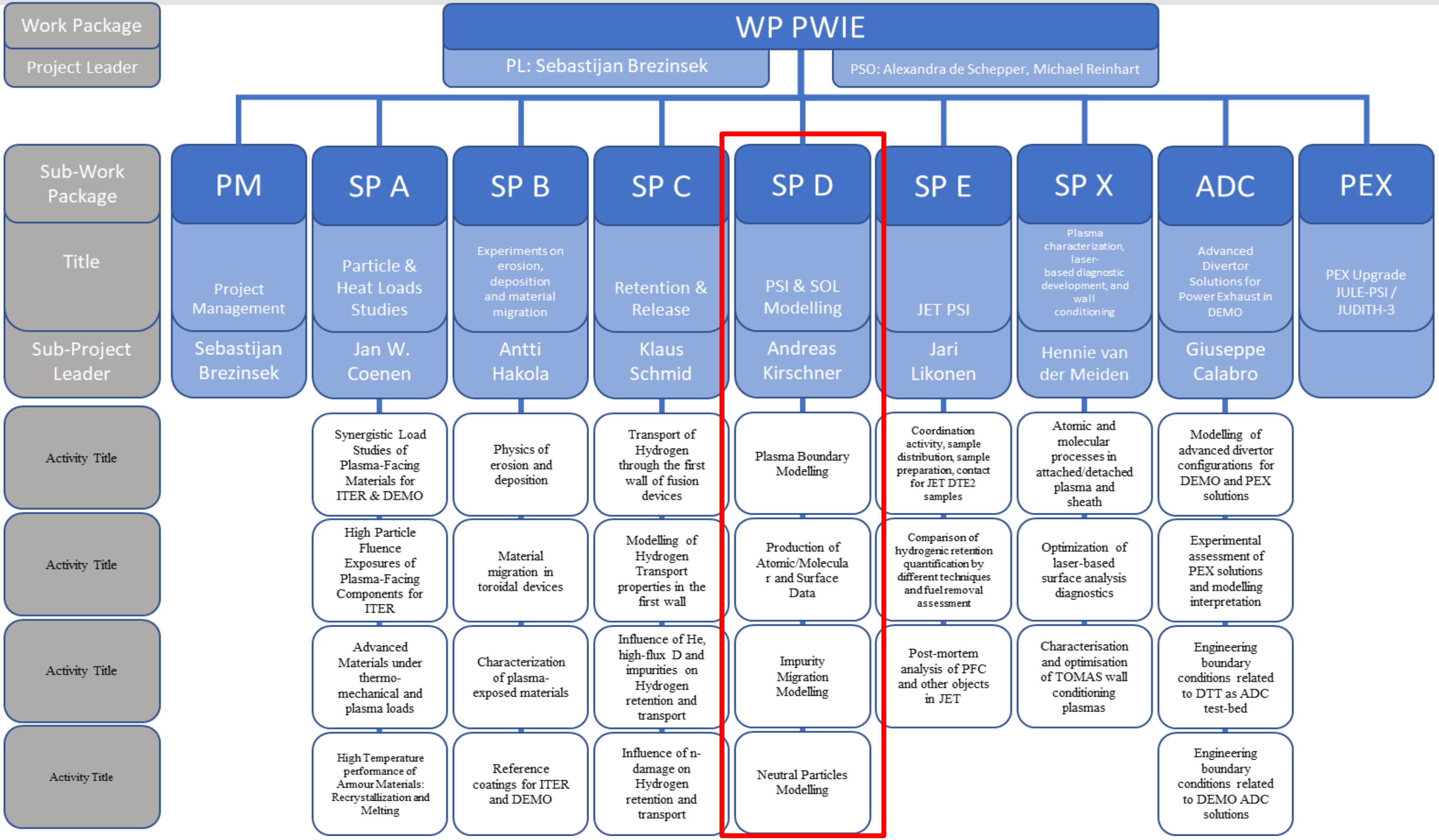
PWIE 2022/2023: SP D



SP D Tasks 2022 (1)

Activity	Deliverable ID(s)	Task Title
		SP D.1 Plasma boundary modelling
SP D.1	D001	Plasma background parameters of WEST for modelling of impurity migration experiments (focus on He and D discharges) (CEA)
SP D.1	D002	Plasma background parameters of linear devices (in particular MAGNUM-PSI) for modelling of impurity migration experiments (DIFFER)
SP D.1	D003	Plasma background parameters of GyM for modelling of impurity migration experiments (ENEA)
SP D.1	D004	Plasma background parameters of W7-X for modelling of impurity migration experiments as well as PSI-2 (FZJ)
SP D.1	D005	Characterization of the emissive and collisional plasma sheath (considering ELMy discharges, rough surfaces, DT plasma) (IPP.CR)
SP D.1	D006	Semi-empirical analytic expressions of emitted current escaping form tungsten surfaces (inter- and intra-ELM conditions) (VR)
SP D.1	D007	Plasma background parameters of AUG and JET-ILW for modelling of impurity migration experiments (VTT)
		SP D.2 Production of atomic/molecular and surface data
SP D.2	D001	Dust production model for anomalous events and detached conditions (CEA)
SP D.2	D003	D3.1: Effect of seeding projectiles (e.g. Ar, Kr) on tungsten sputtering, D3.2: Electron impact cross sections (ionization, excitation), D3.3 Combine BCA and MD at transition from low energies to BCA limit (OAEW)
SP D.2	D004	Erosion information of surfaces including morphology, roughness, fuzz (OAEW)
SP D.2	D005	Model for dust production from melting; prediction of dust formation from molten metal, droplet ejection (VR)
SP D.2	D006	D6.1: Erosion and retention properties of redeposited tungsten, D6.2: Interaction potential of tungsten to be used for sputtering/reflection modelling , D6.3: Sputtering and reflection yields for various kinds of tungsten morphologies (VTT)
SP D.2	D007	Upgraded atomic/molecular database and CRM for molecules (VTT)
SP D.2	D008	Erosion information of 2D surfaces (various morphologies) in comparison to experiments (MPG)

SP D Tasks 2022 (2)

Activity	Deliverable ID(s)	Task Title
		SP D.3 Impurity migration modelling
SP D.3	D001	ERO2.0 simulations of tungsten transport in WEST, determination of main tungsten sources in WEST, comparison with spectroscopy (CEA)
SP D.3	D002	ERO2.0 simulations of dynamic morphology studies in GyM, ERO2.0 simulations of the transport of sputtered material in GyM, Global ERO2.0 modelling of erosion/deposition in AUG (ENEA)
SP D.3	D003	~~D3.1: Model of morphology effects & comparing of modeling results w. experimental ion beam data,~~ D3.2: Local modelling of 13C MPM injection experiment at W7-X & comparison to post-mortem data, D3.3: Erosion, impurity migration & deposition modelling for JET-ILW, incl. recessed areas (FZJ)
SP D.3	D004	D4.1: Predictive tungsten migration in W7-X, D4.2: Beryllium/tungsten migration with realistic 3D ITER first wall (MPG)
SP D.3	D005	ERO simulations of AUG and JET-ILW erosion and migration experiments (including nitrogen, tungsten and beryllium) and comparison with experimental data (VTT)
SP D.3	D006	Dust adhesion and self-charging (VR)
		SP D.4 Neutral particles modelling
SP D.4	D001	Updated version of DIVGAS and benchmarking simulations studying the newly developed features of the code on the example of DEMO divertor (KIT)
SP D.4	D002	Atomic and molecular fluxes to the wall surfaces (VTT)

SP D.1: Plasma boundary modelling

- Provide plasma background parameters to be used in impurity migration codes
- Provide details of sheath characteristics
- Devices mainly involved: WEST, (AUG), JET-ILW, MAGNUM-PSI, GYM, (PSI-2), W7-X

- Many results have been produced: some examples will be presented in the following …
- No major issues occurred

Deliverable: *D001, D002, D003, D004, D005, D006, D007*
Status: *completed / partially completed in 2022 (as planned)*
Modelling*: SOLEDGE-EIRENE, SOLPS-ITER, EMC3-EIRENE, PIC codes*

Human Resources: *total 22 PM*
Involved RU: *CEA, DIFFER, ENEA, FZJ, IPP.CR, VR, VTT*
Linked WP or TSVV: *TSVV 5 , 6, 7, WP TE, WP W7X*

SP D.2: Production of atomic/molecular & surface data

- Provide erosion and reflection data considering morphology effects, roughness, fuzz, re-deposited material
- Main focus on tungsten materials. Projectiles: seeding species, hydrogen isotopes
- Provide data for dust formation
- Provide atomic data, molecular data for CRM

- Many results have been produced: some examples will be presented in the following …
- No major issues occurred

Deliverable: *D001, D003, D004, D005, D006, D007, D008*
Status: *completed / partially completed in 2022 (as planned)*
Modelling*: MD codes, BCA codes, …*

Human Resources: *total 22 PM*
Involved RU: *CEA, OEAW, VR, VTT, MPG*
Linked WP or TSVV: *TSVV 5, 6, 7, WP TE*

SP D.3: Impurity migration modelling

- Impurity migration and resulting erosion/deposition in comparison to experiments (mainly WEST, JET-ILW, AUG, W7-X, GYM)
- Consideration of dynamics of morphology
- Predictive modelling for ITER with realistic 3D wall
- Dust adhesion

- Many results have been produced: some examples will be presented in the following …
- No major issues occurred

Deliverable: *D001, D002, D003, D004, D005, D006*
Status: *completed / partially completed (as planned)*
Modelling*: WALLDYN, ERO2.0 (ERO), …*

Human Resources: *total 31 PM (2 PM moved to SP B)*
Involved RU: *CEA, ENEA, FZJ, MPG, VTT , VR*
Linked WP or TSVV: *TSVV 5, 6, 7, WP TE, WP W7X*

SP D.4: Neutral particles modelling

- Modelling of neutral particle gas dynamics and exhaust (DEMO)
- Estimation of neutral fluxes to wall (to be used in migration codes for erosion)

- Many results have been produced: some examples will be presented in the following …
- No major issues occurred

Deliverable: *D001, D002*
Status: *completed / partially completed in 2022 (as planned)*
Modelling*: DIVGAS, EIRENE*

Human Resources: *total 11 PM*
Involved RU: *KIT, VTT*
Linked WP or TSVV: *TSVV 5, 6, 7, WP TE*

SP D results obtained in 2022 and plans for 2023

some examples

Remark: *details of tasks for 2023 and manpower provisional*

SP D.1: D001 – Plasma background for WEST

CEA 2PM

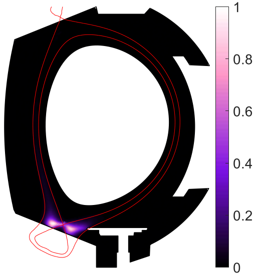
G. Ciraolo, N. Fedorczak, Y. Marandet, M. Raghunathan, S. Di Genova, H. Yang

➢ More details: see dedicated talk

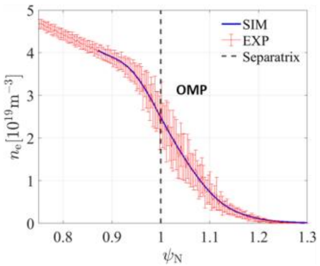
- <u>For Deuterium plasma discharges</u> : The set of 2D plasma backgrounds simulated with SOLEDGE-EIRENE has been increased with new cases compared with experimental data

Example:
WEST #56420

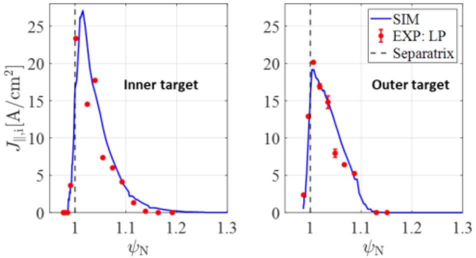
Prad [MW/m³]



electron density profile at the outer mid-plane

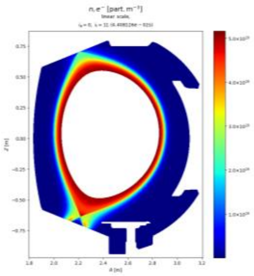


Parallel ion saturation current at the inner (left) and outer (right) divertor targets

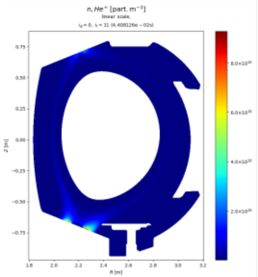


- We have also started to simulate <u>Helium plasma backgrounds</u>, see a first example below

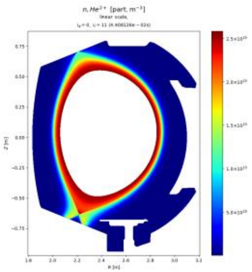
2D map of electron density



2D map of He+ density



2D map of He++ density

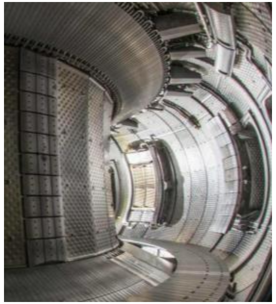


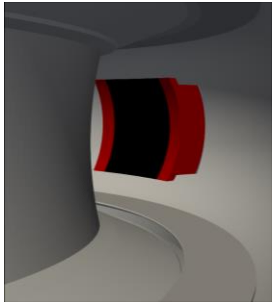
SP D.1: D001 – Plasma background for WEST

CEA 2PM

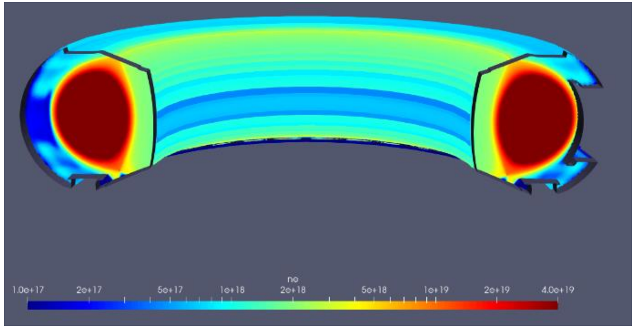
G. Ciraolo, N. Fedorczak, Y. Marandet, M. Raghunathan, S. Di Genova, H. Yang

- For Deuterium plasma discharges : In order to investigate the role of toroidally localized objects, we are performing 3D transport SOLEDGE simulations with a **non-axysimmetric wall**

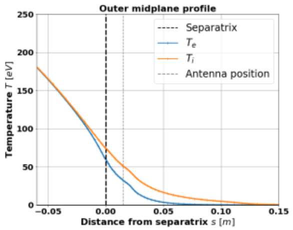


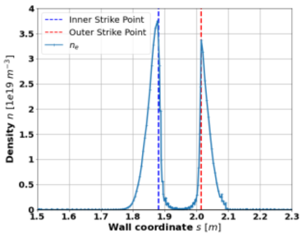


3D map of the electron density obtaind with a toroidally localized antenna limiter

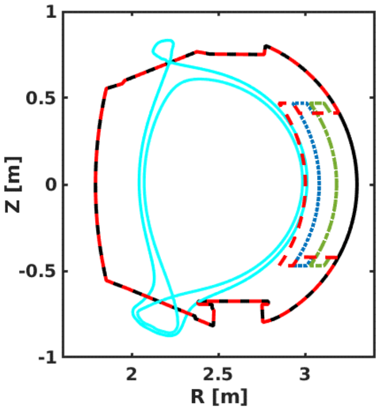


Example of outer midplane and target profiles





Ongoing 3D plasma background transport simulations considering several positions of the antenna limiter



SP D.1: D001 – Plasma background for WEST

CEA 2PM

G. Ciraolo, N. Fedorczak, Y. Marandet, M. Raghunathan, S. Di Genova, H. Yang

Plan for 2023: 2PM

- Modelling of plasma backgrounds for WEST, one focus on long-pulse, high-fluence discharges

SP D.1: D002 – Plasma background for MAGNUM-PSI

J. Gonzalez, E. Westerhof

DIFFER 2PM

EIRENE – Eunomia comparison: huge difference in the implementation of plasma-neutral collision process was found between Eirene and Eunomia

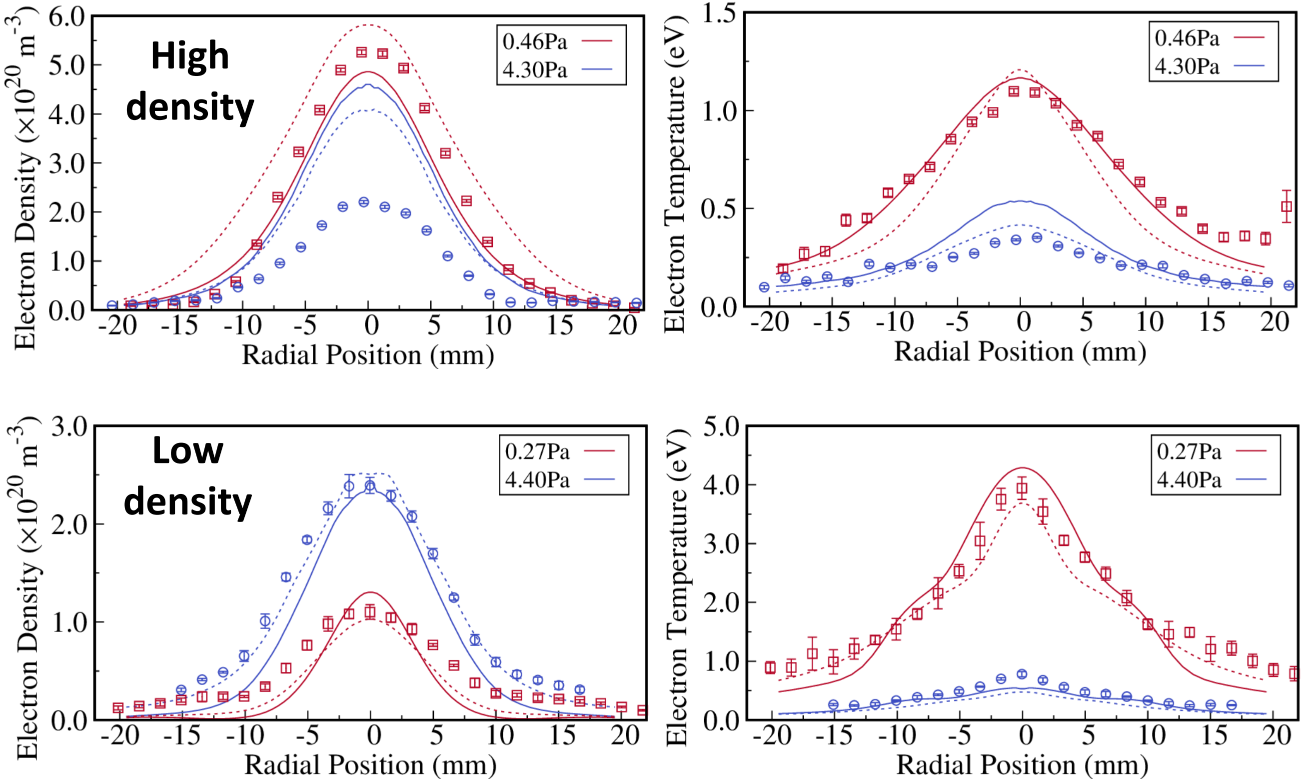
- Right now, SOLPS-ITER can reproduce previous results obtained with B2.5-Eunomia for Magnum-PSI simulation.
- Discrepancies still appear for some cases (*e.g.* high plasma density case with high neutral pressure in the target chamber).
- SOLPS-ITER is able to provide converged solutions in situations where B2.5-Eunomia had issues, probably because of the huge plasma sources computed.
- Discrepancies are being analysed right now: effect of vibrational states, missing collision process or not properly represented for very low plasma temperatures (T_e < 0.2eV)…
- The discrepancies in the plasma sources lead to completely different *free-parameters*: plasma potential at the source (unknown boundary condition) and anomalous transport coefficients.
- Moreover, the resulting neutral distribution in the plasma beam region differs between SOLPS-ITER and B2.5-Eunomia.
- New manuscript summarizing this data is already in the pinboard and will be submitted to PPCF.
- New experimental campaign to measure plasma potential at the source and neutral distributions at the target in a wide range of plasma scenarios will be carried out soon.

SP D.1: D002 – Plasma background for MAGNUM-PSI

DIFFER 2PM

J. Gonzalez, E. Westerhof

Electron density and temperature profiles



SOLPS-ITER (solid lines)

B2.5-Eunomia (dashed lines)

TS (data points)

at the TS target position at two target neutral pressures

J. Gonzalez, E. Westerhof

DIFFER 2PM

Coupling with FE target model

- Magnum-PSI SOLPS-ITER case has been coupled with a FE model to self-consistently describe target properties.
- Currently working in making the coupling general as right now it is case-specific.
- Also working in self-consistently coupling additional parameters to the surface temperature. Particular interest in liquid targets.

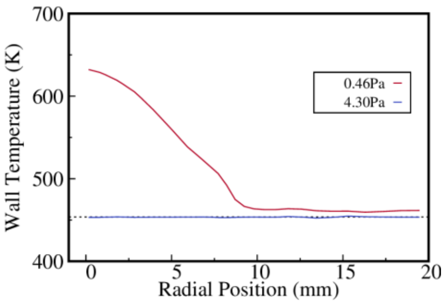


Fig. 8: Surface temperature at the target calculated by the 2D finite Element wall model.

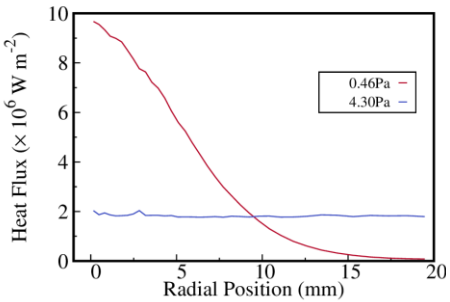


Fig. 9: Heat flux going through the target

SP D.1: D002 – Plasma background for MAGNUM-PSI

J. Gonzalez, E. Westerhof

DIFFER 2PM

Other works

- Simulations for the Vapour Box experiment in Magnum-PSI. Still waiting for experiments for comparison and validation of cases with and without lithium. Paper for simulations in pinboard.
- Comparison with D-Li experiments performed in Magnum-PSI. First simulations of Magnum-PSI using D. Good agreement also with Dummy case involving D and not Li.
- Integration of linear devices in SOLPS-ITER workflow. Now it is much more easier to use DivGeo to generate cases for linear devices, particularly Magnum-PSI, which aids in the generation of cases and the exchange of knowledge between linear devices and tokamaks.

SP D.1: D002 – Plasma background for MAGNUM-PSI

DIFFER

Plans for 2023: 2PM

- Additional comparison between SOLPS-ITER and B2.5-Eunomia when new experimental data is available.
- Continue with the implementation of the FE target model.
- Analyse discrepancies with experiments.
- Add to Eirene the capability to output sources per collision term, which would aid in analysing relevant collision process in Magnum-PSI (and other devices).
- Simulation of smaller linear device UPP, also operated at DIFFER.

SP D.1: D003 – Plasma background for GyM

ENEA 2PM

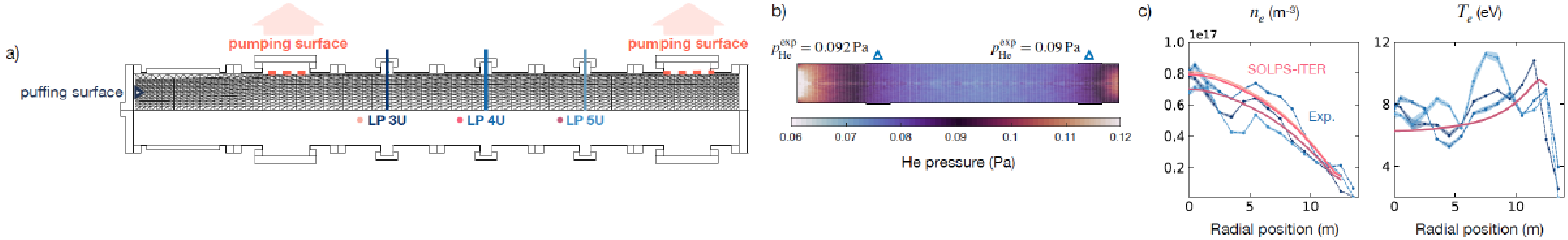
M. Passoni, E. Tonella, G. Alberti, A. Uccello

➢ More details: see dedicated talk

Benchmark of SOLPS-ITER simulations with experimental LP data from GyM (fig.1)

- Optimisation of simulation input (recycling coefficients, D_n, P_{ext}) to obtain good agreement with GyM experimental Langmuir probes (LP) data in the full machine configuration - **completed**

Fig.1 *a) Setup for benchmark of experiments with SOLPS-ITER. b) Helium gas pressure. c) Comparison between SOLPS-ITER simulations and exp. LP results.*



SP D.1: D003 – Plasma background for GyM

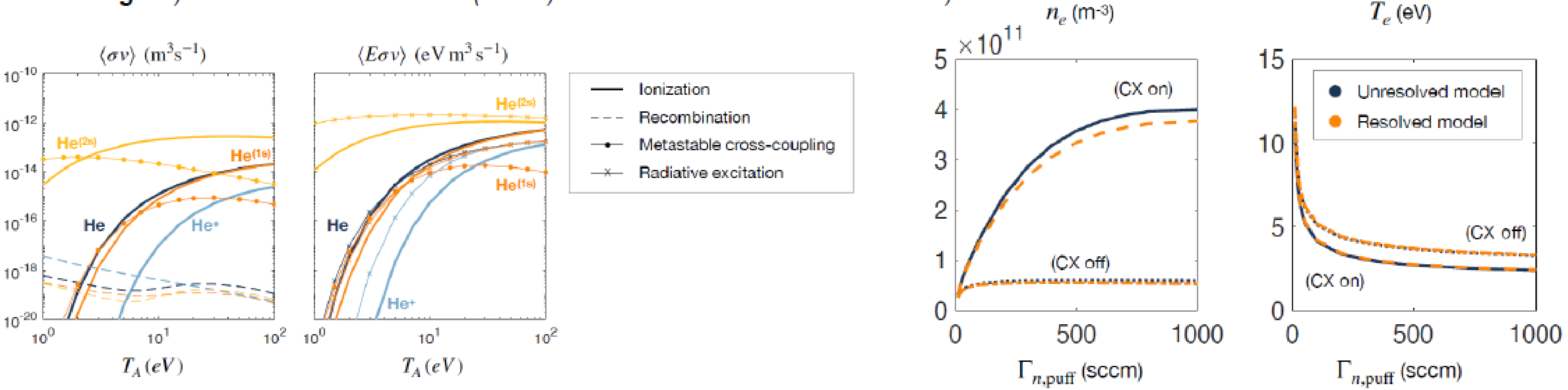
M. Passoni, E. Tonella, G. Alberti, A. Uccello

ENEA 2PM

Investigation of He metastable states (MS) in low-temperature plasmas (fig2.a)

- Implementation of MS resolved model (ADAS rate coefficients) in the 0D model [Tonello E. et al, NF 2022], already benchmarked with SOLPS-ITER. Results show small difference between metastable resolved and un-resolved models in GyM conditions (fig2.b)- **completed**
- Implementation of MS in EIRENE input file - **ongoing**

***Fig.2** a) Reaction rate coefficients (ADAS) for He with metastables resolved. b) results of 0D model resolved vs. un-resolved.*



SP D.1: D003 – Plasma background for GyM

ENEA

Plans for 2023: 2PM

- **Assess the effect of metastable He atoms**
  i. Perform SOLPS-ITER simulations including the MS states of He, using the prepared EIRENE input file (within 2022).

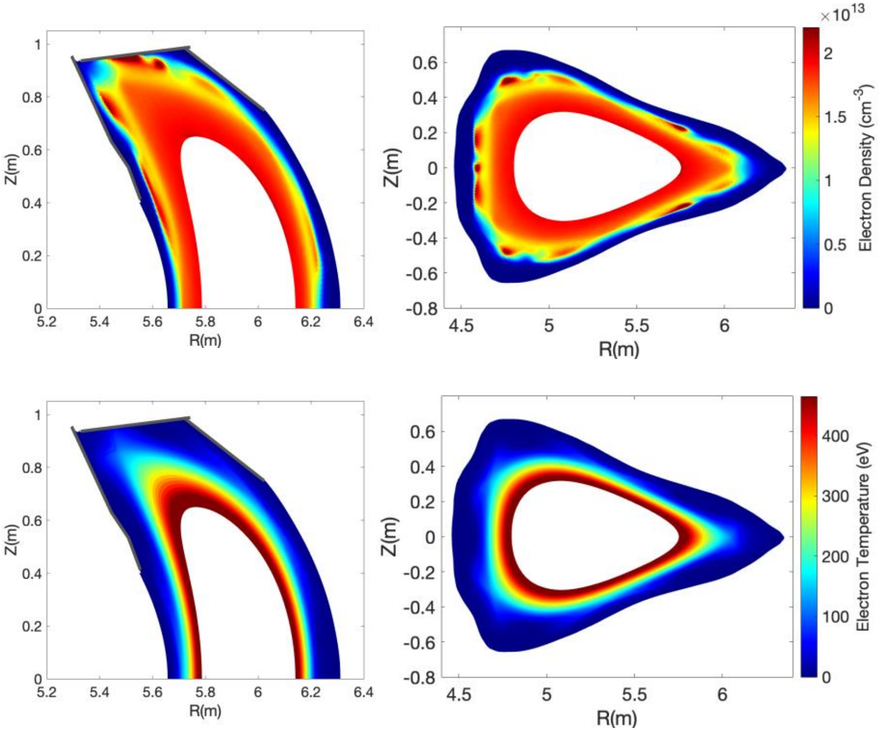
- **Initial development of the sample-holder geometry**
  i. Analysis of the LPs experimental data with sample-holder and investigation of the best strategy to perform the corresponding SOLPS-ITER simulations.
  ii. Study extended-grid code at SOLPS-ITER training workshop (Leuven 14-18/11/2022).

SP D.1: D004 – Plasma background for W7-X & PSI-2

FZJ 4PM

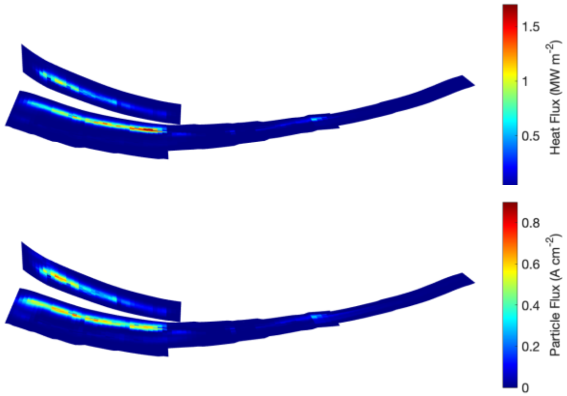
S. Xu

EMC3-EIRENE for W7-X: example case



Half of the bean shape cross-section

Triangular shape cross-section



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3D equilibrium is calculated by HINT with beta effects and plasma current effects being considered.

* S. Xu et al., Submitted to Nuclear Fusion

SP D.1: D004 – Plasma background for W7-X & PSI-2

FZJ

Plan for 2023: 4PM

- Focus on EMC3-EIRENE for PSI-2, "standard" plasma solution, including He

SP D.1: D005 – Sheath characteristics

IPP.CR 5PM

D. Tskhakaya, M. Komm, A. Podolnik

- BIT1 code has been updated to include higher ionized states of Ne (and Ar) → more than 1000 new processes. Simulation accuracy limits maximum ionized state to 4.
- We performed sets of inter-ELM SOL modelling via BIT1 for basic high performance scennarios for COMPASS-U and ITER (see details on the next slides) [1].
- In both cases ion temperature was low leading to W sputtering negligible. Important to note that this result helds even for impurity unseeded COMPASS-U SOL.

ITER modelling

Ne seeded type-I ELMy shot (IMAS IDS number: 122408/3)
OMP parameters are from SOLPS-ITER run: T_e = 160 eV, T_i= 300 eV, n_e= 4x10^{19} m^{-3} (3rd magnetic flux tube)

	Only	Ne$^+$	Ne$^{+i<5}$	
	ID	OD	ID	OD
$T_{e,\,OD}$	2.0	3.5	2.2	2.5
$T_{i,\,OD}$	2.1	4.2	2.4	2.8

- BIT3 modelling of the 3D plasma sheath (ongoing in 2022)

SP D.1: D005 – Sheath characteristics

IPP.CR 5PM

D. Tskhakaya, M. Komm, A. Podolnik

SPICE2 – SHEATH SIMULATIONS

SPICE2 used in quasi-1D regime to provide baseline data for comparison with future upgrades

AIMS

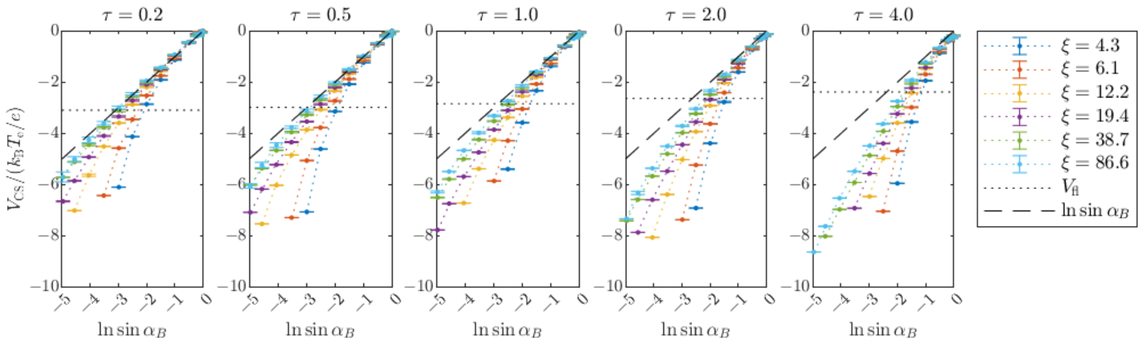
- Study sheath profiles in potential, density, averaged velocities.
- Use simulated profiles for particle tracing (probe application).
- Investigate validity of fluid assumptions [Stangeby NF 2012] for shallow angles and wide range of potential.

PARAMETERS

Magnetization $\xi = r_L/\lambda_D$, temperature ratio $\tau = T_i/T_e$, sheath potential drop V and magnetic field inclination angle α_B scans performed.

EXAMPLE RESULTS

Magnetic pre-sheath drop calculated from the condition $u_z = c_s$ (fig. below). Fluid approach holds for high ξ, also the condition on Debye sheath existence is more strict.



SP D.1: D005 – Sheath characteristics

IPP.CR

Plans for 2023: 5PM

- W-sputtering during ELMs at (COMPASS-U) and ITER.
- Continue BIT3 modelling of the 3D plasma sheath
- Inter- and intra-ELM SOLs for JET, AUG, ITER as input for migration codes
- ELM buffering at JET with Ar seeding
- Sheath for rough surface

SP D.1: D006 – Emissive sheath

S. Ratynskaia, P. Tolias and support from M. Komm, A. Podolnik (IPP.CR)

VR 4PM

- More details: see dedicated talk

- It has been demonstrated that the multi-emissive sheath treatment (relevant for ITER) leads to escaping current densities that are typically **3-5 times larger** than those resulting from the thermionic sheath treatment (relevant for present-day tokamaks)
- Benchmarking of the semi-empirical description of the SEE current density, the EBS current density, the electrostatic field at the wall and the field-assisted thermionic current density against SPICE2 PIC simulations for IVT & OVT intra-ELM conditions.
- Benchmarking of the semi-empirical description of the total escaping current density against SPICE2 PIC simulations for IVT & OVT intra-ELM conditions and comparison with the Richardson-Dushman expression.

SP D.1: D006 – Emissive sheath

VR

Plans for 2023: 4PM

- Semi-empirical analytical description of the multi-emissive collisionless ITER sheath at **normal inclination angles** has been successfully completed.

- Semi-empirical analytical description of the multi-emissive collisionless ITER sheath at **oblique inclination angles** is the next objective [up to the end of 2023].

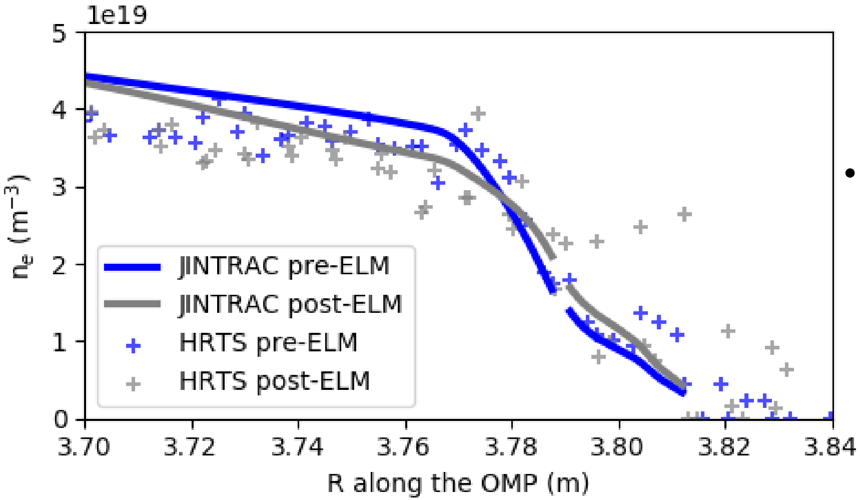
    - The first sets of ITER intra-ELM PIC simulations at grazing inclination angles have been performed and will soon be analyzed.
    - A concrete simulation plan will be devised in order to maximize the physics input that is necessary for the construction of a semi-empirical description.

SP D.1: D007 – Plasma background for AUG & JET-ILW

M. Groth, H. Kumpulainen, N. Horsten, R. Mäenpää

VTT 3PM

Validated ELMy H-mode EDGE2D-EIRENE & JINTRAC solutions produced for W transport modelling



- The studied scenarios include:
  - 18-36 MW of heating power
  - Vertical-horizontal and corner-corner divertor configurations
  - Deuterium and tritium plasmas

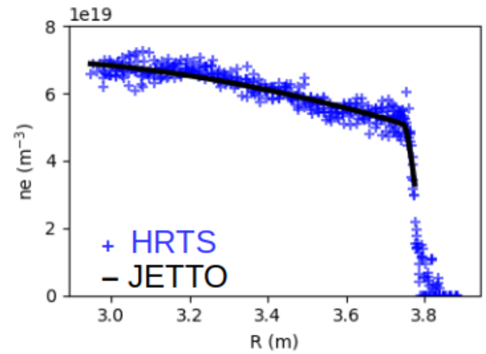
- Time-dependent solutions validated against:
  - Upstream n_e, T_e, T_i profiles
  - LFS target n_e, T_e, j_{sat} profiles
  - ELM-resolved time-evolution of:
    - Pedestal n_e, T_e, plasma stored energy
    - Heat loads on targets
    - Divertor D-alpha and Be II emiss.

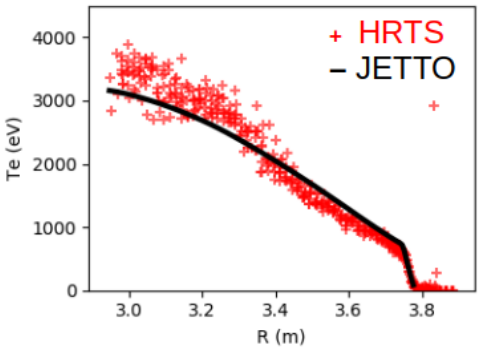
SP D.1: D007 – Plasma background for AUG & JET-ILW

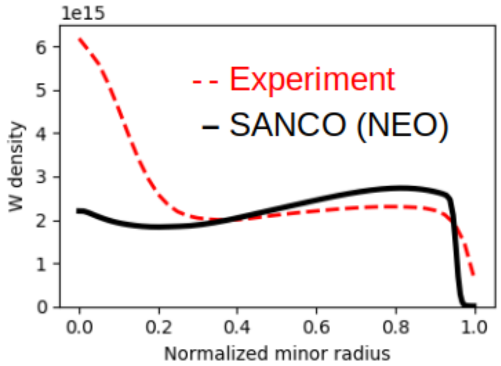
M. Groth, H. Kumpulainen, N. Horsten, R. Mäenpää

VTT 3PM

JINTRAC modelling with NEO aims to predict core W density based on edge ERO2.0 W predictions







- Main ion conditions from Bohm/gyro-Bohm and neoclassical transport, fitted to measurements
- W boundary condition iterated to match ERO2.0 predictions of W density at the pedestal top
- More turbulent transport than expected in the core, work in progress

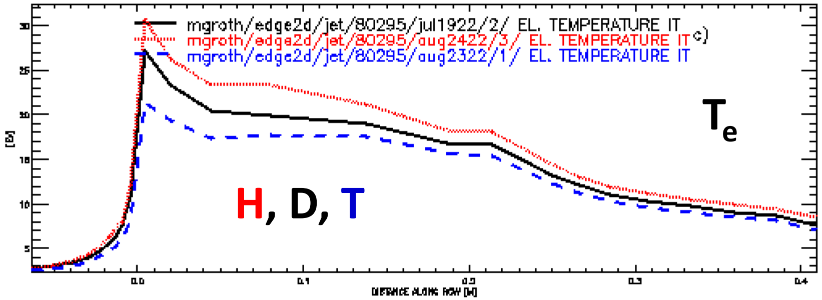
SP D.1: D007 – Plasma background for AUG & JET-ILW

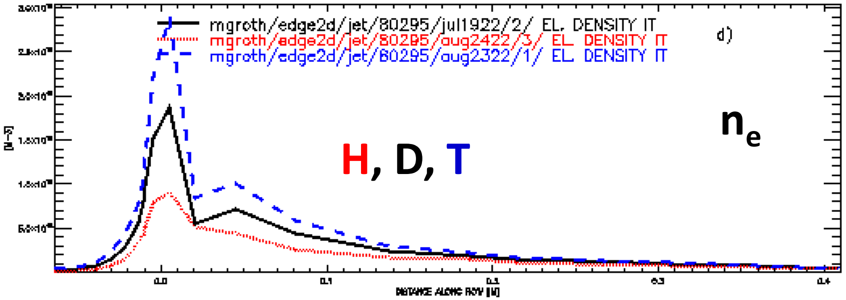
M. Groth, H. Kumpulainen, N. Horsten, R. Mäenpää

VTT 3PM

EDGE2D-EIRENE and JINTRAC were performed for JET L-mode and ELMy H-mode plasmas

Example: inner target profiles for ohmic phase





- Assuming same transport coefficients for H, D and T
- Experimentally, nearly the same profiles were observed
- Radial diffusivities will be varied to match the measured profiles

SP D.1: D007 – Plasma background for AUG & JET-ILW

VTT

Plans for 2023: 3PM

- EDGE2D-EIRENE for H, D, T isotope dependence of Be and W erosion in L-mode and H-mode plasmas
- ELM resolved EDGE2D-EIRENE, JINTRAC and ERO2.0 simulations for W erosion and transport, core contamination
- OEDGE simulations of JET Raised Inner Strike Point configuration, comparison to Balmer spectroscopy
- **EDGE2D-EIRENE and SOLPS-ITER helium plasmas for JET and AUG**

SP D.2: D001 – Dust production

CEA 2PM

A. Michau, K. Hassouni

- More details: see dedicated talk

Nano-particle formation:

2 sources identified

1. **Fate of W droplet ejected from the wall** :
   - Vaporisation : existing models
   - Nucleation in the non-equilibrium vapor cloud : existing models
   - Charging in the plasma
   - charge effect greatly affect the behaviour od droplet in E/B fields

2. **Sputtering of W surface followed by molecular growth**
   => Data need for charged W_m^+ clusters
   More precisely : determine the $W_n^{q+}/W^{0/+}$ coagulation probabilities

SP D.2: D001 – Dust production

A. Michau, K. Hassouni

CEA

Plan for 2023: 2PM

- Connection to experimental results
- To be discussed …

SP D.2: D003 – Tungsten sputtering and ionisation data

ÖAW 3PM

M. Probst, S. Huber, J. Romero, D. Süß

- More details: see dedicated talk

1. Detailed analysis of Be/D sputtering:
angular distributions, analytical formulas for sputtering, T dependence ... has been published. (*Nucl. Fusion* ***62*** *(2022) 066024,* DOI:10.1088/1741-4326/ac592a), also comparisons of energy distributions between MD and analytical formulas and some relations have been discovered.

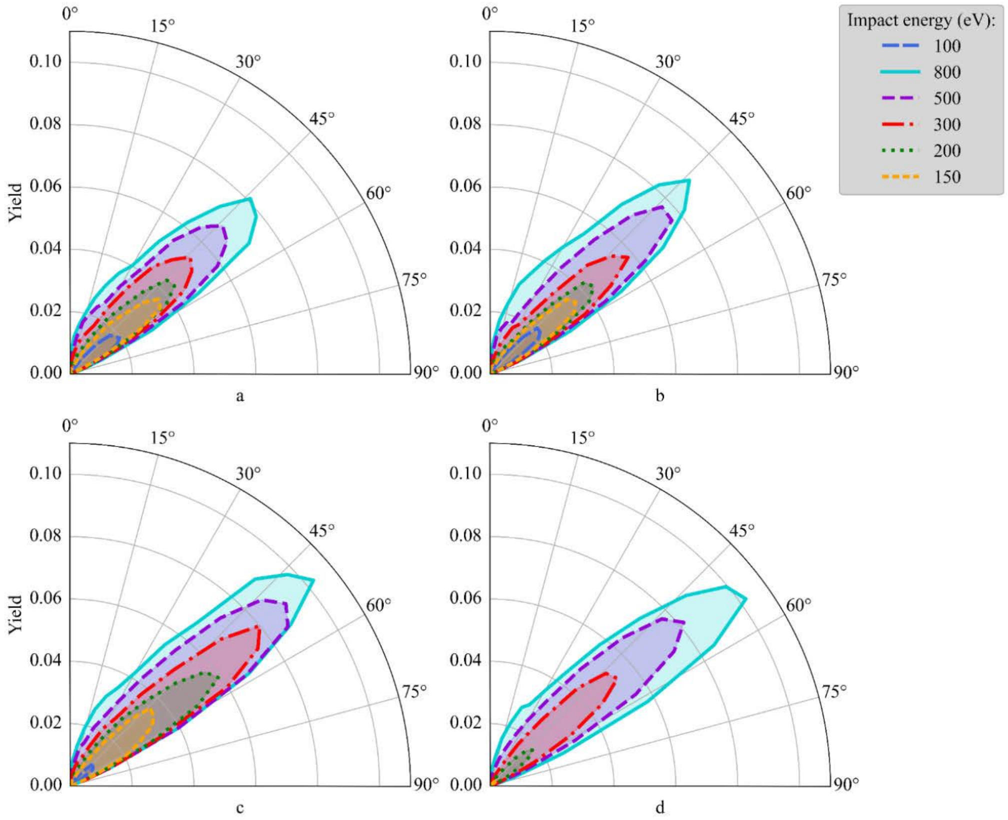
2. First results of the simulations of the Ar/W system:
published in *Eur. Phys. J. D (2022) 76:169,* DOI:10.1140/epjd/s10053-022-00495-3

3. Calculations of new electron-impact ionization:
for neutral and ionic species of molecules containing Fe and Cr (*J. Phys.: Condens. Matter 34 (2022) 374001)*

SP D.2: D003 – Tungsten sputtering and ionisation data

ÖAW 3PM

M. Probst, S. Huber, J. Romero, D. Süß



Example:

Polar plots of the yields and angles of sputtered W atoms as a function of the Ar incident energy for incident angles 0°, 20°, 40° and 60°

ÖAW

Plans for 2023: 3PM

- Sputtering W-O system
- Consideration of further seeding species (Kr, Xe)
- Sputtering of Eurofer

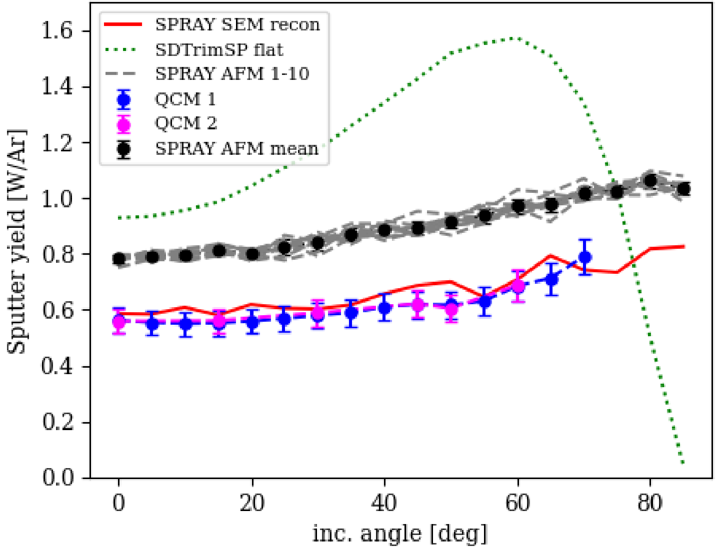
SP D.2: D004 – Erosion data: morphology effects

Ch. Cupak, M. Fellinger, P. Szabo, F. Aumayr

ÖAW 2PM

SPRAY code simulations: *oriented rough surface*

Benchmark of SPRAY with QCM, comparison to MD (see Helsinki SP-D task):
Nano-columnar W (NCW) samples, 1keV Ar^+



- 10 AFM images used as SPRAY input
- Also SEM reconstructed input used
- Synergy with SP-B task of TUW

- Effective sputter yield in very good agreement with QCM (and MD sim.) for SEM reconstructed input

=> Benchmark of SPRAY successful

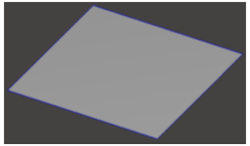
Paper published in Physical Review Materials

SP D.2: D004 – Erosion data: morphology effects

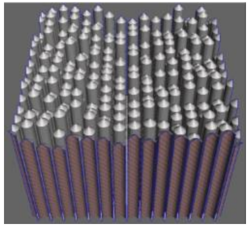
Ch. Cupak, M. Fellinger, P. Szabo, F. Aumayr

ÖAW 2PM

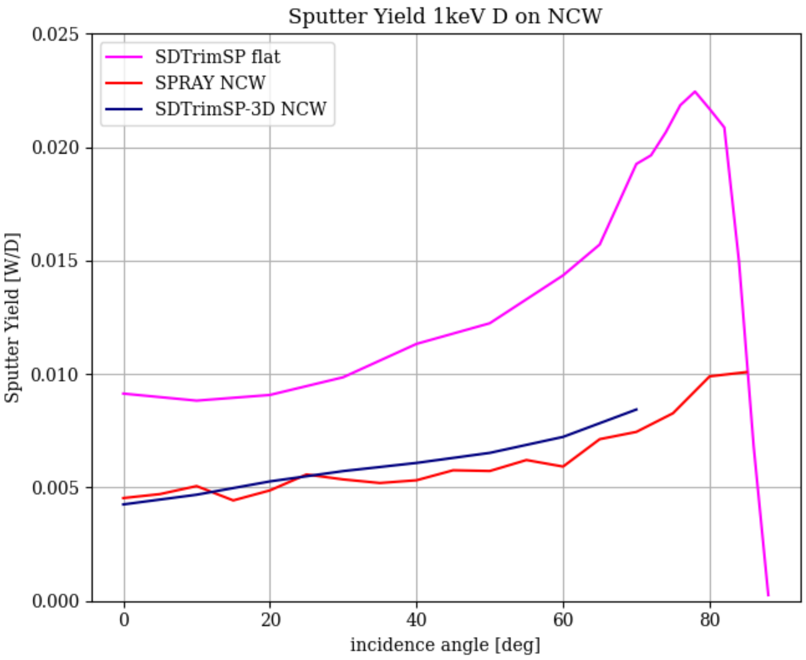
Further simulations for 1 keV D^+ irradiation
Comparison SPRAY with SDTrimSP-3D:



Flat W



SEM recon NCW



- SEM reconstructed input used
- 1keV D^+ ions used (longer range)
- SDTrimSP-3D allows transmission through NCs
- Effective sputter yields in very good agreement between SPRAY and SDTrimSP-3D,
- suggests no transmission effects
- MD data from Helsinki soon

Task solved

SP D.2: D004 – Erosion data: morphology effects

ÖAW

Plan for 2023: 2PM

- Modelling of available experiments (MAGNUM-PSI, W erosion, redeposited material, angular distribution, dynamic evolution of fuzz)
- Large SPRAY study to find an optimised configuration of nano-columnar W surfaces with overall minimal sputter yields
- Use this optimised configuration for creation of a real sample surface (on a QCM resonator) for experiments (synergy with SPB) to study static and dynamic sputtering properties
- Make SDTrimSP-3D and MD simulations (the latter in cooperation with Univ. Helsinki, Nordlund Group) to compare experimental and numerical results
- Validate the fluence-durability of such surface structures

SP D.2: D005 – Dust production from melting

VR 7PM

N. Scapin, M. Crialesi-Esposito, L. Brandt, S. Ratynskaia, L. Vignitchouk

➢ More details: see dedicated talk

- Attempts at designing highly customizable set-ups in ANSYS Fluent
- Include surface-dependent (especially temperature-dependent) effects (e.g. radiation cooling, vaporization, thermo-field emission) as boundary conditions at the metal's free surface *without having to model the gas/plasma*
- Tests with temperature-dependent vaporization heat flux and recoil force (no mass transfer) as extra source terms
- The vapor pressure force term seems to cause numerical instabilities in the form of spurious free-surface oscillations at the mesh cell scale

SP D.2: D005 – Dust production from melting

VR

Plan for 2023: 6PM

- Complete code transfer of knowledge
- Resume heat solver implementation and testing if time permits
- Continue designing ANSYS Fluent set-ups with better customizability to include a wider variety of plasma-surface interactions processes

SP D.2: D006 – Erosion data: morphology, redeposits

VTT 5PM

F. Granberg, A. Lopez-Cazalilla, F. Kporha, K. Nordlund

Tasks in 2022:

- Further investigation of effect of different surface morphologies
  - Comparison with experiments and other methods, where applicable
  - Article published in PRM in collaboration with TU Vienna & Univ. Poli. Madrid
- Further investigation of erosion of redeposited tungsten
  - Ongoing:
    - Paper on effect of single & cumulative irradiation of nanostructures submitted (minor revision)
    - Our focus for latter part of 2022
- Investigate the effect of interatomic potential choice
  - Ongoing
    - Tests comparing classical and Machine Learning (ML) interatomic potentials ongoing

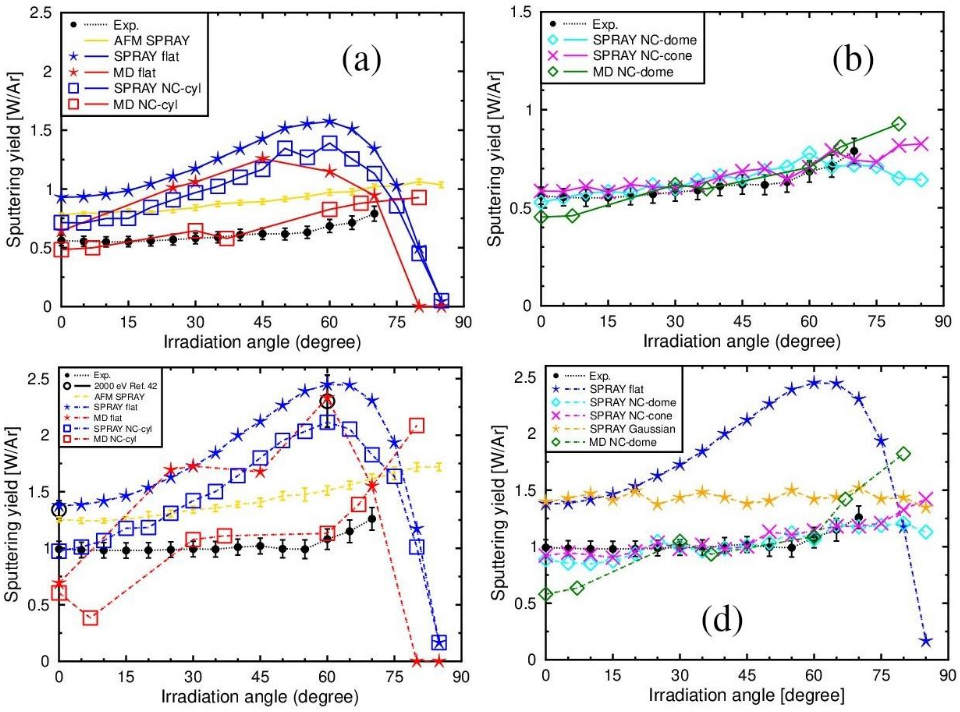
SP D.2: D006 – Erosion data: morphology, redeposits

F. Granberg, A. Lopez-Cazalilla, F. Kporha, K. Nordlund

VTT 5PM

Sputtering of W nanopillars:

- MD show very good agreement with experiments without any adjustable parameters
- SPRAY, a raytracing simulation technique show sensitivity to the shape of the nanopillar. Eg. There is a need to include the half-sphere on the pillars to obtain good results (”dome” results have the half-sphere on top.) These are more realistic, as the pillars do not have hard egdes.



SP D.2: D006 – Erosion data: morphology, redeposits

F. Granberg, A. Lopez-Cazalilla, F. Kporha, K. Nordlund

VTT 5PM

Investigate the effect of interatomic potential choice:

- It is known that the interatomic potential in MD simulations can and most likely will affect in principle everything, at least to some extent.
- In order to see how robust the commonly used potentials are, we have started to do simulations with both classical potentials as well as with newly developed Machine Learning (ML) interatomic potentials. The latter which should be more accurate and should yield more reliable results.
- This task has been started and benchmarks and comparative studies with commonly used potentials have started. However, even though the ML potentials should yield more reliable results, they are orders of magnitude slower, which limits the parameter space that can be explored. This study will hopefully verify that the much CPU lighter potentials can be used for certain applications in the future, and there is only need for the CPU heavy simulations for some cases.

SP D.2: D006 – Erosion data: morphology, redeposits

VTT

Plan for 2023: 5PM

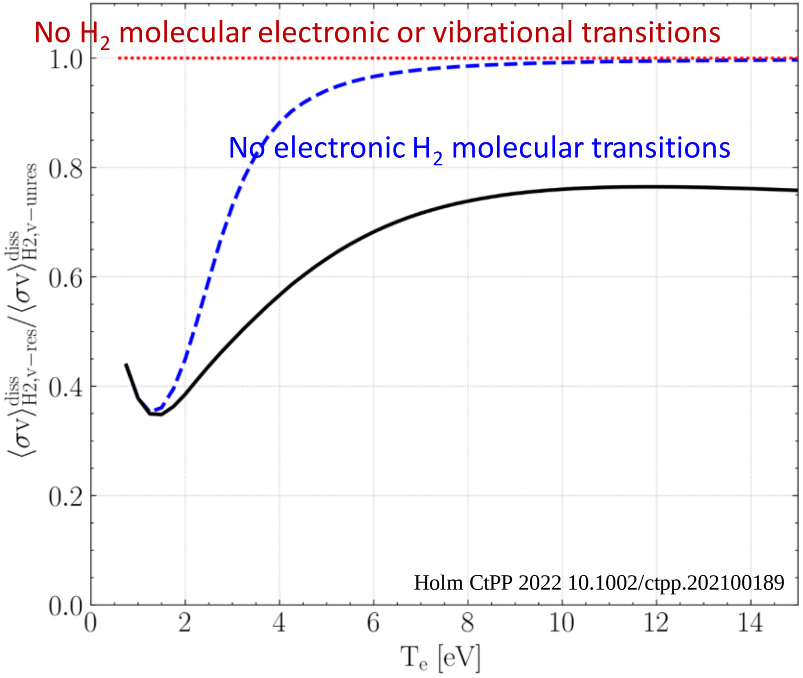
- Continue the work on effect of surface morphology and structure on the sputtering yields, and the effect of redeposited tungsten in these cases.
- Use of more accurate interatomic potentials. Mainly focusing of different ML/AI potentials, that should show superior accuracy to commonly used classical potentials.
  - quite computationally heavy and discovered that utilizing light elements as ions (H/D/T and He) will require huge simulation cells.
  - these cells are much larger than previously used, but seems to be necessary to use these large ones to obtain reliable results.
  - solve this by investigating, calculating correction factors for simulations with smaller cells - would be sufficiently small for sputtering simulations, even with computationally heavy ML/AI potentials.

SP D.2: D007 – Atomic/molecular data, CRM

M. Groth, A. Holm

VTT 1PM

Collisional-radiative processes for hydrogen molecules (and atoms) were revisited in AMJUEL (used in EIRENE) comparing vibrational resolved & vibrationally unresolved cross-sections and reaction rates



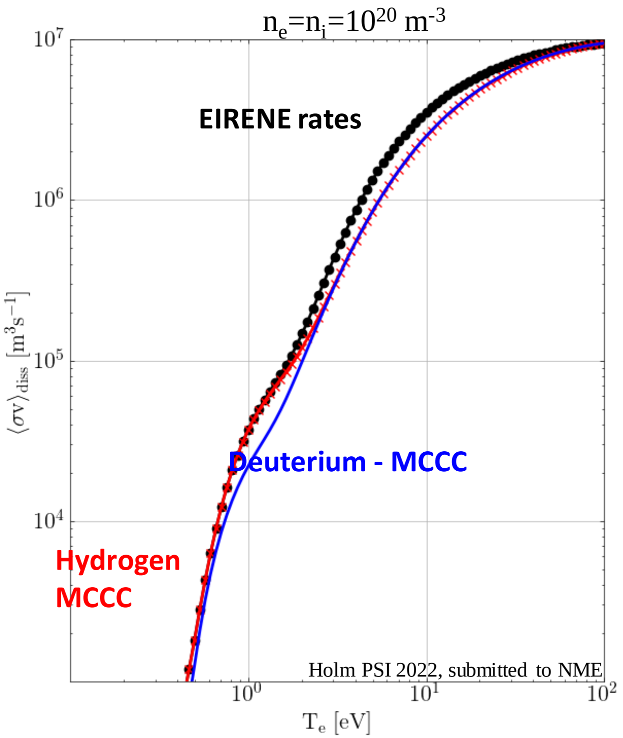
- Different CR processes cause up to 60% difference in dissociation rates
- Impact strongest in the T_e=0.5–4 eV range, where molecular processes strongest
- Electronic transitions affect T_e>4 eV
- Vibrational transitions affect T_e<4 eV

SP D.2: D007 – Atomic/molecular data, CRM

VTT 1PM

M. Groth, A. Holm

Molecular-convergent close-coupling (MCCC) data predicts an isotope effect on dissociation for T_e=0.7-3 eV



- Predicted isotope effect strongest for temperatures associated with detachment onset and detached conditions

- MCCC data indicates weaker dissociation of both H_2 and D_2 for T_e>3 eV compared to EIRENE data (AMJUEL, HYDHEL, H2VIBR)

SP D.2: D007 – Atomic/molecular data, CRM

VTT

Plan for 2023:

- Move to TSVV?

SP D.2: D008 – Erosion data: morphology effects

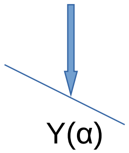
U. v. Toussaint, R. Preuss

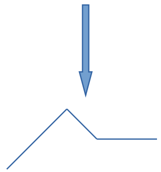
MPG 2PM

- More details: see dedicated talk

SDTrimSP-surrogate : present and ongoing work

- Extension of fast ML-based predictor for large-fluence induced morphology changes:
  - present:
    - large-scale cluster-based computation of database (i.e. Y(α_1, α_2, α_3)) : (instead of Y(α)) should be completed by end of August 2022





  - coming next (= until end of this year)
    - Multivariate GP- or Student-t based regression of database, followed by implementation in
    - Dynamical PDE-based predictor for morphology evolution and
    - validation of ML model against 2D-SDTrimSP (and assessment of limitations)

In case of success, extension to 3D is computationally expensive (4 or 9 angles) but straightforward

SP D.2: D008 – Erosion data: morphology effects

MPG

Plan for 2023: 2PM

- Model developments will be mainly included in TSVV
- SP D: effect of crystal orientation on W sputtering

SP D.3: D001 – Migration modelling for WEST

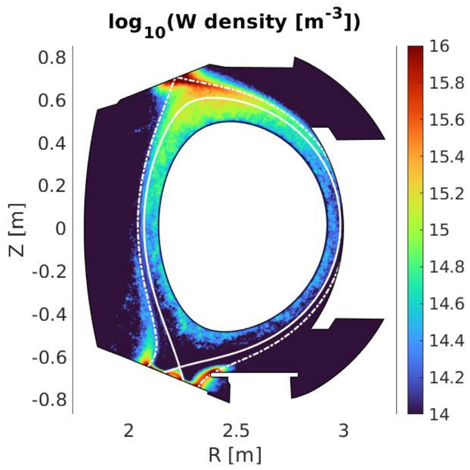
CEA 2PM

G. Ciraolo, N. Fedorczak, Y. Marandet, M. Raghunathan, S. Di Genova, H. Yang

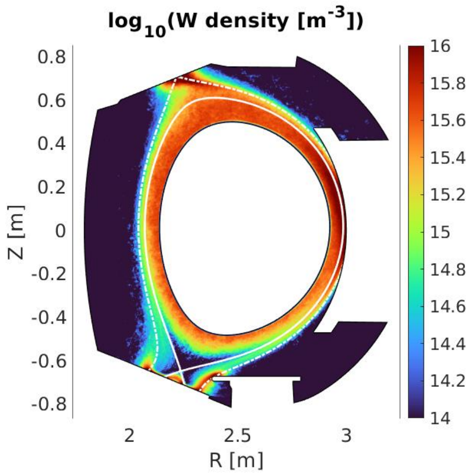
- More details: see dedicated talk

  - **Modelling W erosion and migration with ERO2.0: an example on the role of Antenna limiter**

Without Antenna erosion



With Antenna erosion



Example of the set up of a simulation	
radial transport	Diffusive process with $D_{an} = 0.3\ \mathrm{m}^2/\mathrm{s}$
Collisional forces	Kinetic friction forces F_0, Kinetic thermal forces $F_{\nabla T}$
Sheath physics	Electron density and electrostatic potential linked with Boltzmann factor: $n_\mathrm{e} = n_0 \exp\left(-\frac{\phi}{k_\mathrm{B} T_\mathrm{e}}\right)$
Plasma impurities	Uniform 3% Oxygen mixture from O^{1+} to O^{8+}

- Investigation of the erosion of each « main PFC » (lower divertor, upper divertor, antenna limiter etc..) and in the contamination of core plasma
- Ongoing comparison between the results obtained from 2D and 3D plasma backgrounds

SP D.3: D001 – Migration modelling for WEST

CEA

Plan for 2023: 2PM

- Continuation of migration modelling: W source, transport and screening
- One focus on long-pulse, high-fluence discharges

SP D.3: D002 – Migration modelling for GyM

ENEA 5PM

M. Passoni, E. Tonella, G. Alberti, A. Uccello

- More details: see dedicated talk

Morphology evolution studies

- First ERO2.0 simulations performed on CAD drawn pyramids exposed to He-plasma to identify numerical parameters influencing morphology evolution - **completed**
- Analysis of experimental results in GyM (under SP B1) – **completed**
- Comparison with ERO2.0 simulations - **ongoing**

SP D.3: D002 – Migration modelling for GyM

ENEA 5PM

M. Passoni, E. Tonella, G. Alberti, A. Uccello

Global erosion/deposition studies in GyM (fig.3)

- Advancement of 2021 activity including iron (Fe) erosion/deposition evaluation (main component of GyM steel), as a function of bias voltage applied to GyM walls - **completed**
- Analysis of bushings erosion, considering both total deflection of plasma ions in the sheath and no deflection - **completed**

Related publication: *under review for Nuclear Fusion*

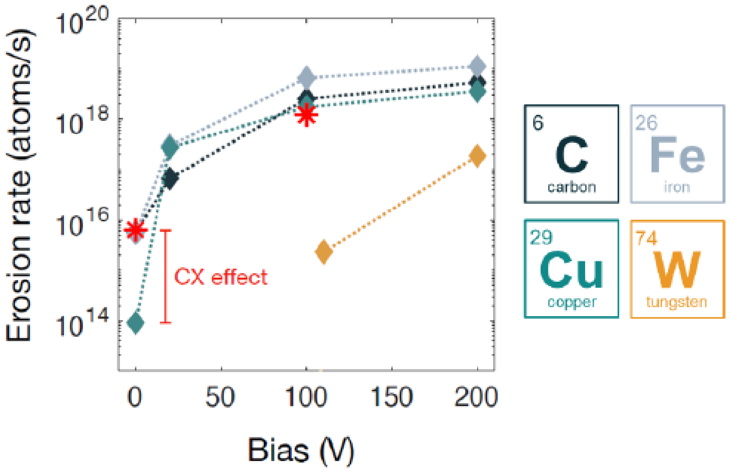


Fig.3 *Overall erosion rate of GyM walls as function of wall material and bias voltage applied.*

SP D.3: D002 – Migration modelling for GyM

ENEA 5PM

M. Passoni, E. Tonella, G. Alberti, A. Uccello

Global erosion/deposition studies in AUG (fig.4)

- Simulations considering SOLPS-ITER D-plasma (discharge #35617), full-W 3D walls and 80° toroidal sector with periodic BC - **completed**
- Investigation of the effects of plasma extrapolation to walls surface method and shadowing - **completed**

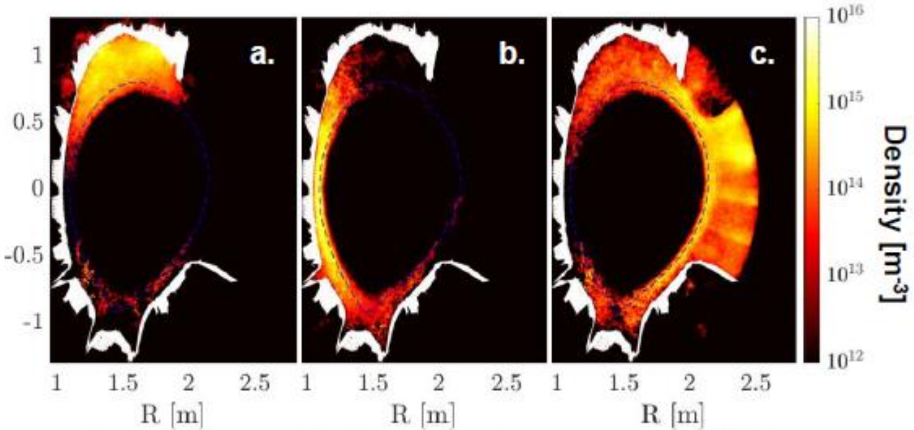


Fig.4 *Density of W particles eroded from a) upper wall, b) inner wall and c) outer wall.*

SP D.3: D002 – Migration modelling for GyM

ENEA

Plans for 2023: 5PM

- **Morphology evolution studies:**
  1. Progress the comparison between ERO2.0 simulations of AFM-generated surfaces and experimental results, possibly reducing experimental uncertainties and tuning ERO numerical parameters to match observed data (within 2022).

- **Global ERO2.0 in GyM:**
  1. First simulations with sample-holder, to study erosion and migration of exposed materials.

- **Global ERO2.0 in AUG:**
  1. Consider other important parameters influencing first wall erosion (erosion due to charge-exchange neutrals and plasma molecules).
  2. Performing similar analysis using recently SOLPS-ITER calculated He-plasma in AUG, in comparison to experimental results (if available).

- **DTT studies** for standard divertor…

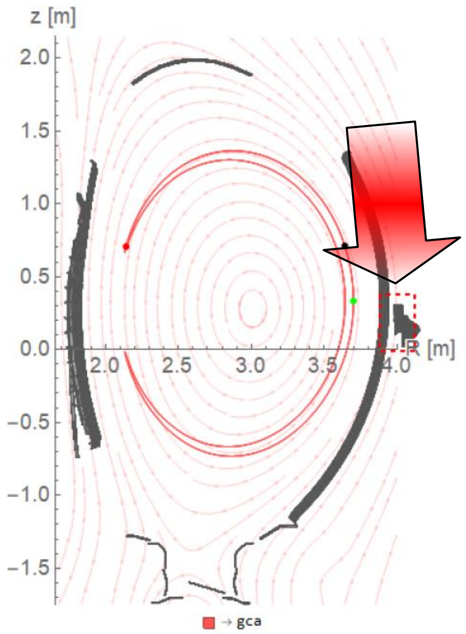
SP D.3: D003 – Migration modelling for JET-ILW, W7-X and morphology studies

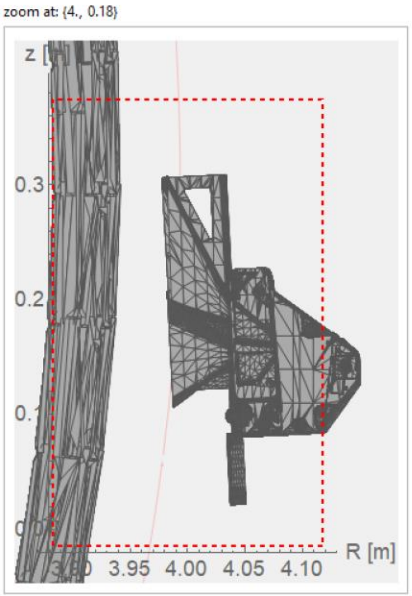
J. Romazanov, A. Kirschner, H. Xie, …

FZJ 15PM

➢ More details: see dedicated talk

Modelling PWI for JET mirror assembly





ITER-like mirror test assembly (ILMTA): 3D model was imported into ERO2.0 global model for JET

- CX neutral distributions at ILMTA from EIRENE (provided by VTT)
- To be included into ERO2.0

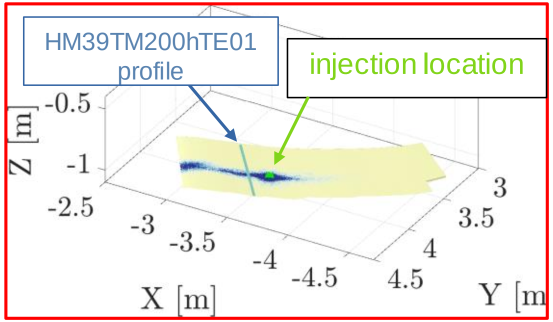
J. Romazanov, A. Kirschner, H. Xie, …

FZJ 15PM

Modelling the W7-X ^{13}C tracer injection experiment: ERO2.0

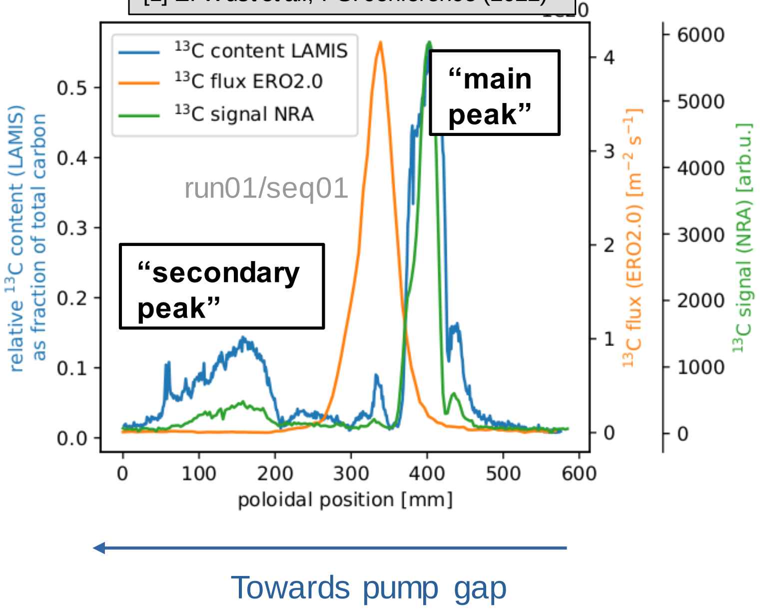
First benchmark of ERO2.0 ↔ post-mortem analysis available.
Further analysis and simulation improvements ongoing.

ERO2.0 simulation of ^{13}C



poloidal profile of ^{13}C

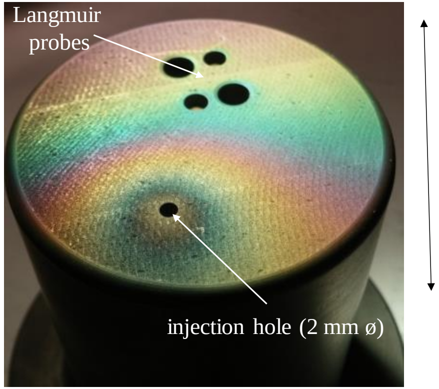
[1] E. Wüst et al., PSI conference (2022)



J. Romazanov, A. Kirschner, H. Xie, …

FZJ 15PM

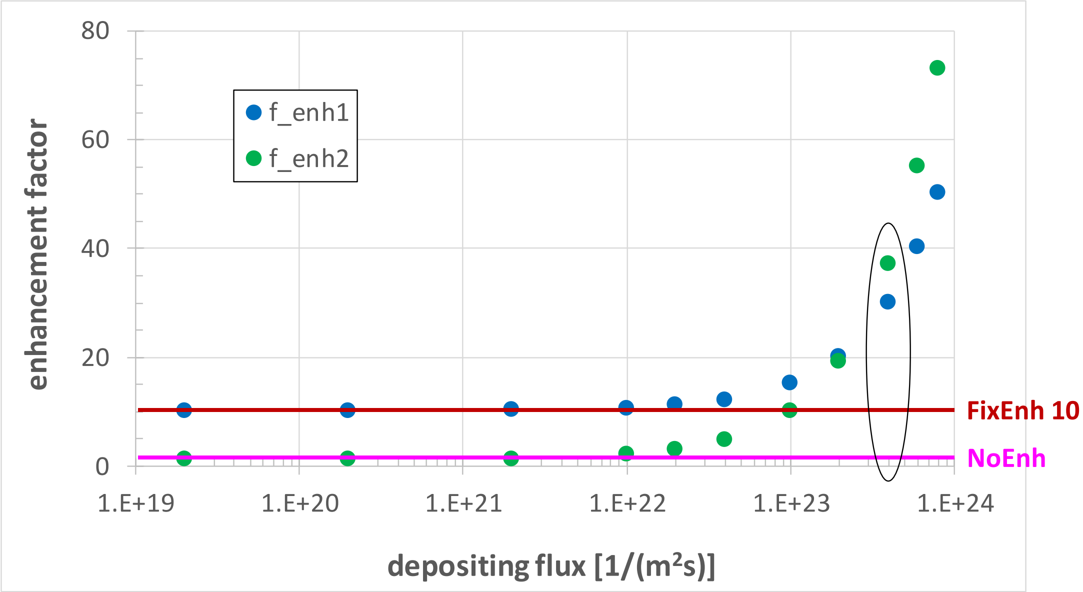
Modelling the W7-X ^{13}C tracer injection experiment: ERO



Manipulator head after exposure (2 discharges with $^{13}CH_4$)

^{13}C deposition efficiency ~1%

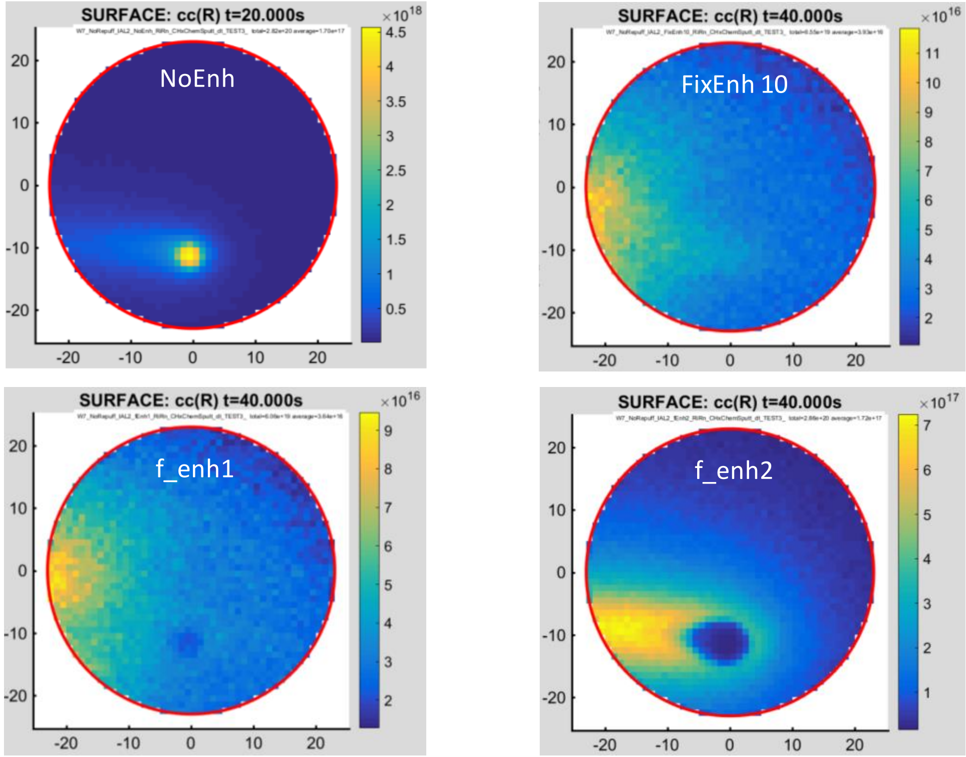
Assumptions for in-situ enhanced re-erosion factor:



J. Romazanov, A. Kirschner, H. Xie, …

FZJ 15PM

Modelling the W7-X MPM ^{13}C tracer injection experiment: ERO



^{13}C deposition efficiency

Rion05, Rn09

Run	
NoEnh	~14%
FixEnh 10	~0.1%
fenh 1	~0.1% (->0?)
fenh 2	~6%

Exp **~1%**

FZJ

Plan for 2023: 16PM

- W7-X simulations: detailed comparison with post-mortem data, further parameter studies (global and local simulations)
- JET mirror assembly: ERO2.0 runs with neutrals, comparison to post-mortem
- Simplified fuzz-model for ERO2.0 under consideration …

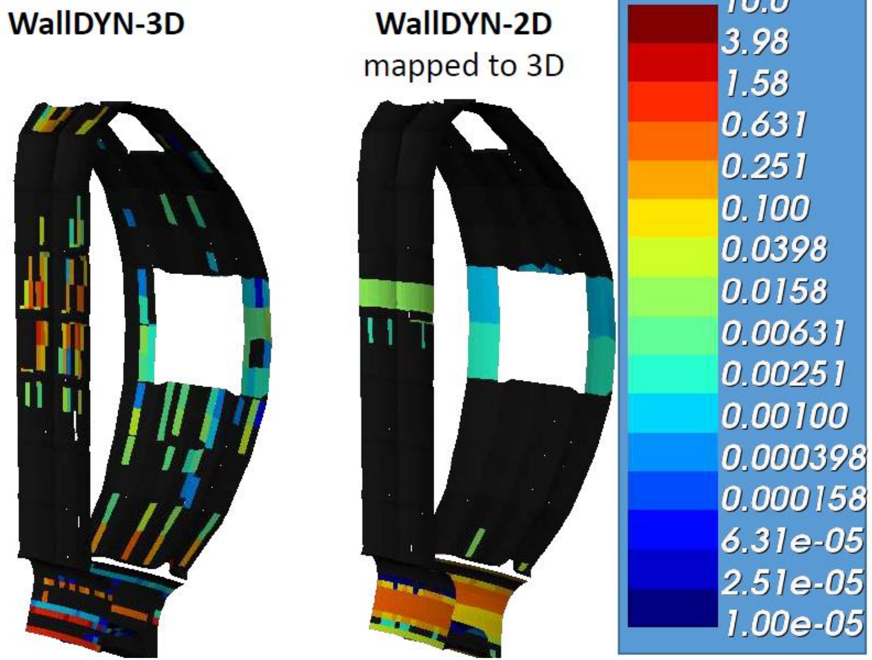
MPG 2PM

K. Schmid

3D WallDYN for ITER

Influence of 3D shaped Be wall on Be layer formation

Be-layer growth rate ($10^{20} m^{-2} s^{-1}$)



- Be deposition in main chamber higher in 3D case

  → Effect of shadowed regions in between shaped Be tiles

  - ❑ **2D: 8% on first wall** Factor 5!
  - ❑ **3D: 43% on first wall** (**Depends on wall-plasma**)

- Total Be erosion:
  - ❑ 2D: 1.3E20 (Be/sec)
  - ❑ 3D: 1.6E20 (Be/sec)

→ Total Be source similar
BUT the layer distribution is different

SP D.3: D004 – Migration modelling for ITER & W7-X

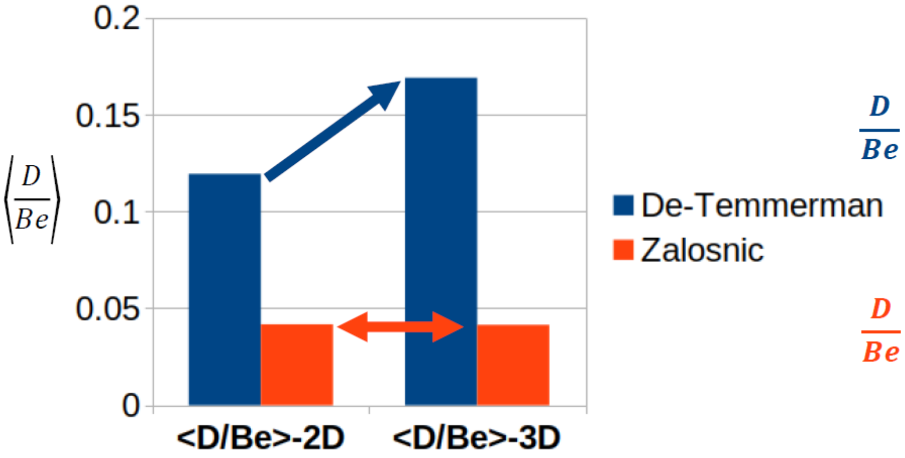
K. Schmid

MPG 2PM

3D WallDYN for ITER

Influence of 3D shaped Be wall on T retention

Define mean $\left\langle \frac{D}{Be} \right\rangle = \frac{Be\text{−}Layer\ growth\ rate\ (\frac{Be}{s})}{D\text{−}co\text{−}deposition\ rate\ (\frac{D}{s})}$



$\frac{D}{Be} \sim E^{1.34\pm0.15}$

$\frac{D}{Be} \sim E^{0.79\pm0.18}$

Depending on scaling law: shaped wall increases retention slightly (x1.5) or has little effect

More details: PSI 2022 contribution

MPG

Plans for 2023: 2PM

- W7-X: WallDYN with 3D shaped wall
- Continue 3D ITER modelling: further comparison with ERO2.0, high density cases

SP D.3: D005 – Migration modelling for AUG & JET-ILW

VTT 4PM

A. Hakola, A. Järvinen

Migration modelling of AUG erosion experiments

- Change from ERO to ERO2.0: installation on local VTT cluster
- AUG erosion experiments (focus on L-mode and H-mode in D): Preparation of ERO2.0 simulations …

SP D.3: D005 – Migration modelling for AUG & JET-ILW

VTT

Plan for 2023: 4PM

- **ERO2.0 simulations for AUG erosion experiments**

SP D.3: D006 – Dust adhesion

VR 3PM

S. Ratynskaia, P. Tolias

- More details: see dedicated talk

- Fully retarded Lifshitz theory calculations have been performed for fusion relevant dust-wall combinations from the Hamaker non-retarded limit up to the Casimir asymptotic limit within the proximity force approximation or Derjaguin approximation.
- A novel compact semi-empirical expression has been proposed for the separation-dependence of the Hamaker coefficient that has been demonstrated to be very accurate for any metal-metal combination embedded in vacuum or water [Tolias, Surf. Sci. **723** 122123 (2022)].
- Fully retarded Lifshitz theory calculations will be performed for fusion relevant dust-wall combinations from the Hamaker non-retarded limit up to the Casimir asymptotic limit without invoking the proximity force approximation. These are computationally heavy calculations that are expected to be finished by the end of 2022.

SP D.3: D006 – Dust adhesion

VR

Plan for 2023: 3PM

- The first accurate W-on-W adhesion measurements will be carried out within 2022. The analysis of the new experimental results will most likely finish at the beginning of 2023.
- Corresponding adhesive force calculations are foreseen

SP D.4: D001 – Gas dynamics and exhaust for DEMO

C. Tantos, S. Varoutis, Y. Igitkhanov, C. Day

KIT 9PM

Improved DIVGAS code for DEMO

Necessary input for DIVGAS: plasma solutions for ADC not yet available
=> in 2022: concentrate on SN configuration

- The DIVGAS boundary conditions have been extracted based on the SN fluid plasma simulations (detached case) provided by Fabio Subba.
- The plasma input includes several macroscopic parameters of neutrals, such as the atomic and molecular deuterium density, temperature and velocity as well as the corresponding quantities for the impurities (helium and argon).
- The 2021 SN baseline DEMO divertor design with a liner has been used. The official 3D CAD file can be found in the following link: https://idm.euro-fusion.org/default.aspx?uid=2P57HS. For all the ongoing simulations a 2D cut of the divertor cassette has been extracted.

SP D.4: D001 – Gas dynamics and exhaust for DEMO

C. Tantos, S. Varoutis, Y. Igitkhanov, C. Day

KIT 9PM

Improved DIVGAS code for DEMO

- A large number of simulations are in progress, covering a wide range of the involved parameters, i.e. 6 indicated values of the pumping speed and 4 values of the incoming flux varying with respect to the reference Φ^{+}_{ref} obtained by the plasma simulations as follows: $0.2\Phi^{+}_{\mathrm{ref}}$, Φ^{+}_{ref}, $2\Phi^{+}_{\mathrm{ref}}$, and $5\Phi^{+}_{\mathrm{ref}}$.
- All the aforementioned simulation cases are running in MARCONI HPC, with the available computational resources being allocated under the project TOK-KIT.
- Based on the progress of the work so far no delays are foreseen and by the end of this year all the obtained numerical findings will be reported.

SP D.4: D001 – Gas dynamics and exhaust for DEMO

Plan for 2023: 9PM

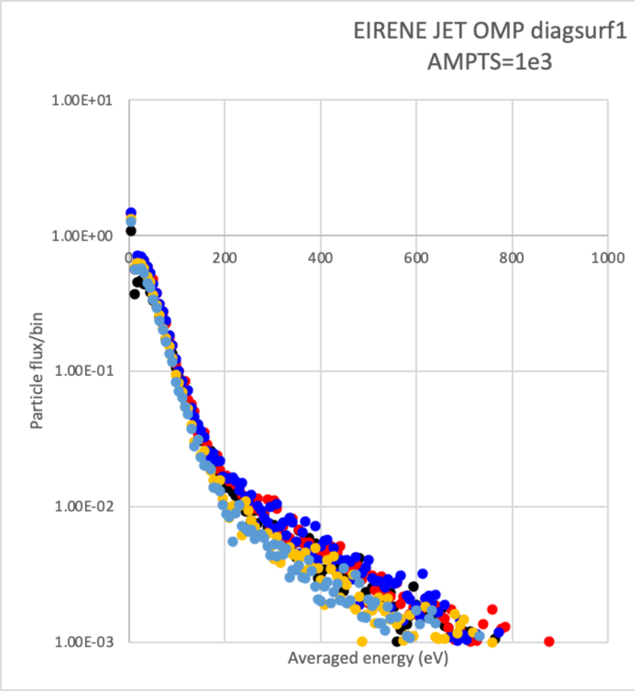
- DIVGAS simulations for DEMO ADC scenario (XD)

SP D.4: D002 – Neutral fluxes

VTT 2PM

M. Groth, H. Kumpulainen, N. Horsten, R. Mäenpää

A port and a EIRENE diagnostic surface at the OMP vessel was introduced to measure D^0 CX fluxes to a mirror assembly



- Sufficient statistic achieved for total neutral histories > $1x10^6$ particles
- Decay of fluxes in energy range 0.1 to 200 eV independent of grid, EDGE2D-EIRENE and assumed port geometry
- Assuming a halo plasma (of up 1.0 eV and $5x10^{18}$ m^{-3}) in the far SOL/port box reduces the CX D0 fluxes by up to 30%

SP D.4: D002 – Neutral fluxes

VTT 2PM

M. Groth, H. Kumpulainen, N. Horsten, R. Mäenpää

Plan for 2023: 2PM

- Extension of EDGE2D-EIRENE domain at outer midplane, energy and angle resolved EIRENE neutral fluxes (-> assessment of mirror performance in JET)

SP D Milestones for 2023

WM1	SP D	Set of dedicated plasma backgrounds for JET-ILW, WEST, AUG, W7-X, JT60-SA and linear device discharges (PSI-2, MAGNUM-PSI, UPP) to be used as input for impurity migration. Sheath and SOL characteristics to be used as input for impurity modelling (intra- and inter-ELM). (ITER)	31.12.2023
WM2	SP D	Set of novel reflection and sputtering data for W considering morphology, crystal orientation and redeposits. Provision of dust production models. (DEMO+ITER)	31.12.2023
WM3	SP D	Benchmark and predictive modelling of erosion sources, impurity migration, and resulting net erosion/deposition for specific set of well characterised JET-ILW, WEST, AUG, W7-X, DTT and linear device discharges. Refined predictive modelling of ITER with ERO2.0 and WallDYN-3D regarding first wall and divertor erosion. (ITER)	31.12.2023
WM4	SP D	Upgraded DIVGAS neutral particle code applied to ADC divertor configurations in DEMO. Provision of neutral flux distributions to wall and recessed areas. (DEMO)	31.12.2023

SP D Deliverables for 2023

SP D Deliverables 2023

SP D1

- Modelling (SOLEDGE3X-EIRENE) of background plasmas for WEST to be used as input for migration modelling: focus on long-pulse, high fluence discharges (CEA)
- Modelling (SOLPS-ITER) of background plasmas for linear devices MAGNUM-PSI and UPP to be used as input for migration modelling (DIFFER)
- Modelling (SOLPS-ITER) of background plasmas for linear device GyM to be used as input for migration modelling: inclusion of sample holder (ENEA)
- Modelling (EMC3-EIRENE) of background plasmas to be used as input for migration modelling: focus on PSI-2, including He (FZJ)
- PIC modelling of sheath and SOL including transients and surface roughness (IPP.CR)
- PIC modelling for emissive sheath at hot surfaces with focus on oblique angles (VR)
- Modelling (SOLPS, EDGE2D-EIRENE) of background plasmas for JET-ILW and AUG, including He plasmas (VTT)
- Modelling of background plasmas for JT60-SA (ERM)

SP D2

- Development of dust formation models for tungsten: nucleation and sputtering (CEA)
- Calculation of sputter yields, reflection coefficients for tungsten and EUROFER, considering seeding species and the W-O system (ÖAW)
- SDTrimSP-3D and SPRAY modelling of erosion including morphology, roughness, fuzz. Comparison to experiments and MD modelling (ÖAW)
- Model development for production mechanisms for dust formation from melting (VR)
- Production of erosion yields for W considering morphology and redeposits W, comparison to SDTrimSP-3D and experiments, study on more accurate interaction models (VTT)
- Calculations of the effect of crystal orientation on tungsten sputtering (MPG)

SP D3

- ERO modelling of W sources, transport and screening in WEST with focus on long-pulse, high fluence discharges (CEA)
- ERO modelling of erosion, migration in GyM including the sample holder, ERO2.0 modelling for AUG (including He plasmas, first wall erosion) (ENEA)
- ERO2.0 modelling of impurity migration in DTT (ENEA)
- ERO modelling of impurity migration in W7-X and JET-ILW, implementation of simplified fuzz model into ERO2.0 (FZJ)
- WallDYN 3D modelling for W7-X, WallDYN modelling with realistic 3D ITER wall, comparison to ERO2.0 (MPG)
- ERO2.0 modelling for AUG erosion experiments (VTT)
- Dust adhesion and self-charging (VR)

SP D4

- DIVGAS code development and modelling of neutral particle gas dynamics and exhaust for DEMO with advanced scenario (XD) (KIT)
- Post- processing of plasma modelling with SOLPS or OSM/EIRENE to get neutral fluxes to the walls in particular for JET-ILW to be used in ERO2.0 (VTT)