TSVV 6 – Impurity Sources, Transport, and Screening

G. Ciraolo on behalf of the TSVV 6 team

EUROfusion Science Meeting - TSVV Final Reports (2021-2025) - Part II – Jan 28, 2026

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TSVV 6: Impurity Sources, Transport, and Screening

Aims

- **Establish an integrated modelling suite to predict the W impurity distribution** in ITER and DEMO, including W source generation, W screening, W transport, W exhaust and its impact on the plasma performance.

- Develop **3D kinetic transport models for heavy impurities** (including W) and seeding species like Ar, Kr, Xe in the SOL and pedestal regions of DEMO.

- **Assess the effects of 3D perturbations** and ELM suppression techniques **on the W impurity distribution in ITER** reference scenarios, along with their implications for DEMO.

TSVV 6: Impurity Sources, Transport, and Screening

Key Deliverables

1. **Validated suite of 3D codes** and **transport models to describe in an integrated way the W content** and **its distribution in metallic devices**, in particular DEMO and ITER, with discrimination of main chamber and divertor sources, screening, transport, and exhaust along with its impact on the main plasma dynamics and performance.

2. **Assessment of** the W influx, W screening, and **W transport** in **ITER plasmas envisaged for pre-fusion and fusion power** operation with **semi-detached divertor** and **application of resonant magnetic perturbations for ELM suppression**. Discussion of the impact on a potential loss of semi-detachment and ELM suppression on the W influx, W screening, and W transport in those ITER scenarios.

3. **Applications of the developed model**. Assessment of the **seeding impurity screening and transport** in DEMO and **ITER scenarios**

CONSORTIUM AND PARTICIPANTS (5 ppy in total)

Team member	Beneficiary	2021	2022	2023	2024	2025
G Ciraolo	CEA	8	8	8	8	8
H Bufferand	CEA	6	6	6	4	4
N Rivals	CEA	0	0	0	4	4
E Gravier	CEA/UL	5	5	5	3	3
M Raghunathan	CEA/AMU	6	6	6	0	0
R. Dull	CEA/AMU	0	0	0	0	4
Y. Marandet	CEA/AMU	4	4	4	4	0
D. Harting	FZJ	8	6	6	6	6
S. Rode	FZJ	6	6	6	0	0
J. Romazanov	FZJ	0	4	6	6	6
A. Knieps	FZJ				6	6
H. Kumpulainen/ R. Maenpaa / M. Groth	VTT (Aalto Univ)	6	6	6	6	6
J Koerfer	EPFL	0	0	0	6	6
J Graves	EPFL	0	0	0	1	1
M. Eder	OEAW (Graz TU)	6	6	6	0	0
ACH resources	**ACH**	**1**	**1**	**1**	**6**	**6**
TOTAL pm		59+1	59+1	59+1	54+6	54+6

TSVV 6: Impurity Sources, Transport, and Screening

Expertise / codes

- **CEA / FR-FCM** : SOLEDGE3X-EIRENE, GYSELAX
- **FZJ** : EMC3-EIRENE and KIT module, ERO2.0
- **AALTO UNIV**. : integrated modeling core-edge JET plasma, W transport with JINTRAC-ERO2.0 package
- **GRATZ TU:** kinetic modeling of ion transport with GORILLA code (2021-2023)
- **EPFL**: theoretical framework, W transport in 3D equilibria with VENUS-LEVIS code (2024-2025)

- **PROJECT ORGANIZED WITH RESPECT TO THE 3 KEY DELIVERABLES**

TSVV 6: Impurity Sources, Transport, and Screening

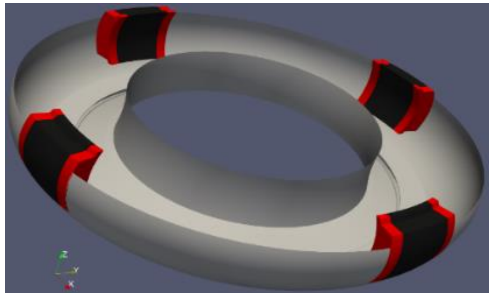
Key Deliverable 1: Validated suite of 3D codes and **transport models to describe in an integrated way the W content** and **its distribution in metallic devices**, in particular DEMO and **ITER**, with discrimination of main chamber and divertor sources, screening, transport, and exhaust along with its impact on the main plasma dynamics and performance.

- Task 1: **Numerical development and verification** of **SOLEDGE3X, EMC3-EIRENE and ERO2.0** codes.
- Task 2: **Gysela and VENUS-LEVIS code development** for investigation for W transport in the **edge region**
- Task 3: **Validation of numerical tools** on selected experiments on **WEST, W7-X and JET**

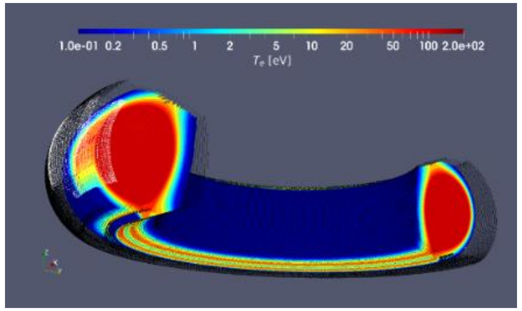
SOLEDGE3X-ERO2.0 3D workflow: numerical developments and validation on WEST experiments

- INVESTIGATION OF **W CORE CONTAMINATION** IN **WEST 3D WALL GEOMETRY** DUE TO ANTENNA LIMITER

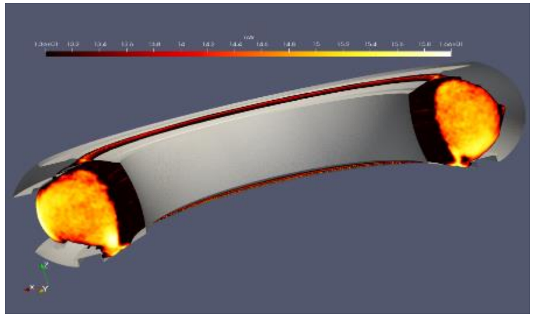
3D non-axsymmetric wall :
Radial Outer Gap: 1.5 cm

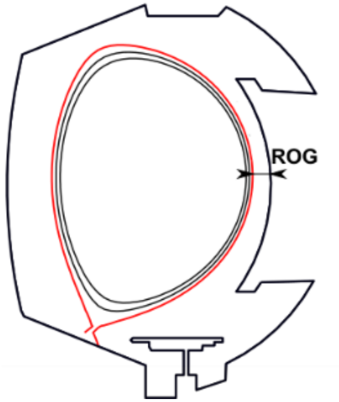


SOLEDGE3X plasma background

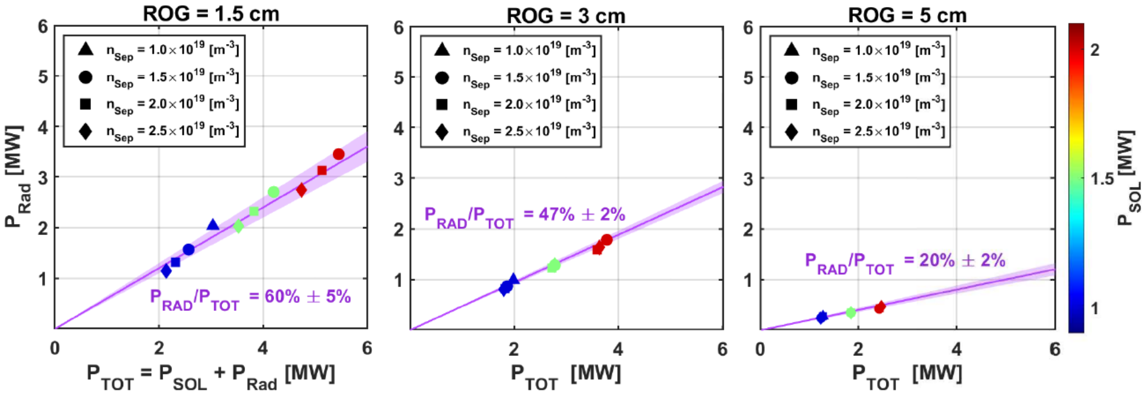


3D density map of W obtained with ERO2.0 using SOLEDGE3X plasma backrgound





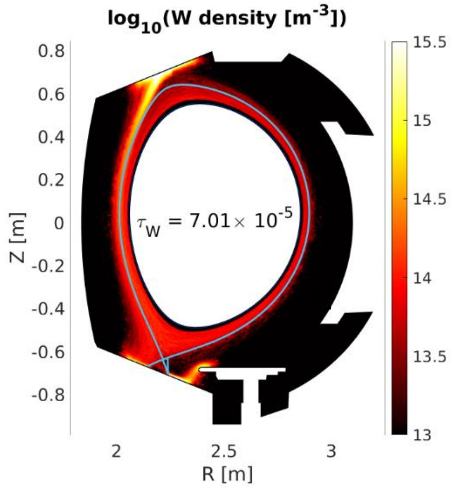
- **Simulations results predict** strong **role of the antenna limiter** in the tungsten contamination of core plasma depending on the distance from the plasma (ROG parameter)
- **The predictions have been validated against WEST experiments**

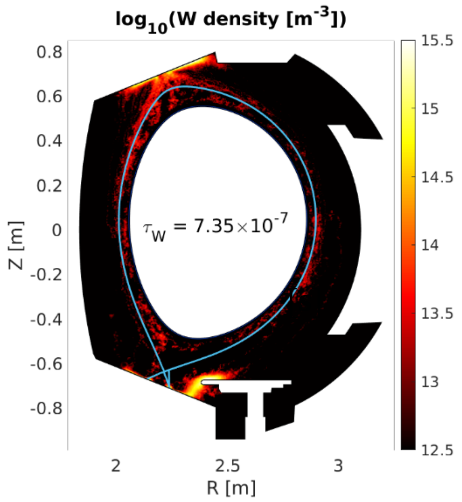


S. Di Genova et al., Nuc. Fus. 2024
G. Ciraolo et al PSI 2024

Improving W migration description in ERO2.0

Old version

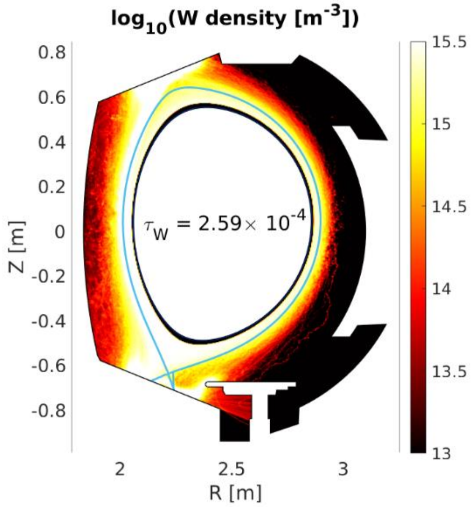


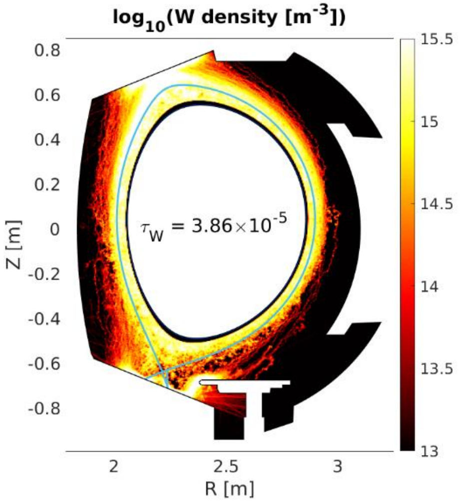


Code update	
Collisional forces	friction forces F_0, thermal forces $F_{\nabla T}$
Sheath physics	Electron density with Boltzmann factor: $n_\mathrm{e} = n_0 \exp\left(\frac{\mathrm{e}\phi}{k_\mathrm{B} T_\mathrm{e}}\right)$

With the new version, penetration of W into the core region increases accordingly to experimental measurements

New version





S. Di Genova et al NME. (2023)
S. Di Genova, PhD manuscript (2024)

SOLEDGE3X-ERO2.0 3D workflow: numerical developments and validation on WEST experiments

INVESTIGATION OF W CORE CONTAMINATION IN WEST **3D MAGNETIC GEOMETRY (IMPACT OF MAGNETIC RIPPLE** ON TARGET HEAT FLUX AND W EROSION AND MIGRATION)

Two approaches currently used:

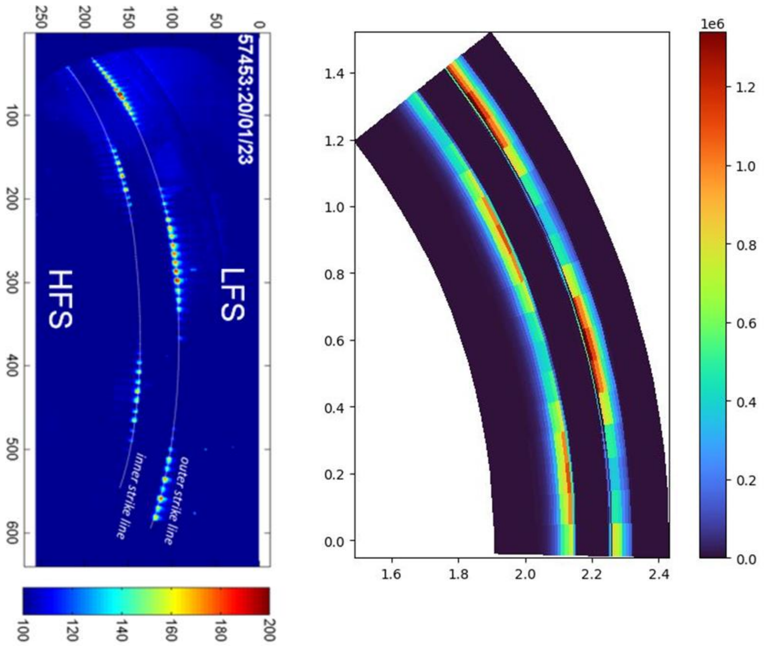
1) B_{ripple} is added as a perturbation on the axysimetric B

- Increased numerical costs as parallel operators are now coupled between (geometric flux surfaces): one 3D system must be solved instead of N^{FS} independent 2D systems for parallel viscosity and parallel heat fluxes
- Non standard radial BC with parallel fluxes into the core and first wall

2) Implementation of 3D NON-AXISYMMETRIC meshes aligned to perturbed flux surfaces

- **New plasma and wall mesh generated**
- Power and density scans performed → results close to the experimental values with ripple effect
- **ERO2.0 data analysis on going** → post-processing tools to be optimized

[R. Dull et al, Nuc. Mat. Energy (2024)]

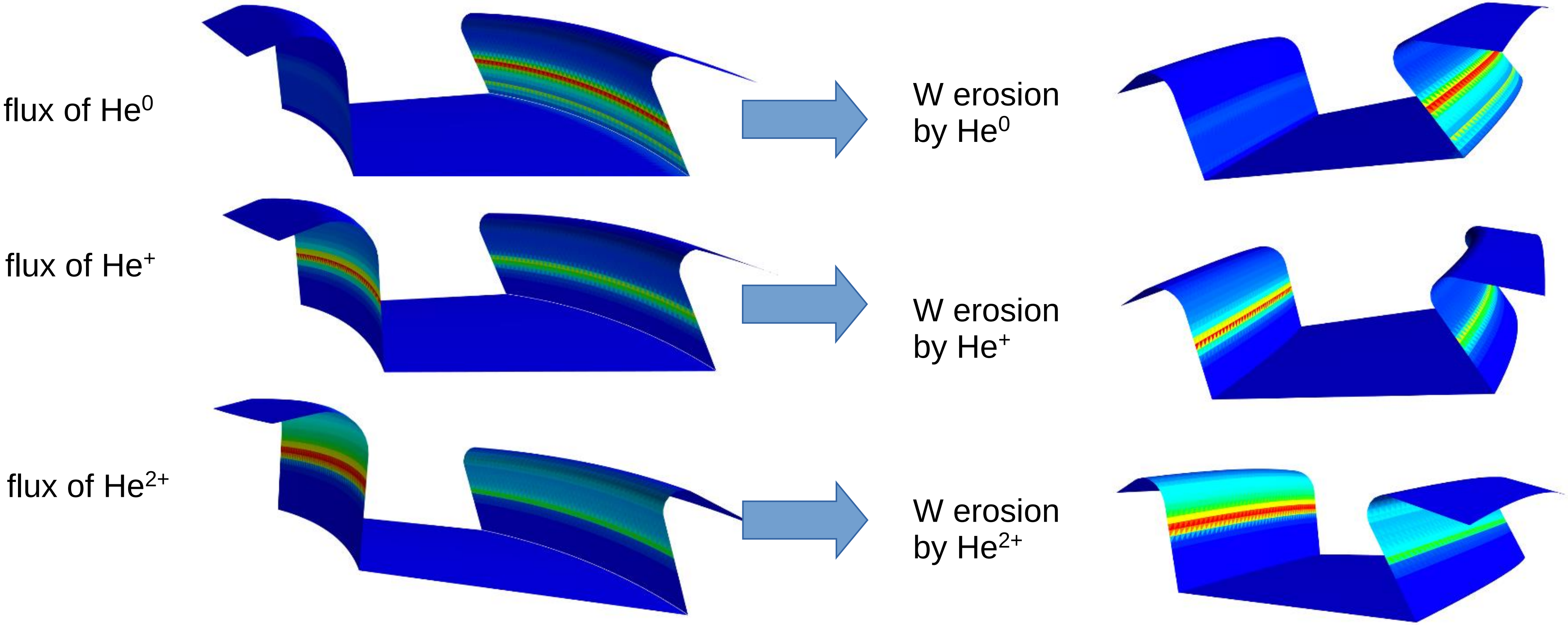


Top view of heat flux on divertor: experiments (IR camera) on WEST (left) and simulations with SOLEDGE3X (right)

ERO2.0 CODE DEVELOPMENT

- **Old version**:
  - **only** constant concentrations **of incoming background particles** could be defined (fraction of electron flux) - e.g. 50% He^+, 50% He^{2+}
- **New version:**
  - **allows to define spatially varying concentrations of incoming background particles including neutrals (decoupled from electron flux)**

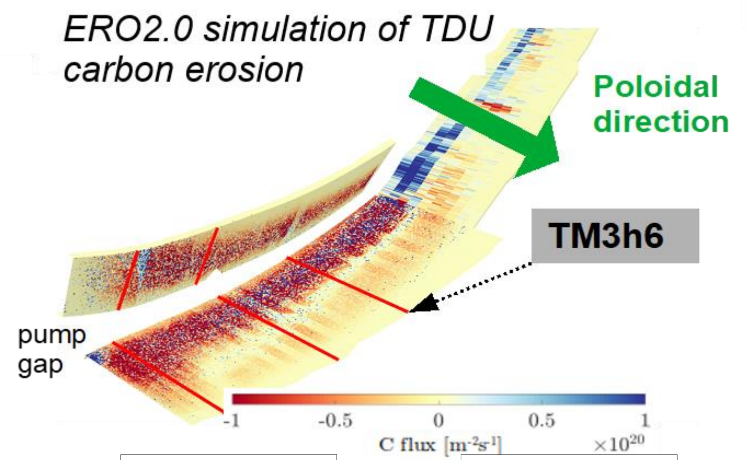
> Important for Helium plasmas (He^+/He^{2+} ratio), oxygen impurities @WEST, seeding impurities, ...

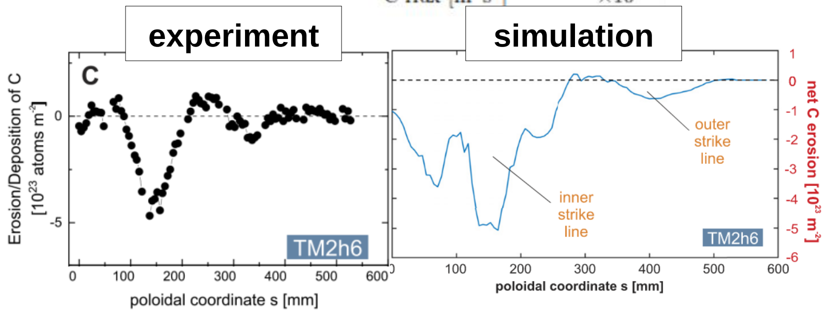


EMC3-EIRENE + ERO2.0 WORKFLOW: VALIDATION ON W7-X

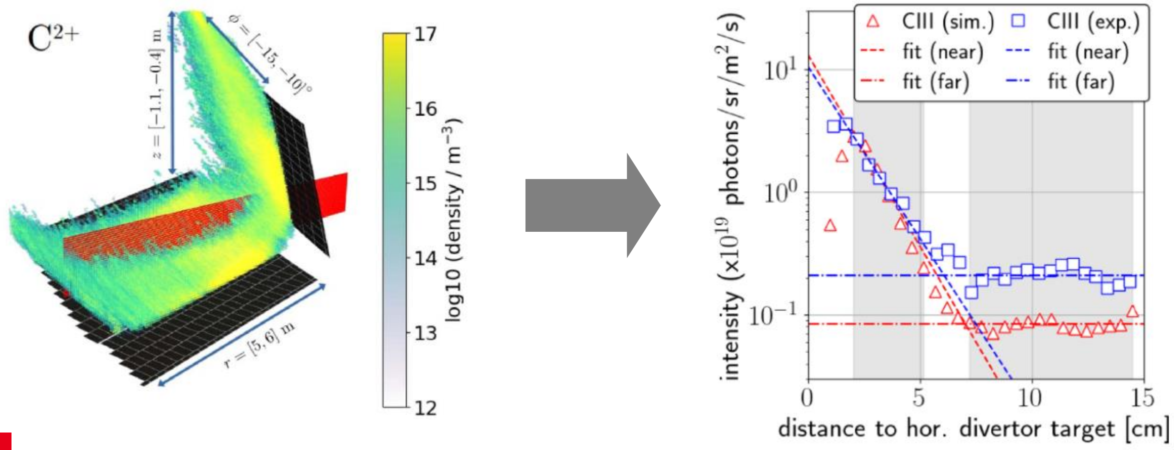
- **W7-X simulations:**
  - **Develop EMC3-EIRENE + ERO2.0 integrated 3D workflow**
  - **Validate the workflow using W7-X experiments**

- **intrinsic ^{12}C erosion and transport:**
  - Comparison with **post-mortem data** [1-3] and **spectroscopy** [4]





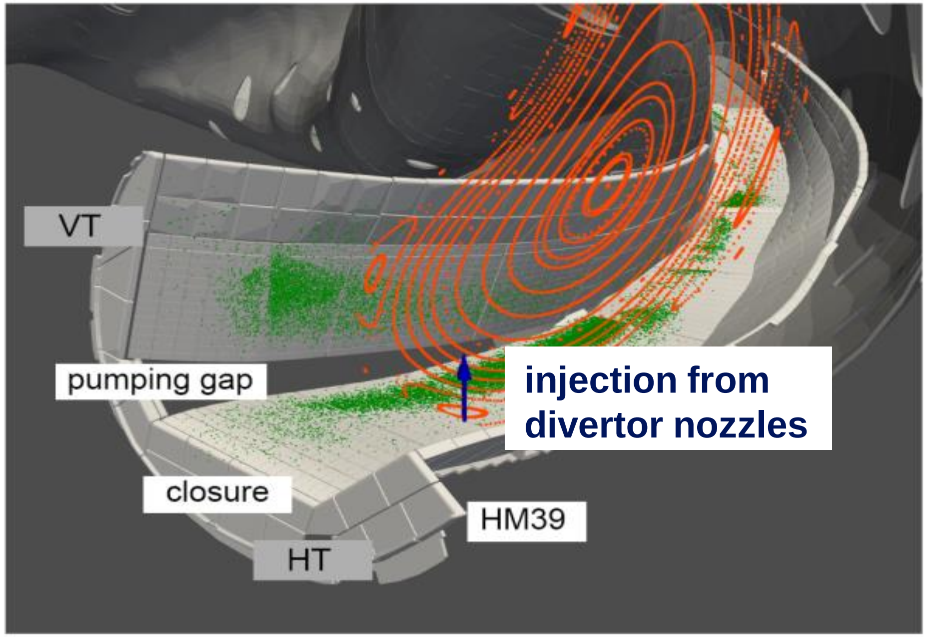
Experimental benchmark via carbon line emission spectroscopy

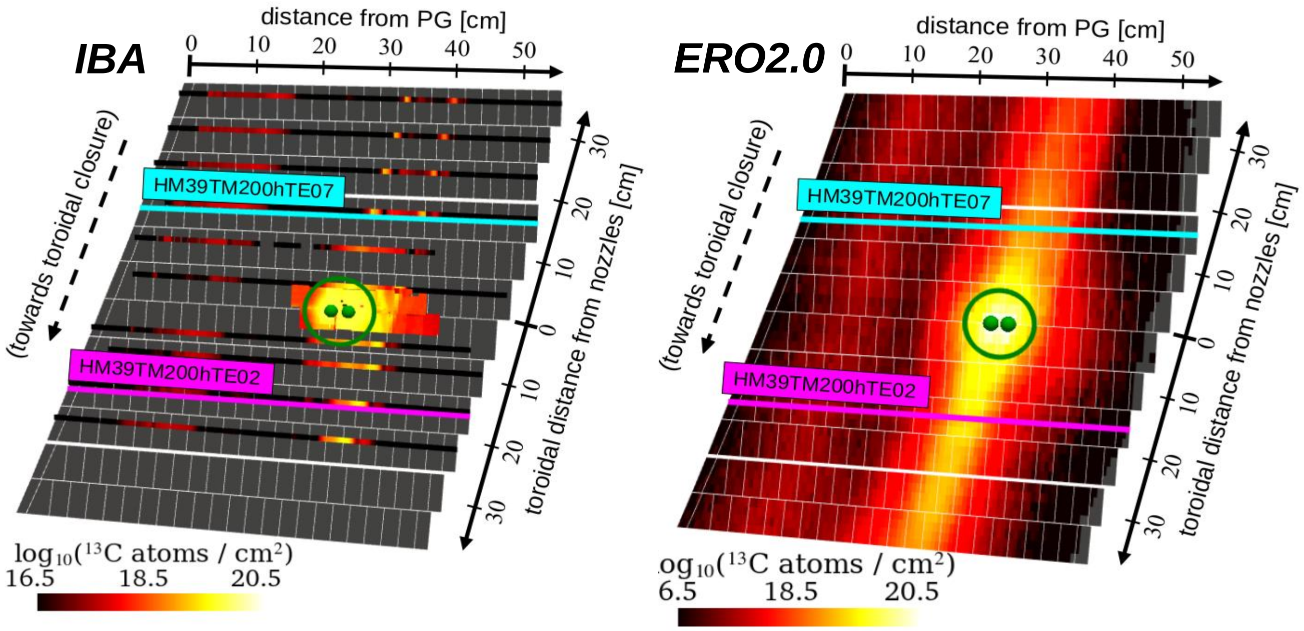


[1] S. Brezinsek et al., NF 2021
[2] C.P. Dhard al., Phys. Scr. 2021
[3] M. Zhao et al., NF 2022
[4] J. Romazanov et al., NF 2024

EMC3-EIRENE AND ERO2.0 SIMULATIONS AND VALIDATION ON W7-X

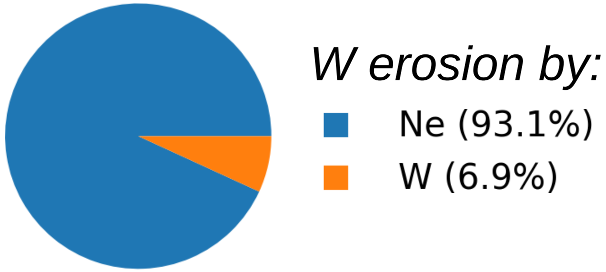
- **W7-X simulations:**
  - **Develop EMC3-EIRENE + ERO2.0 integrated 3D workflow**
  - **Validate the workflow using W7-X experiments**
- **injection of ^{13}C marker impurities:**
  - Comparison with post-mortem profiles [1-3]



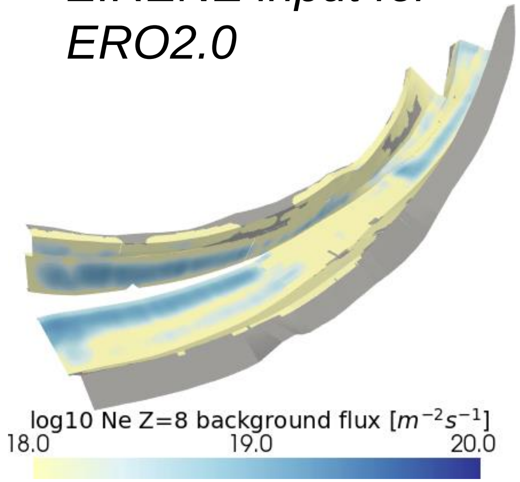


[1] E. Wüst et al., NME 2022
[2] C. Kawan et al., NME 2024
[3] J. Romazanov et al., PSI conference 2024

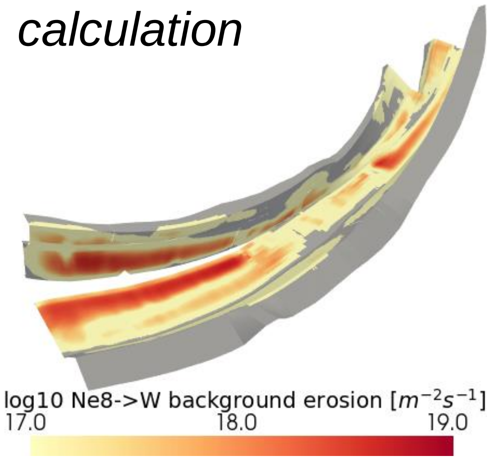
- **W7-X simulations:**
  - **Develop EMC3-EIRENE + ERO2.0 integrated 3D workflow**
  - **First predictions for W7-X with full-W PFCs**



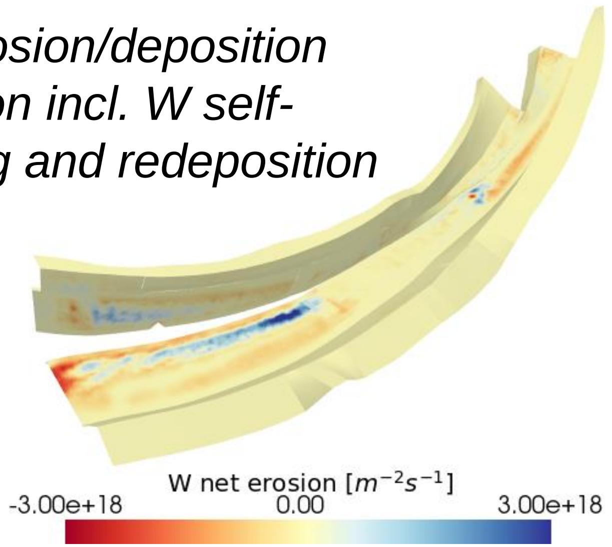
Example of EMC3-EIRENE input for ERO2.0



Example of ERO2.0 gross erosion flux calculation



W net erosion/deposition distribution incl. W self-sputtering and redeposition



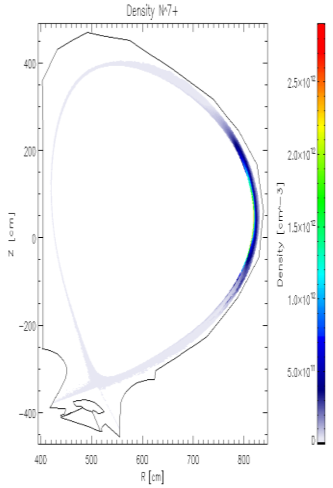
[1] J. Romazanov et al., EPS conference 2025

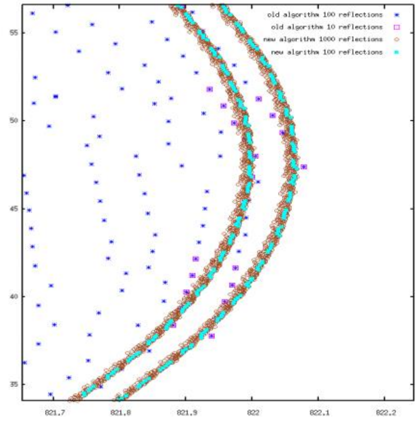
3D KINETIC IMPURITY MODELING WITH EIRENE KIT MODULE

EUROfusion

- Kinetic ions followed by **guiding centre** approximation
- New accurate **implementation of grad-B and curvature drift-movement**
  - **Completely redesigned core part of KIT with EMC3** (field aligned local curvilinear coordinate system of the EMC3 cell)
  - **Banana orbit correctly described**
- Re-designed treatment of anomalous diffusion
  - Add time step limit to avoid huge diffusion steps

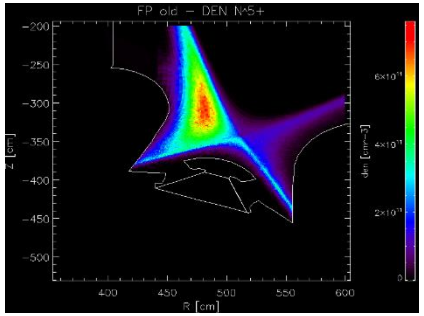
- **TEST simulations for Nitrogen seeding with an ITER plasma background**





Banana orbit correctly described

- BUT still **unphysical accumulation of Nitrogen N5+ in the HFS divertor region**



[HARTING D. et al., Nucl. Mater. Energy ***33,*** *101279 (2022)]*

3D KINETIC IMPURITY MODELING WITH EIRENE KIT MODULE

EUROfusion

New Fokker-Planck collision operator was implemented

- Now properly treats scattering of ions out of the magnetic mirror regions
- Friction with background species included
- Strongly reduced confinement compared to simple energy relaxation scheme
- **Same Fokker-Planck operator as in ERO2.0** but missing thermal force

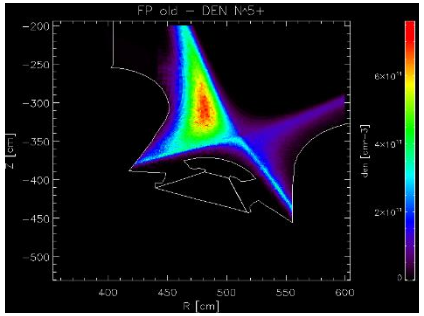
Time step control for MC integration of FP operator **is vital**

- Two time step controls were implemented
  - Time step as **fraction** (10^{-4}) from **Spitzer slowing down time** τ_s
  - **Adaptive time step control** algorithm (**factor 5-10 faster**)

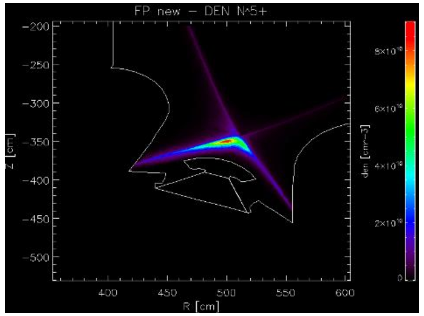
- **Benchmark with ERO2.0** shows **good agreement both for light and heavy impurities**

- **TEST simulations for Nitrogen seeding with an ITER plasma background**

Old FP operator



New FP operator



[HARTING D. et al., Nuclear Materials and Energy 42 (2025) 101887]

Next steps:

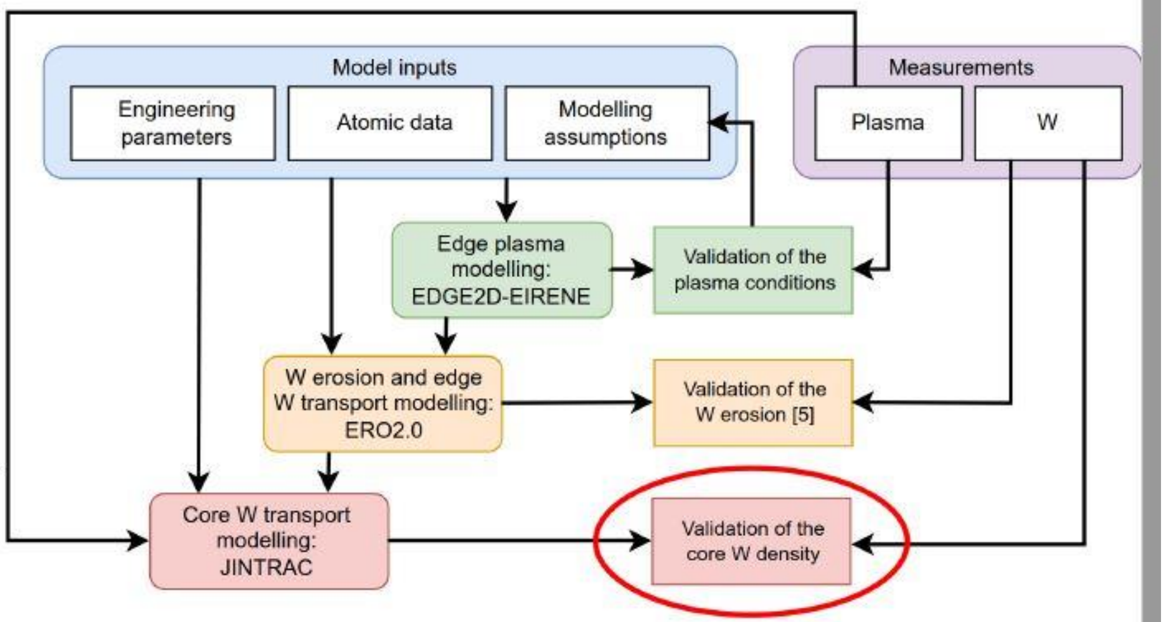
- **Include** missing **thermal force** (inline with ERO2.0)
- Continue **detailed benchmark with ERO2.0** including **recycling Impurities**
- Compare **kinetic low Z impurity** simulation to **fluid solution**

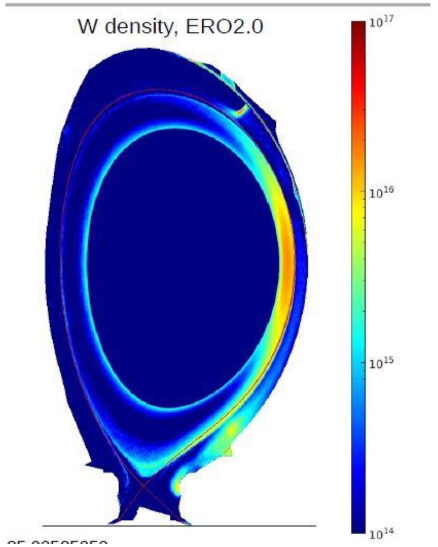
cea

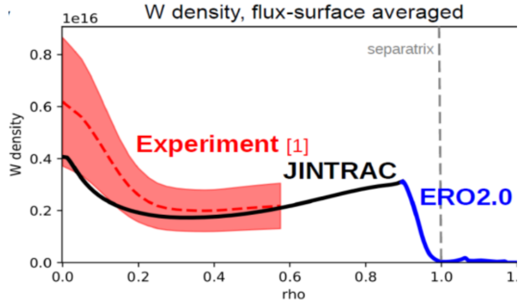
JÜLICH Forschungszentrum

Task 3 for key deliverable 1: Validation of numerical tools on selected experiments on WEST, W7X and JET

- The plasma conditions are simulated in EDGE2D-EIRENE [1] (JINTRAC [2]) by adjusting uncertain parameters to optimise agreement with measurements
- W erosion and edge transport is predicted using ERO2.0 [3]
- The predicted W density at the pedestal top (ρ = 0.9) is used as the boundary condition for predictive W core transport simulations using JINTRAC
  → Earlier validation of JINTRAC W core transport [4] extended to cover the SOL and W erosion from ERO2.0
- **No information from W diagnostics is used to fit the predictive W simulations**







- High-power type-I ELMy H-mode experiments
  - 18-36 MW of heating
  - V5/C and C-C configurations, focus on V5/C
  - Both deuterium and tritium

→ *EPS 2023 invited talk by H Kumpulainen*

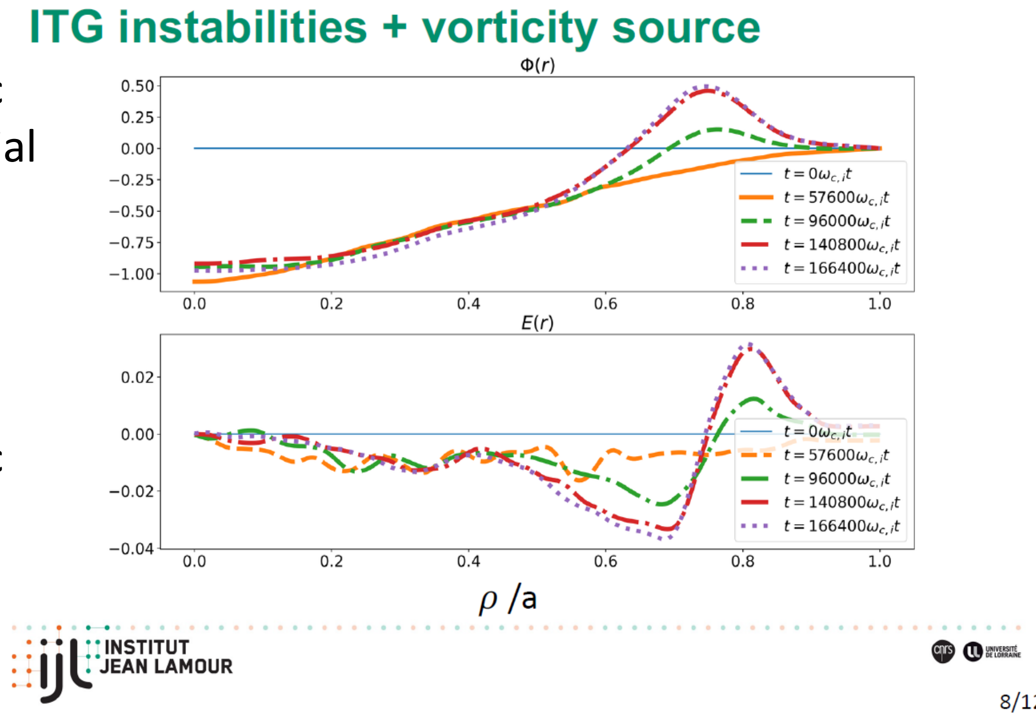
Task 2 for key deliverable 1: Gysela code development for investigation for impurity transport in edge region

ID	Milestone-description	participants	Target date
M1.19	**Implementation of a source term in the vorticity equation of GyselaX code**	E. Gravier, PhD student CEA/UL (funded by other means)	12/2021
M1.20	**Generation of transport barriers by sheared poloidal flows, triggered by a vorticity source** (poloidal momentum), with GyselaX code.	E. Gravier, PhD student CEA/UL (funded by other means)	12/2022

In collaboration with TSVV 1 and 4

Electric potential radial profile

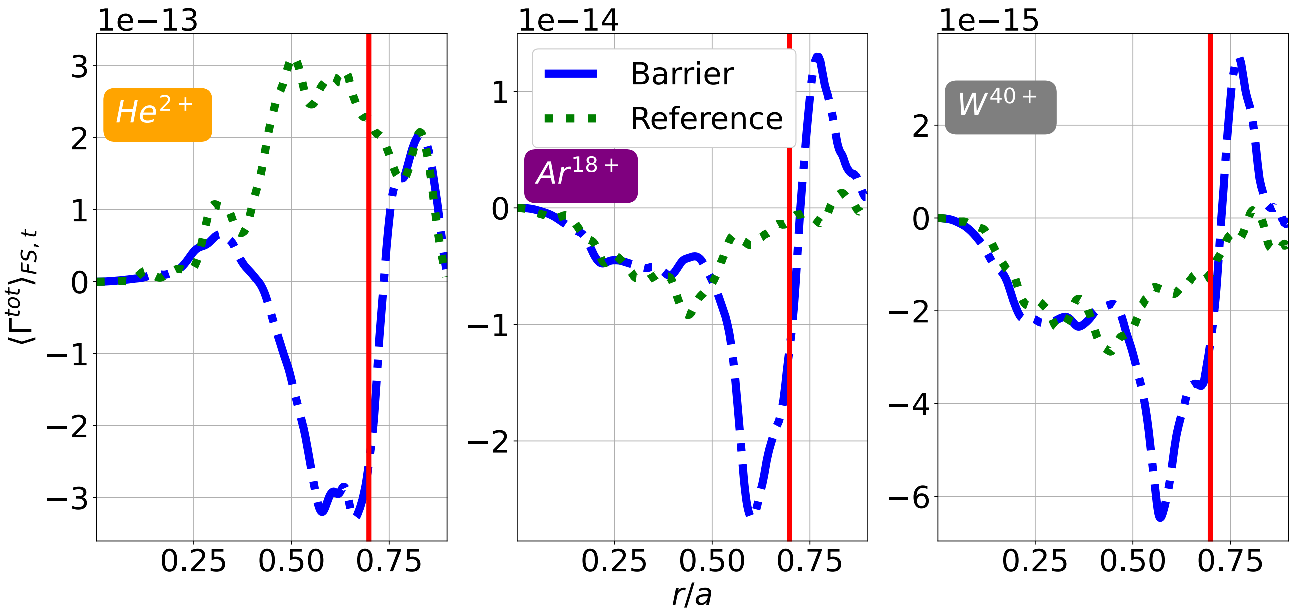
Radial Electric field profile



E Gravier, G Lo Cascio (IJL and Univ. Lorraine)

- Strong reduction in turbulent transport for helium
- Strong negative flux on the inside of the barrier avoids particles to leave core region
- Positive flux on the outside region prevents particles to contaminate the core
- Effective barrier: enhanced confinement

- Vorticity source injects poloidal asymmetries of pressure anisotropy $\partial_\theta \Pi_\parallel$
- Leads to increased neoclassical fluxes at source location, not fully realistic
- Work required to create a poloidal momentum source without poloidal asymmetries !



Total impurity flux with (dashed-dotted blue lines) and without (dotted green lines) the transport barrier. Red vertical line indicates vorticity source position.

Analysis of simulation results ongoing for estimation of **effective radial transport coefficient**

- Integrated modeling: need for radial profiles of transport coefficients

W turbulent flux [C. Angioni 2012]

$$\frac{\Gamma^{turb}(\mathrm{W})}{n_\mathrm{W}} = -D_\mathrm{n}\frac{1}{n_W}\frac{\partial n_W}{\partial r} - D_T\frac{1}{T_W}\frac{\partial T_W}{\partial r} - D_u\frac{\partial \Omega_\phi}{\partial r} + V_p$$

Diffusion — Thermo-diffusion — Roto-diffusion — Pure convection

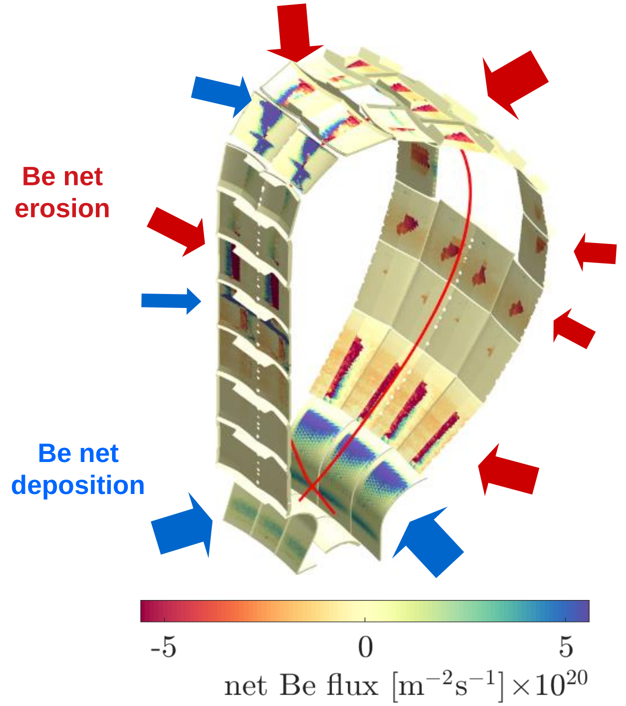
Diffusion — Full convection

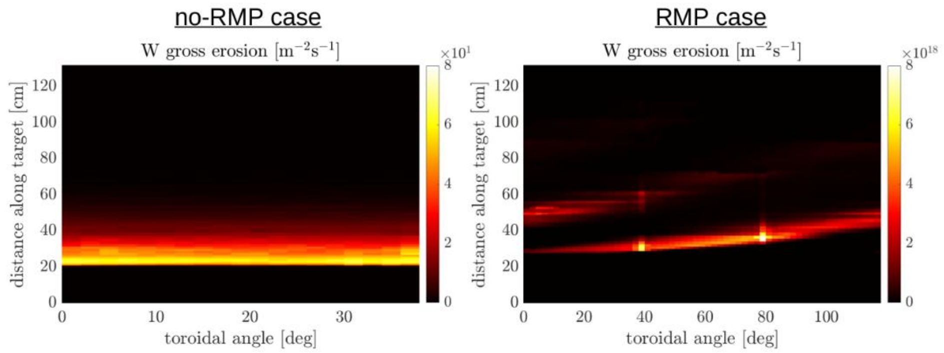
[G. Lo-Cascio et al., *Controlling impurity transport in 5D gyrokinetic simulations using a transport barrier,* Nucl. Fusion 65, 056021 (2025)]

Key Deliverable 2: Assessment of the W influx, W screening, and W transport in ITER plasmas

EMC3-EIRENE + ERO2.0 simulations for ITER plasma

- **ERO2.0 runs using 2D ITER plasma backgrounds (OEDGE):**
  - Previous work (*J. Romazanov et al. CPP-2019, NME-2021, NF-2022*) focused on Be FW erosion
  - Next step: repeat with considering the W divertor
- **ERO2.0 runs using 2D/3D ITER plasma backgrounds with+w/o RMPs (EMC3-EIRENE)** is work-in-progress:
  - 4 EMC3-EIRENE PFPO plasma backgrounds by Heinke Frerichs: 2 with and w/o RMPs, each in low + high density
  - Implementation of EMC3-EIRENE to ERO2.0 data transfer was adapted to tokamaks
  - **First preliminary W gross erosion obtained on inner target for low-density case**
  - Under investigation: improvement of B-field interpolation





Work done at the beginning of the project before the change to full W wall

Since then **new activity recently done at FZJ** with full W wall (**presented at PWIE annuel meeting**)

Key Deliverable 2: Assessment of the W influx, W screening, and W transport in ITER plasmas – SOLEDGE3X modeling

EUROfusion

ID	Milestone-description	participants	Target date
M2.2	2D Plasma background (no RMP)	D. Harting, H. Bufferand, G. Ciraolo, **N. Rivals**	12/2021

- **20MW** **(PFPO-1)**
- **L-mode** transport
- Pure H
- **Advanced options in EIRENE** (elastic ion-molecule col., MAR, neutral-neutral col.)

SOLEDGE3X computational domain

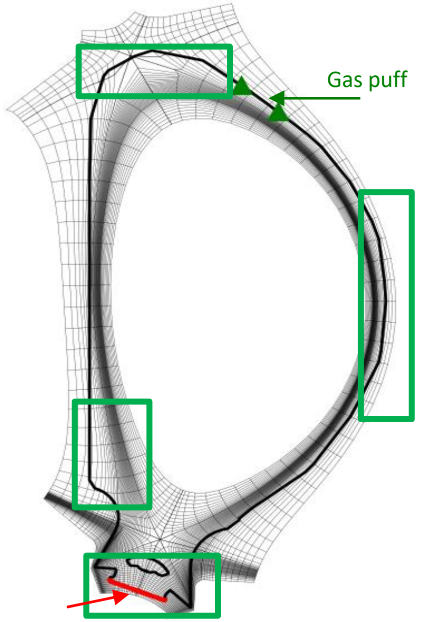
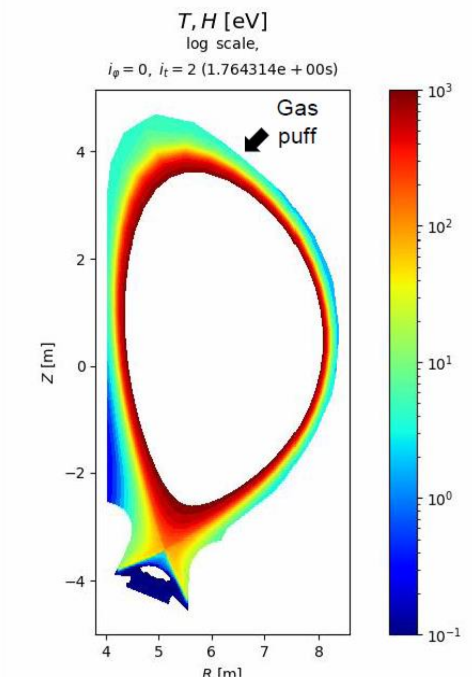


Illustration of case 2297

(mid-upper part of the gas puff scan)

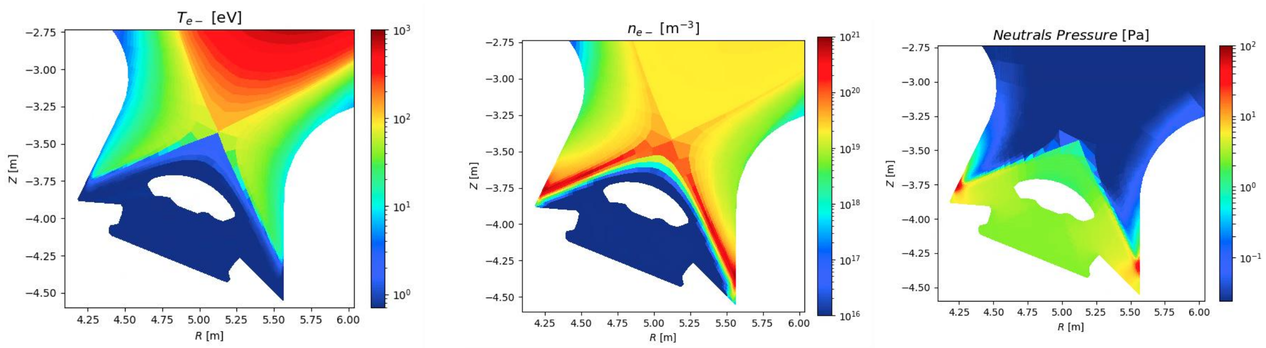


N Rivals (in collaboration with TSVV 3 and IO)

electron temperature

electron density

neutral pressure

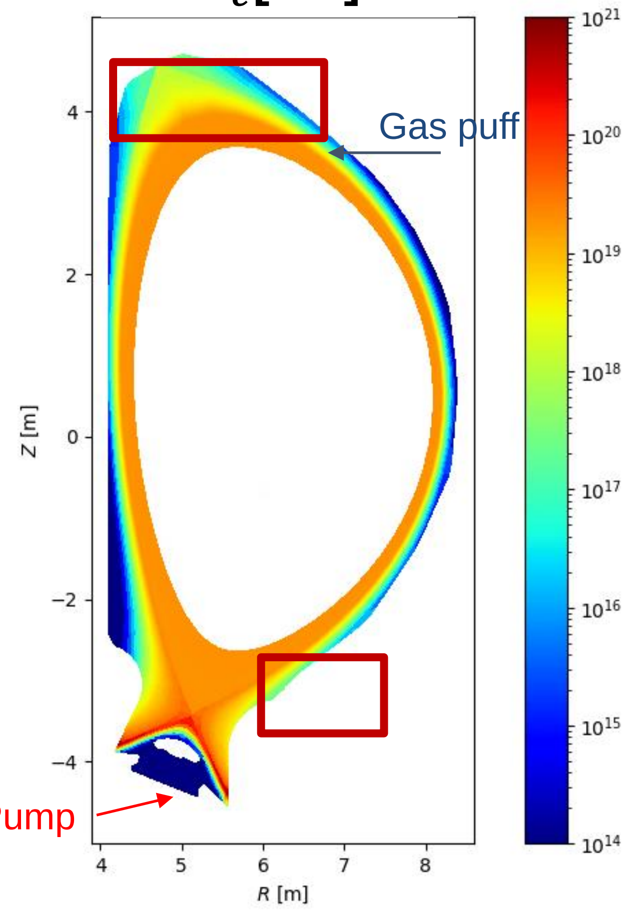


PFPO-1 case, Pure H, 20 MW, throughput = 6.80e+22/s

SOLEDGE3X SIMULATIOND FOR LOW POWER L-MODE ITER CASE: INCREASING THE THROUGHPUT FROM ATTACHED TO SEMI-DETACHED PLASMA

Illustration case at medium throughput (3.31 x 10^{22} $e^{-}.s^{-1}$):

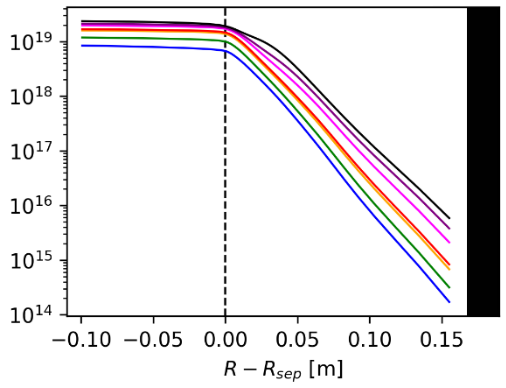
n_e[m^{-3}]



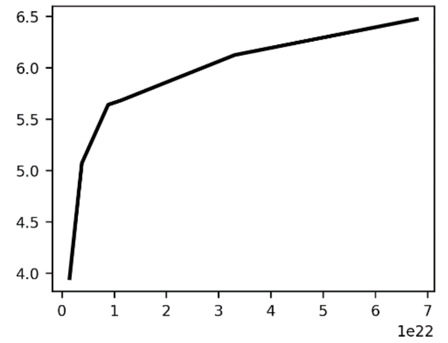
[N. Rivals et al, NME 2022

[N. Rivals et al 2025 Nucl. Fusion 65 026038]

n_e[m^{-3}] OMP

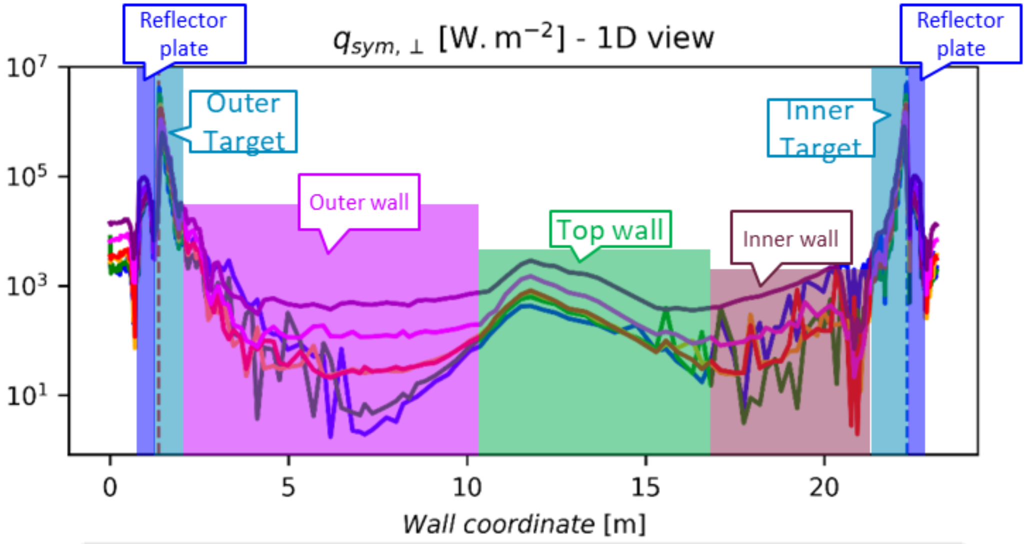


λ_q[mm]



Throughput [$e^{-}.s^{-1}$]:

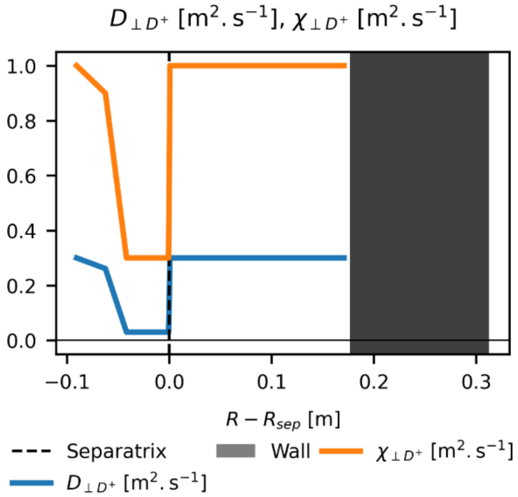
- 1.46e+21 s^{-1}
- 3.81e+21 s^{-1}
- 8.85e+21 s^{-1}
- 1.13e+22 s^{-1}
- 3.31e+22 s^{-1}
- 6.80e+22 s^{-1}
- 1.76e+23 s^{-1}

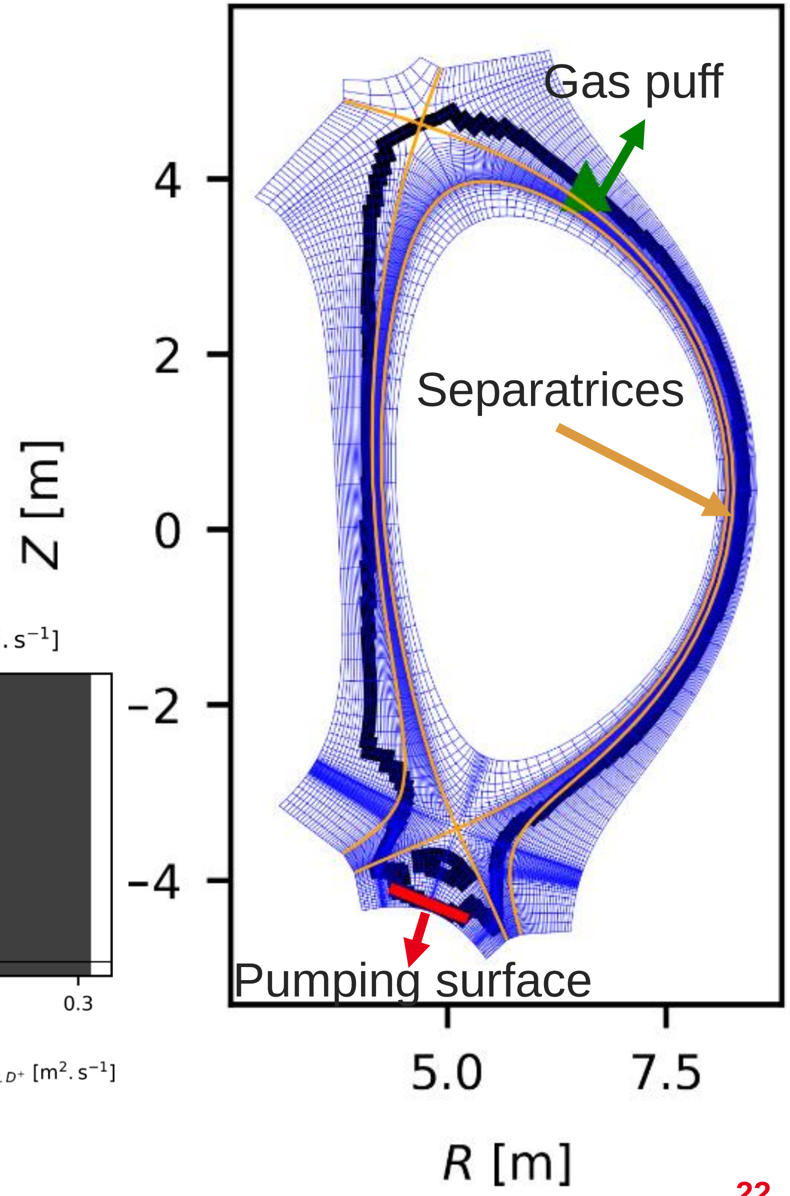


- λ_q increase with throughput
- **Strong plasma-wall interaction**:
  - Top
  - Outer lower wall

100MW D, Ne, He ITER scenarios

- **Input power from core-edge boundary** - 50MW for D^+ + 50MW for e^-
- **Particle influx from the core** - $1.0 \times 10^{22} s^{-1}\ D^+,\ 1.0 \times 10^{20} s^{-1}\ He^{2+}$ (at 1800eV)
- **Impurities modelled**: Ne, He from fusion
- **Fuelling Port, Pump** – top port in the LFS, pumping surface with recycling coeff. = 0.9928
- **Magnetic equilibrium**: d_rsep = 6cm (eq135011r6) wall (w116000r2)
- **Wall material**: **W**
- particle recycling coefficient at wall = 1
- **Neutral Model**: Kotov model with neutral-neutral collisions
- **Drifts, Collisional closure:** No fluid drifts, no currents, Zhdanov closure
- **Transport coefficient profile:** H mode (Far SOL $D_\perp = 0.3\ m^2 s^{-1}, \chi_\perp = 1.0\ m^2 s^{-1}$)

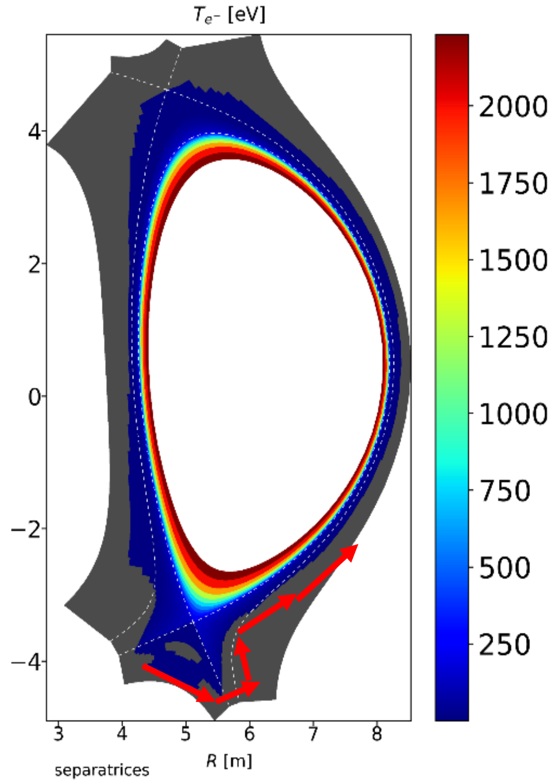


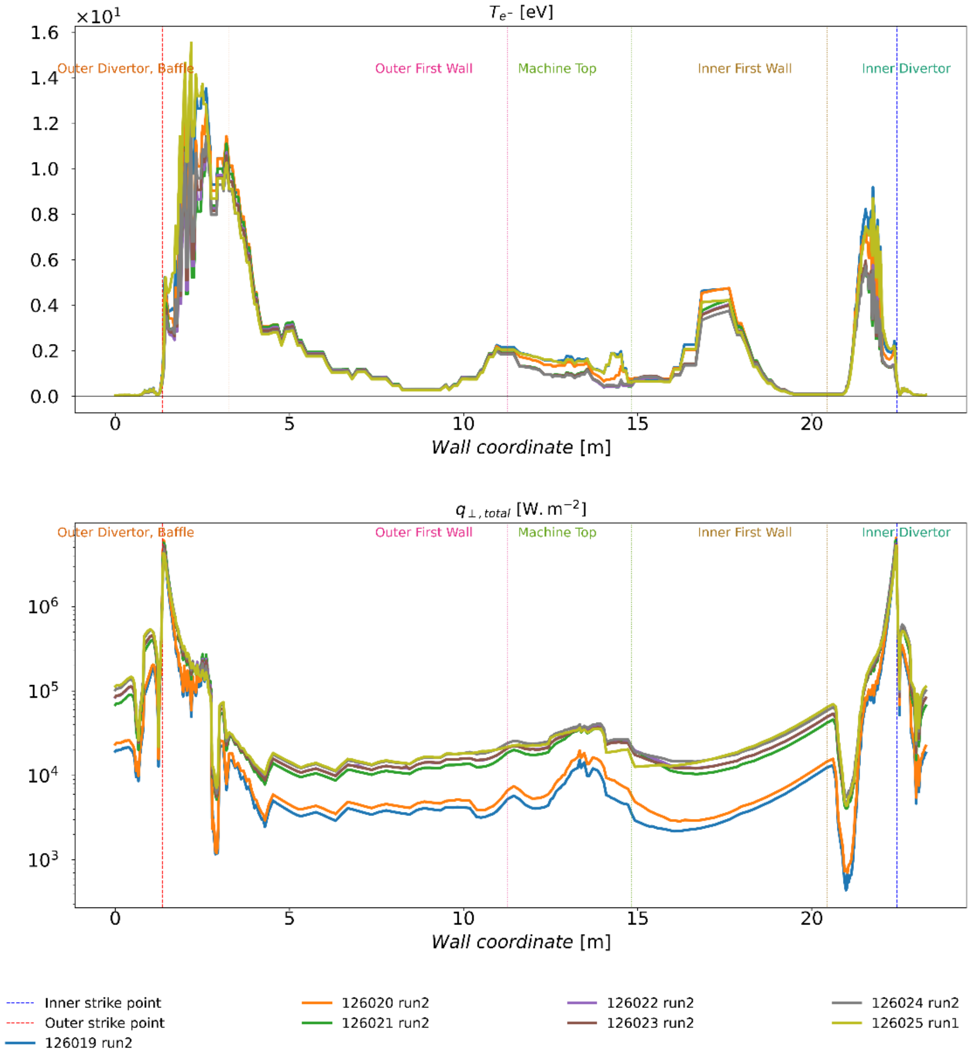


Courtesy S Sureshkumar (in collaboration with TSVV 3 and IO)

100MW D, Ne, He ITER scenarios
First wall conditions and fluxes

- T_e at the outer baffle is ~10eV and is similar regardless of neutral pressure
- Heat flux on the FW is generally larger for higher fuelling scenarios – exception is when Ne concentration is much larger

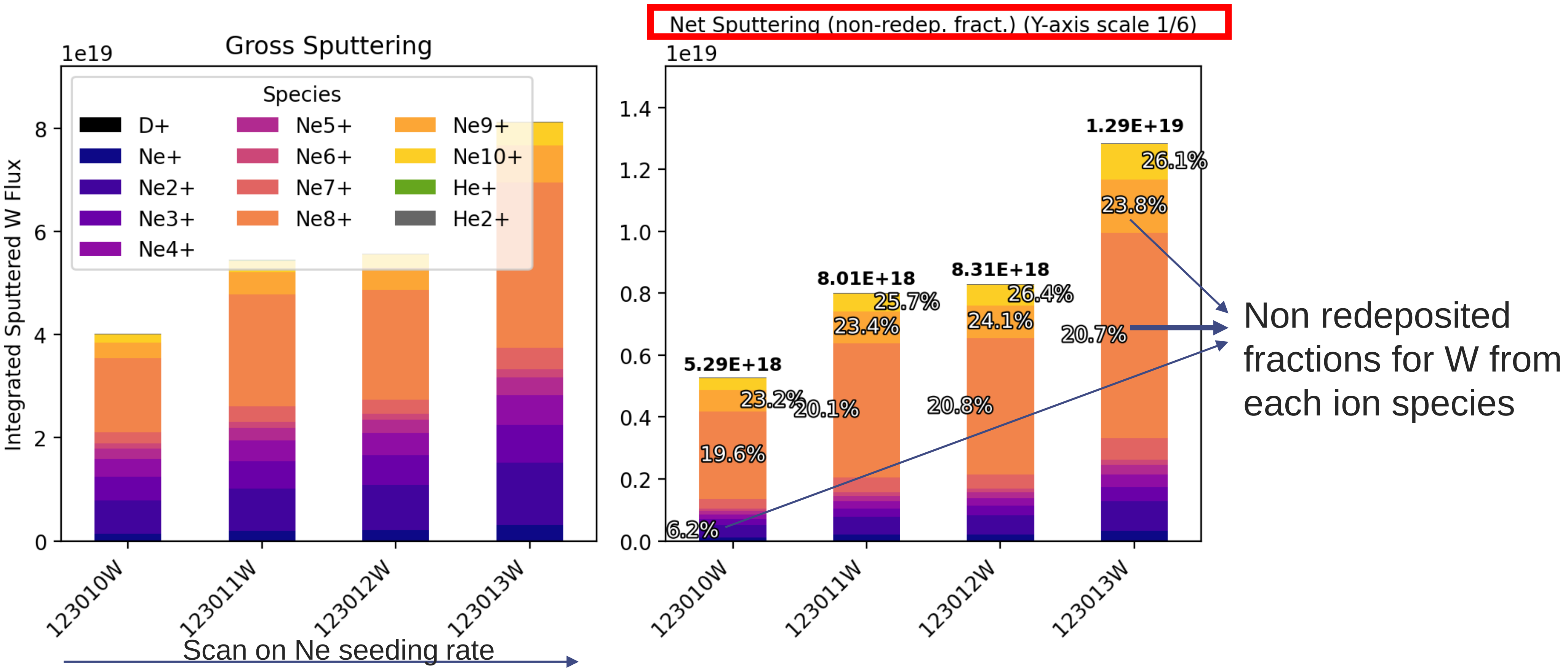




Courtesy S Sureshkumar (in collaboration with TSVV 3 and IO)

Ne8+ largest source of W sputtering

Courtesy
S Sureshkumar
(collaboration with TSVV 3, 5 and IO)



- **Net sputtering estimated using non-redeposited fraction from [8] and modified Thompson distribution [9] for the sputtered energy.**
- ***Ne^{8+}* - still largest W sputtering source**, larger non redeposited fraction for high Z Ne.

[8] D. Tskhakaya, et al, (2015) Nuclear Materials ,463 : 624–628.
[9] N. Mellet et al, (2017) Plasma Physics and Controlled Fusion, 59 (3): 035006.

CODES ACCESSIBILITY, DISSEMINATION and IMASification

EUROfusion

- **All numerical tools accessible** to the eurofusion community (SOLEDGE3X, ERO2.0, etc…)
  - Codes accessible (or soon to be) either through Gateway repository or web-page
  - codes are well-documented, version-controlled

- **Training of new users** has been performed in collaboration with others TSVVs and WP
  - **SOLEDEG3X training workshop (2023)**
  - **ERO2.0 training week last December (2025)**
  - **But also done on an individual basis**

- On-going **IMASification** to allow easy set-up and post-treatment with experiments as well as code comparison
  - Ongoing with SOLEDGE3X and ERO2.0
  - EMC3-EIRENE to be started

Conclusions and perspectives

- **Several major improvements on code developments achieved:**
  - SOLEDGE3X version able to threat **full 3D magnetic and wall geometry** now available
  - ERO2.0 **physics model** strongly enriched
  - EIRENE **KIT module redesigned** on solid basis
  - **3D workflows SOLEDGE3X+ERO2.0 and EMC3-EIRENE+ERO2.0** routinely used for comparison with experiments

- **Several studies on WEST, W7-X and JET for code validation successfully performed**
- **Gyrokinetic modeling of impurity transport** for estimation of **effective radial transport coefficients** ongoing
- **Strong connection with WP PWIE** both on modeling developments and code validation
- **Predictions for ITER** performed with SOLEDGE3X, EMC3-EIRENE and ERO2.0

2026-2027 outlook – TSVV-E: Motivation and context

TSVV-E: Impurity Sources, Transport, and Screening in Metallic Devices

- Develop an integrated modelling suite to predict tungsten (W) impurity distributions (including sources, transport, screening), and assess its impact on plasma performance in ramp-up and steady-state phases. Exploit synergies with TSVV-A through TSVV-D.
- Create and validate 3D kinetic transport models for heavy impurities (including W) and seeding species such as Ar, Kr, and Xe in the edge and scrape-off layer of tokamaks and stellarators.
- Evaluate the effects of 3D perturbations and ELM suppression techniques on W impurity and seed impurity distributions in ITER reference scenarios and their implications for future fusion devices.

- Reduced model development: focus on core-edge integration and pedestal region for improving our **predictive capabilities on W core contamination in H-mode**