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

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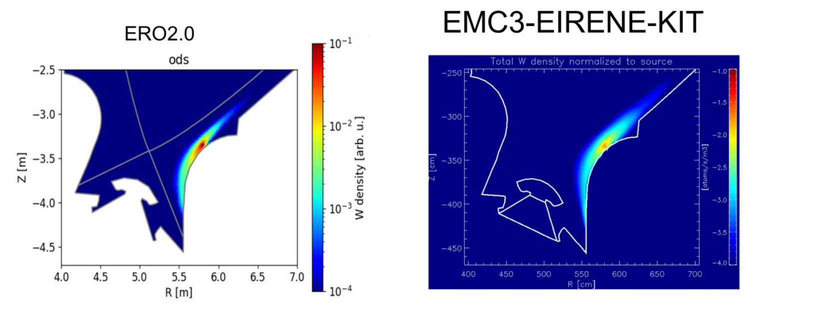
ABSTRACT

- In this poster, we present an overview of the EUROfusion Theory, Simulation, Validation, and Verification project entitled **"Impurity sources, transport, and screening in Metallic Devices" (TSVV E)**. The main goal is the development, verification, and validation of advanced numerical tools in order to **predict impurity sources, transport, and screening in the edge plasmas of tokamak and stellarators, in particular ITER and W7-X, as well as their impact on future fusion devices.** The project is organized in WP related to the **main objectives of the project** :
- **Development of an integrated modelling suite to predict tungsten (W) impurity distributions** and assess its impact on plasma performance.
- **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
- Evaluation of 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.
- **development of fast reduced models,** making possible the scan over several parameters, often too much time consuming for first-principles 3D simulations

KINETIC ION TRANSPORT MODULE

- **3D kinetic description of heavy impurity transport in edge and SOL plasmas,** necessary both for taking into account the finite Larmor radius effects on prompt redeposition and the short lifetimes of lower ionization stages of such impurities. **The Kinetic Ion Transport (KIT) module of EIRENE** (Kinetic ions followed by **guiding centre** approximation) has been chosen as one of the possible solutions for such a description.
- Major improvements have been obtained during these years. For example, the **correct description of grad-B drift and the formation of banana orbits** in the magnetic mirror. **A new Fokker-Planck collision operator has been implemented** which now properly treats the scattering of ions out of the magnetic mirror regions, which takes into account friction with background species.
- First **W simulations** with **EMC3-EIRENE-KIT** achieved (**indication that a large fraction of the lower ionisation stages of W is NOT thermalized with the ion background plasma temperature).**



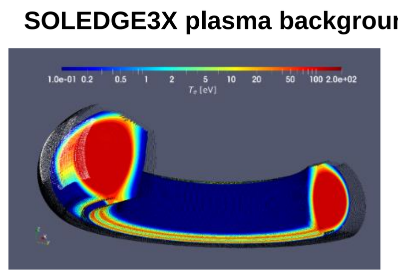
Next steps: Include missing **thermal force** (inline with ERO2.0); Continue Benchmark with ERO2.0 including **recycling Impurities** and **high Z impurities** (e.g. W, Ar); **Compare kinetic low Z impurity** simulation to **fluid solution**

First qualitative comparisons between results from ERO2.0 and KIT module using EMC3-EIRENE ITER plasma background

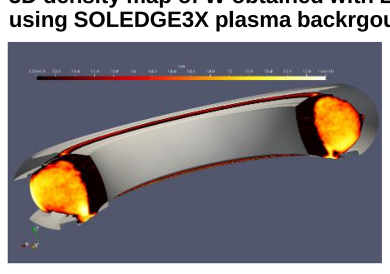
DEVELOPMENT OF NUMERICAL TOOLS FOR 3D SIMULATIONS

- **SOLEDGE3X-ERO2.0 3D workflow: improvements and validation on WEST experiments simulations** in 3D transport mode with a 3D magnetic geometry (ripple effect) and 3D wall (toroidally localized antenna limiter) for providing plasma background to be used for computing W sources and transport with ERO2.0 code

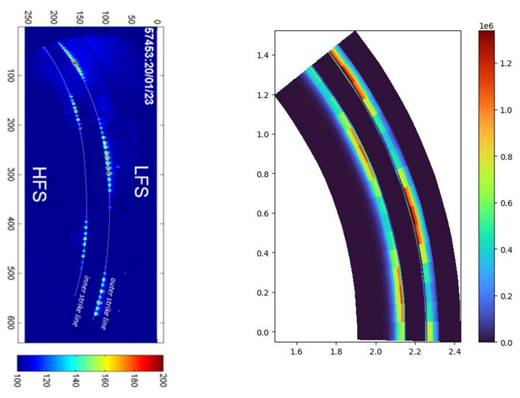
SOLEDGE3X plasma background



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



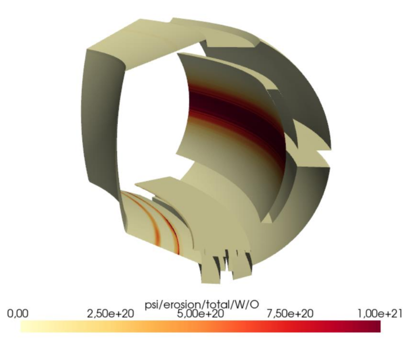
Top view of heat flux on divertor: experiments (IR camera) on WEST (left) and simulations with SOLEDGE3X (right)



Implementation of 3D magnetic equilibria: two approaches currently used:

1) B_ripple is added as a perturbation on the axisymmetric 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

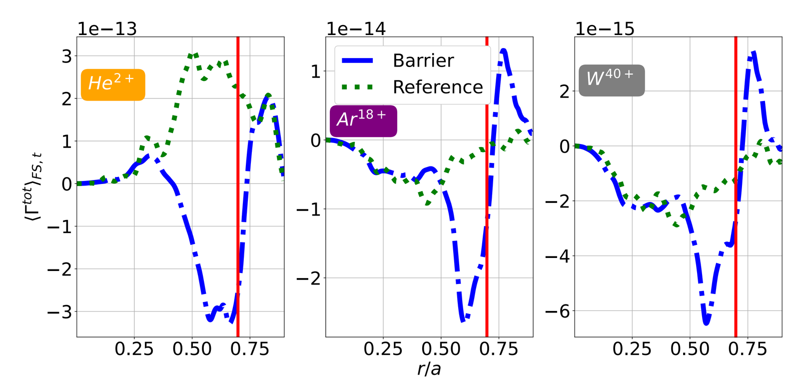
2) Implementation of 3D NON-AXISYMMETRIC meshes aligned to perturbed flux surfaces



Example of 3D computations with ERO2.0 using SOELDGE3X plasma background

IMPURITY TRANSPORT IN EDGE PLASMA WITH GYSELA AND VENUS-LEVIS CODES

- **GYSELA Gyrokinetic modeling of impurity transport in edge and pedestal region:**



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

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

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

Next step: Inclusion of Kinetic Electrons and Temperature Effects in Gysela simulations

- **Venus-Levis drift-kinetic studies to assess 3D equilibria effects on W transport**

The VENUS-LEVIS code will be applied to investigate the **transport of heavy impurities** in the presence **of saturated 3D MHD structures at the edge of high-performance tokamak plasmas**. Of particular interest will be the impact magnetic symmetry breaking associated with in-vessel and ex-vessel coils (using free boundary VMEC) and internally generated structures such as edge harmonic oscillations. The work will self consistently take into account neoclassical toroidal viscosity, centrifugal effects and essential collisional dynamics. A limitation of the current approach is that heavy ion self-collisions cannot yet be included. **Recent development to the code made it fully GPU-accelerated**, enabling fast and massively parallel simulations of millions of particles, which allows for the calculation of neoclassical transport coefficients that are necessary for such problems. The unique features of the VENUS-LEVIS code permits a realistic investigation into the difficulties of sustaining QH-modes in plasmas with a tungsten divertor (due to impurity accumulation in the 3D edge), and the potential impact of EXB flow shear, thermal profiles in the separatrix, and in-vessel and ex-vessel coils. The workplan will follow the following points:

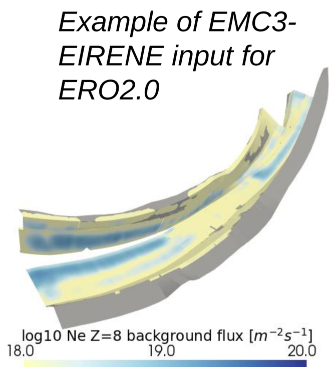
- Comparison of VENUS-LEVIS simulations of heavy and light impurities with Gysela simulations for axisymmetric non-rotating ITER pedestal (W neoclassical transport) plasma
- Generalization of the previous study using VENUS-LEVIS code to include centrifugal effects,
- Generalization of the previous case with VENUS-LEVIS code to include 3D equilibria effects (from RMP coils or/and EHOs) and NTV/flows

Derivation of "reduced" models and (D,v) maps for impurities from VENUS-LEVIS simulations

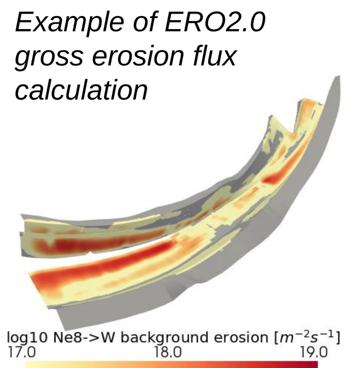
EMC3-EIRENE-ERO2.0 SIMULATIONS OF W7-X EXPERIMENTS

- **Improved 3D grid for ERO2.0:** Background: axis-aligned grid in ERO2.0 limits resolution of imported 3D plasma backgrounds (EMC3-EIRENE, SOLEDGE3X), potentially introducing numerical artifacts. Starting from the present version we will implement **flexible 3D grid in ERO2.0 aligned with the EMC3-EIRENE hexahedral cells**. The validation step will be performed on W7-X with Ne-seeded EMC3-EIRENE plasma background.
- **Charge-Exchange Neutrals (CXN) 3D workflow for ERO2.0:** Background: Workflow for transferring EIRENE-ERO2.0 data about CXN fluxes and energy & angular spectra currently exists only for 2D. **Realistic treatment of CXN is crucial for predicting unscreened main chamber W sources.** The workplan consists in developing a workflow considering complex 3D PFCs in tokamaks with CXN shadowing effects (e.g. JET poloidal limiters) and stellarators. The application cases will be both a W7-X geometry with Ne-seeded EMC3-EIRENE plasma background as well as a WEST geometry using N-seeded SOLEDGE3X background.
- **EMC3-EIRENE + ERO2.0** for **predictions for full-W wall W7-X.**

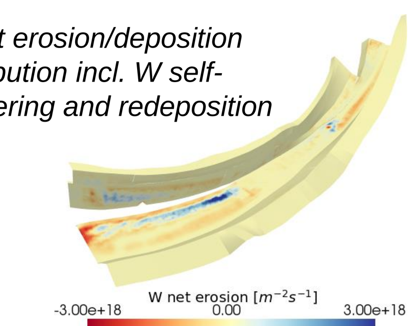
Example of EMC3-EIRENE input for ERO2.0

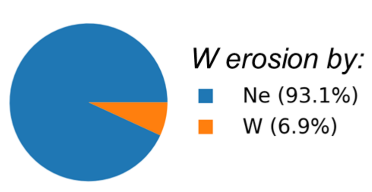


Example of ERO2.0 gross erosion flux calculation



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



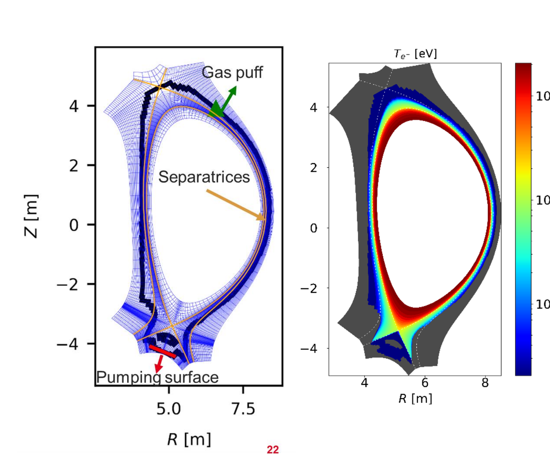


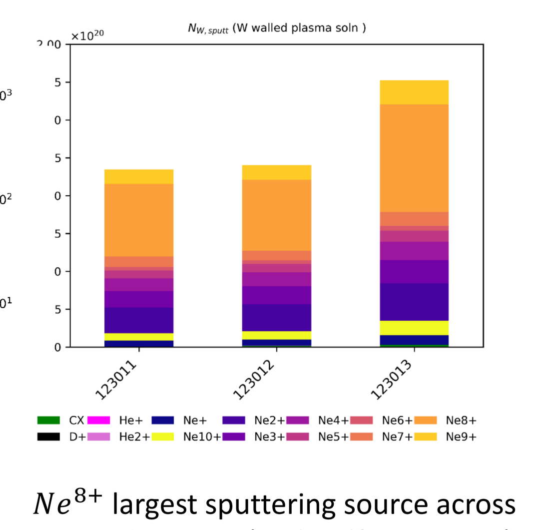
[1] J. Romazanov et al., EPS conference 2025

APPLICATION TO ITER SCENARIOS

- With the change to **W wall**, we started (in collaboration with IO) simulations for **new ITER full power scenarios with W wall and Ne seeding**

Input conditions:
- $P_{sol} = 100\ MW$
- Species: D, Ne – injected from upper gas puff; He fusion product as a flux from core
- H mode – transport barrier with $D_{\perp}^{Far\ SOL} = 0.3 m^2 s^{-1}$ (no balooning or enhanced far SOL transport)
- Scan performed over Ne seeding





- **MAJOR OBJECTIVE: Evaluate the effects of 3D perturbations and ELM suppression techniques on W impurity and seed impurity distributions in ITER reference scenarios**

Ne^{8+} largest sputtering source across Ne seeding scan (excl. self sputtering)

DEVELOPMENT OF REDUCED MODEL AND VALIDATION

- We consider four main reduced models based on existing tools (**SOLEDGE, JINTRAC, AURORA and CoreTeXY**), each of them being more or less advanced in the treatment of key aspects (from PWI interaction up to pedestal and core transport) for predicting W distribution and impact on plasma performances.
- The **TGLF** (gyro-Landau-fluid) model will be **integrated into the Aurora** 1.5D impurity transport forward model: improvements and validation on AUG and WEST experiments
- Workflow **JINTRAC + ERO2.0** (core-edge coupled code package, including JETTO, SANCO, NEO and EDGE2D-EIRENE) and SOLPS-ITER plasma backgrounds as inputs. The workflow will be extended to **JET-ILW limiter plasma configurations** addressing metal erosion and migration in non-diverted plasmas
- **SOLEDGE3X core-edge version**: validation on WEST experiments for W migration and self consistent evaluation ot its impact on plasma performances
- **CoreTeXY:** The code will be improved with core modules for estimation of cross field transport coefficients as well as with PWI models for estimation of W erosion and prompt redeposition. His application to the WEST and AUG experiment
- **The four tools will be improved during the first year of the project** while the second phase will focus on the benchmark and application to selected experiments, in order to **converge toward the most appropriate choices for the different physics aspects treated by them** and for improving their predictive capabilities**. Finally, the new features will be implemented in one (or two) reduced model able to threat all the aspects, from wall erosion up to the impact of migration on plasma performances**

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