



TSVV-D: Plasma-Wall Interactions with Metallic Plasma-Facing Components

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INTRODUCTION

Motivation and context

- In next-generation reactor-scale devices metallic PFCs will be exposed to regimes well beyond those accessible to date: steady-state operation, high neutron fluences and extreme transient loads
- PWI modelling emerges as an indispensable tool for extrapolation beyond present-day facilities
- The project aims to consolidate the PWI modelling and code development activities of TSVV-7 and to further advance the modelling tools to address frontier problems in the field of PWI for devices with metallic walls, focusing in parallel on code validation and development of reduced models, where appropriate, to make the description of complex PWI physics predictive and computationally efficient for integration into design and scenario optimization workflows
- While the focus is on W PFCs in AUG and ITER, the modelling tools and frameworks from this work will be available for application to existing and new devices, including non-D-T machines and future burning-plasma devices subject to significant neutron fluxes

Scientific objectives

- Provide consistent description of W wall impurity sources, transport to the core, re-deposition
- Address W dust inventory evolution and impurity sources from dust ablation in plasma
- Develop physics-informed model of retention driven by neutron-induced material damage
- Enable simulations of poloidally-resolved bulk retention and permeation for different scenarios
- Allow quick estimation of PFC thermal response to REs with different impact characteristics
- Extend the thermo-mechanical response framework to RE-driven PFC explosions of W
- Support validation activities for the entire framework in ASDEX-Upgrade as a relevant full-W machine
- Perform predictive simulations for ITER with improved models
- Comply with EUROfusion standard software requirements and IMAS interfaces

PROJECT IMPLEMENTATION

SP1. Wall lifetime, dust and impurity migration

TASK 1.1: Surrogate models of sputtering and reflection

- Effective erosion yields depend on atomistic material properties and surface morphology, with multi-dimensional PWI-relevant output – differential yields for (re-)emission energies and angles
- Current description is based on tabulated SDTrimSP (binary collision) data and limited set of high-fidelity MD (molecular dynamics) simulations with different data structure descriptions
- A hybrid approach based on active learning scheme is proposed to combine both databases, enabling quick estimates of quantities of interest with high accuracy and combining with the ray-tracing code SPRAY to account for static surface morphology effects via parameterized representation of surfaces

TASK 1.2: Core W density estimates in ERO2.0 and link to core impurity transport simulations

- Wall sources and their screening are essential for estimates of the core contamination
- ERO2.0 addresses primary wall sources and transport across separatrix; core region is grid boundary
- Extension of the ERO2.0 simulation domain to the magnetic axis is proposed, possible due to the new field-aligned grid approach compatible with native grids of edge plasma codes
- Impurity transport coefficients from core transport codes of different fidelity levels (JINTRAC, AURORA)

TASK 1.3: Modelling of electron collection and plasma-induced forces for dust particles

- Dust (re-)mobilization is controlled by competition of plasma-induced and adhesive forces
- Self-consistent PIC simulations are required for proper description of dust charging and screening
- Simulations with recently upgraded code CPIC are proposed to evaluate complex sheath effects under different electron magnetization conditions and for different dust distributions for improved UQ

TASK 1.4: Self-consistent modelling of transport of W impurities from wall and dust sources

- Ablation of dust particles in plasma provides an additional source of impurity atoms with complex distribution within the plasma volume, contributing both to core contamination and PWI
- A static interface between MIGRAIne (dust) and ERO2.0 (impurity) transport was tested under TSVV-7
- Advanced time-dependent framework is proposed to address dust evaporation on proper time scales

SP2. Fuel retention in neutron-damaged wall materials

TASK 2.1: Damage-induced physics-informed trap model based on cluster dynamics

- Earlier developed trap model uses a semi-empirical annealing factor fitted to laboratory experiments
- A physics-informed description of involved defect structures and their dynamics is proposed to be based on a cluster dynamics model and cover broader range of temperature and other conditions
- The new model will be implemented in the reaction-diffusion code FESTIM, focusing on optimization of numerical performance with increased numbers of unknowns and reactions

TASK 2.2: Global-scale modelling of fuel retention, permeation and outgassing

- The hydrogen inventory simulation for PFCs (HISP) framework (now PFC-T-T under ITER development) uses FESTIM as the underlying reaction-diffusion model for global fuel inventory evolution studies
- IMAS-integrated version of PFC-T-T will use data from plasma edge codes for wall-resolved input data
- Simulations of post-discharge outgassing in AUG and predictive simulations for ITER are foreseen

SP3. Consequences of transient events

TASK 3.1: Surrogate models of RE energy deposition & escaping secondary products

- The workflow "RE impact – energy deposition – PFC response" is computationally expensive
- MC simulations provide volumetric energy deposition maps and distribution of secondary products for given RE impact characteristics – basis for reconstruction of arbitrary distributions by superposition
- Surrogate models are proposed for the 4D parameter space using Bayesian or ANN approaches that will feed a 1D heat diffusion solver for quick estimates of melting and identification of cases of interest

TASK 3.2: Modelling W PFC damage for RE impact parameters of relevance to future machines

- The Geant4-MEMENTO workflow (thermal → vaporization and melt losses) is being validated against controlled experiments, the Geant4-LSDYNA workflow (thermo-mechanical → explosive damage and release of debris) is under development for predictions of W damage under RE impacts
- Predictive simulations for selected ITER scenarios will provide information on damage in terms of deformation profiles, lost volume, impact on the cooling system and bond interface temperature, release of debris and their characteristics as well as secondary (non-localized) damage

Steady-state PWI
• Surrogate models for PWI
• W to core, field-aligned grid
• Time-dependent dust evaporation sources
• Validation in AUG
• Predictive modelling and comparison (link TSVV-E)

Dust transport
• Improved electron collection model
• Remobilization by plasma-induced forces
• Time-dependent dust evaporation sources
• Validation in AUG
• Predictive modelling

Fuel retention
• Physics-informed defect annealing model
• Optimization of numerical convergence
• Global framework for reactor scale simulations
• Validation in AUG
• Predictive modelling

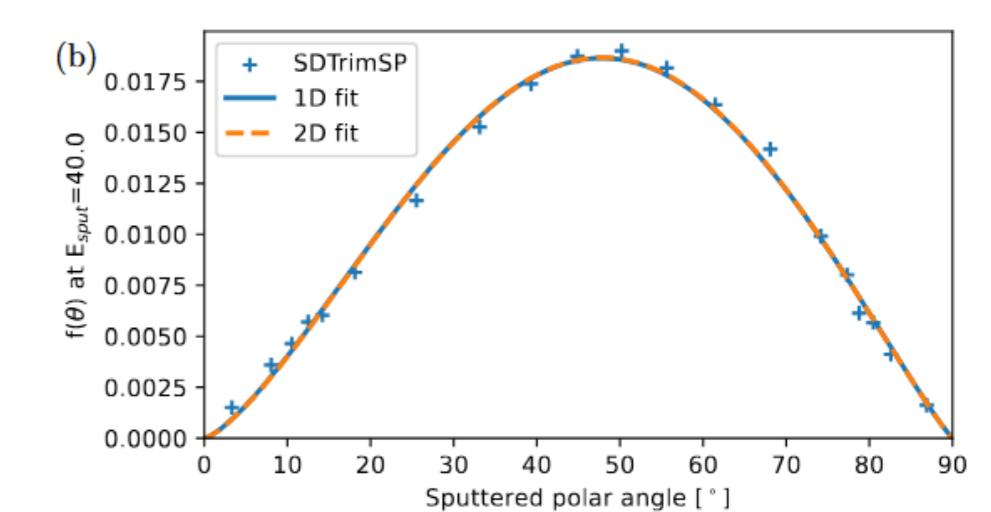
Transient events → RE
• Surrogate models for RE energy deposition and secondary products
• Full thermo-mechanical response model with explosive fragmentation
• Validation in AUG
• Predictive modelling

Analytic fitted descriptions of the SDTrimSP sputtered distributions

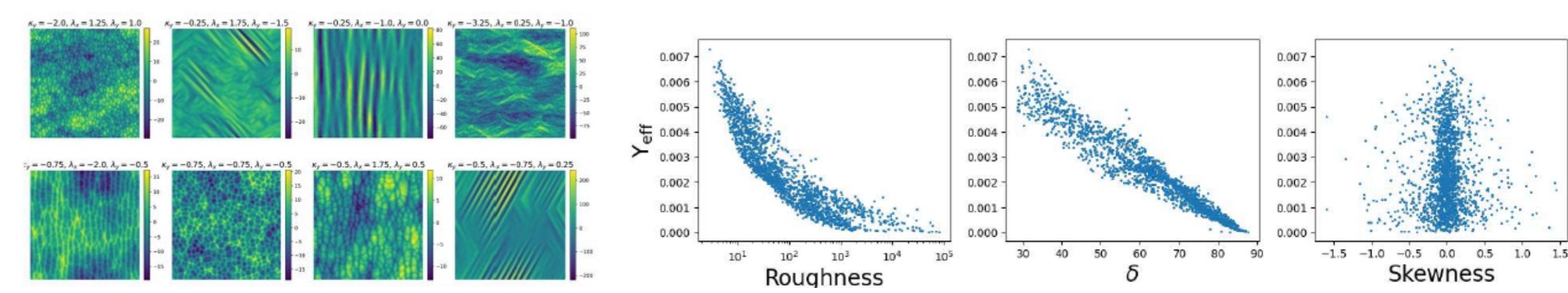
$$f(E) = A_{\text{norm}} E^{C_1} \frac{1 - \sqrt{E/C_2}}{(E + C_3)^{C_1+2}} \quad (1)$$

$$f(E, \theta) = A_{\text{norm}} f(E) \sin^2 \theta \cos^{C_4} \theta \quad (2)$$

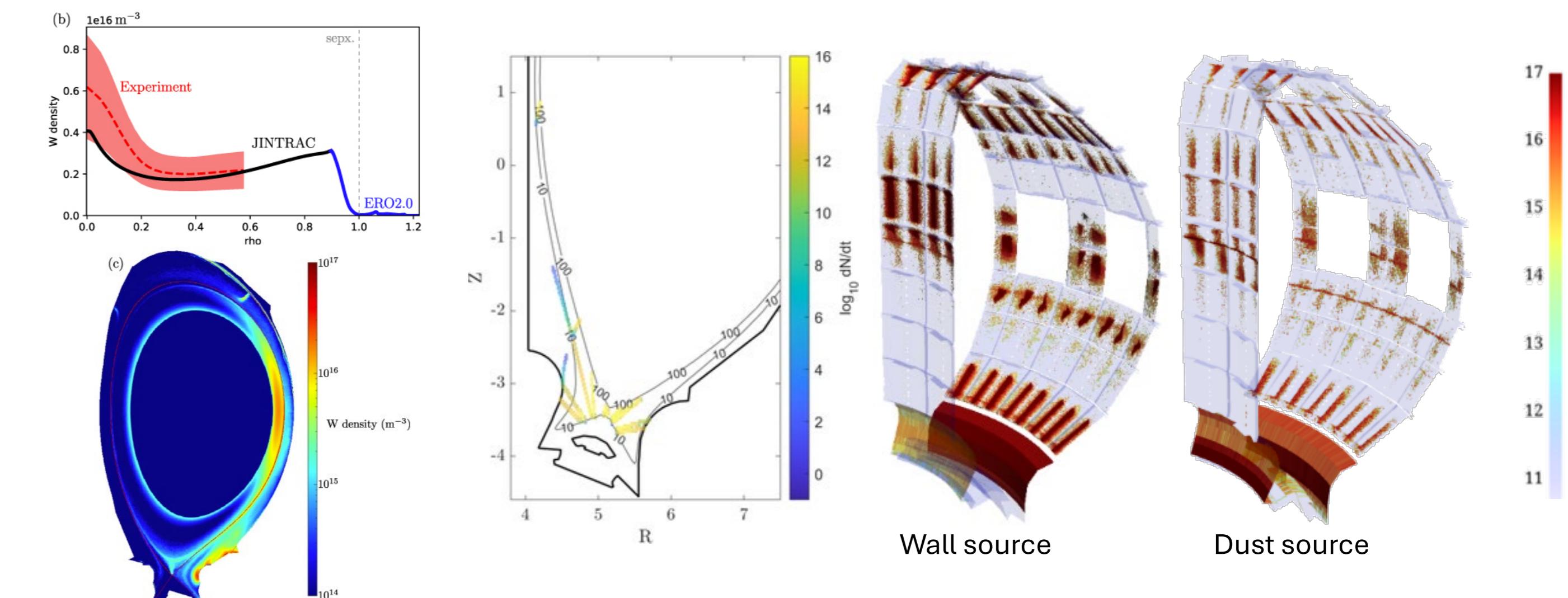
$$f(E, \theta, \phi) = A_{\text{norm}} f(E, \theta) \left(1 + C_6 \cos \phi + C_7 \exp \left(- \left(\frac{\phi - C_8}{C_9} \right)^2 \right) \right) \quad (3)$$



Classification of surface morphology structures and relation of surface properties and effective sputtering yields



W density by ERO2.0 and JINTRAC for JET ELMy H-mode / Gross W deposition in ITER from wall and dust sources



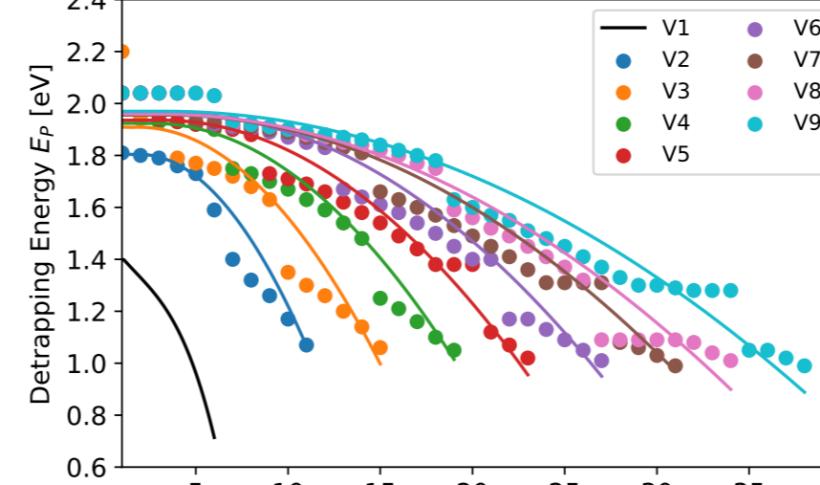
Phenomenological vs cluster dynamics defect model

$$\frac{\partial n_i}{\partial t} = \Phi \cdot K \left[1 - \frac{n_i}{n_{\text{max},\Phi}} \right] - A \cdot n_i \quad A = A_0 \cdot \exp(-E_i/(k_B \cdot T))$$

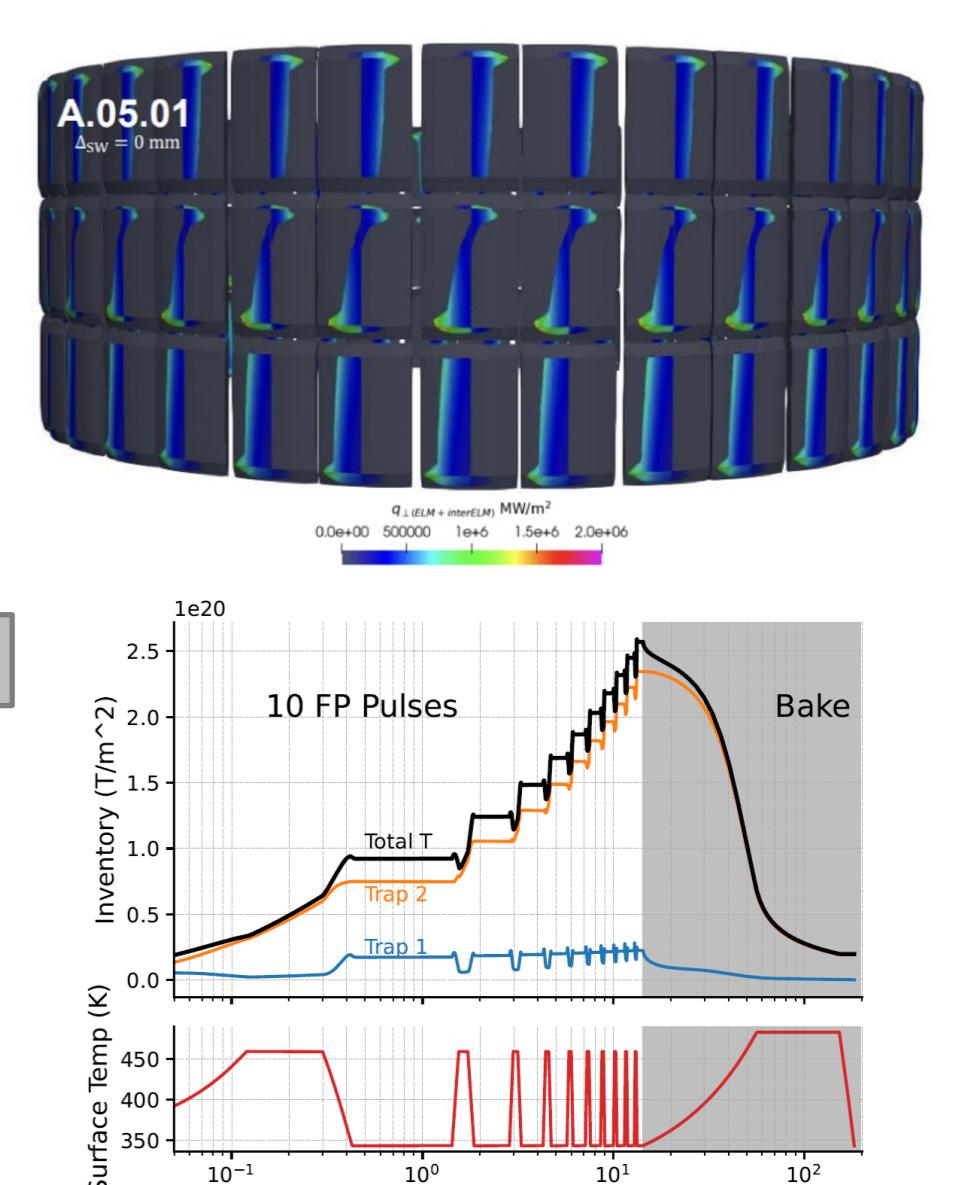
$$\frac{\partial C_{Vi}}{\partial t} = \nabla \cdot (\bar{D}_{Vi} \nabla C_{Vi}) - S_{Vi} D_{Vi} C_{Vi}$$

$$+ b_{Vi+1}^+ C_{Vi+1} C_{Vi-1} - b_{Vi+1}^- C_{Vi+1} C_{Vi} + G_{Vi},$$

$$+ b_{Vi+1}^- C_{Vi+1} C_{Vi} + G_{Vi},$$



Wall-resolved global simulations of fuel retention (ITER)



Loading of ITER first wall due to RE impacts

Surrogate models of RE energy deposition by superposition of profiles for fixed RE (energy; impact angle)

