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Multidimensional, multi-material and multiphysics modelling of Hydrogen transport in ITER

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► **To cite this version:**

Rémi Delaporte-Mathurin, Jonathan Mougenot, Etienne A Hodille, Y. Charles, Christian Grisolia. Multidimensional, multi-material and multiphysics modelling of Hydrogen transport in ITER. 24th International Conference on Plasma Surface Interactions in Controlled Fusion Devices, Jan 2021, Jeju Island, South Korea. hal-03120261

HAL Id: hal-03120261

<https://hal.science/hal-03120261v1>

Submitted on 25 Jan 2021

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INTRODUCTION

- Reproducing experimental results can be **long** and **tedious**
- Is it possible to **automatically fit** a thermal desorption spectrum and **identify materials properties**?
- Can these properties be used to **perform complex multidimensional simulations**?
- Is there a **discrepancy** between 2D and 1D simulations?

METHODOLOGY

Hydrogen transport

$$\frac{dc_m}{dt} = \nabla(D\nabla c_m) + S - \sum_i \frac{dc_{t,i}}{dt}$$

$$\frac{dc_{t,i}}{dt} = k c_m (n_i - c_{t,i}) - p c_{t,i}$$

- Finite Element Methods
- FEniCS backend
- FESTIM code [1]



Heat transfer

$$\rho C_p \frac{dT}{dt} = \nabla(\lambda \nabla T) + Q$$

PROPERTIES IDENTIFICATION

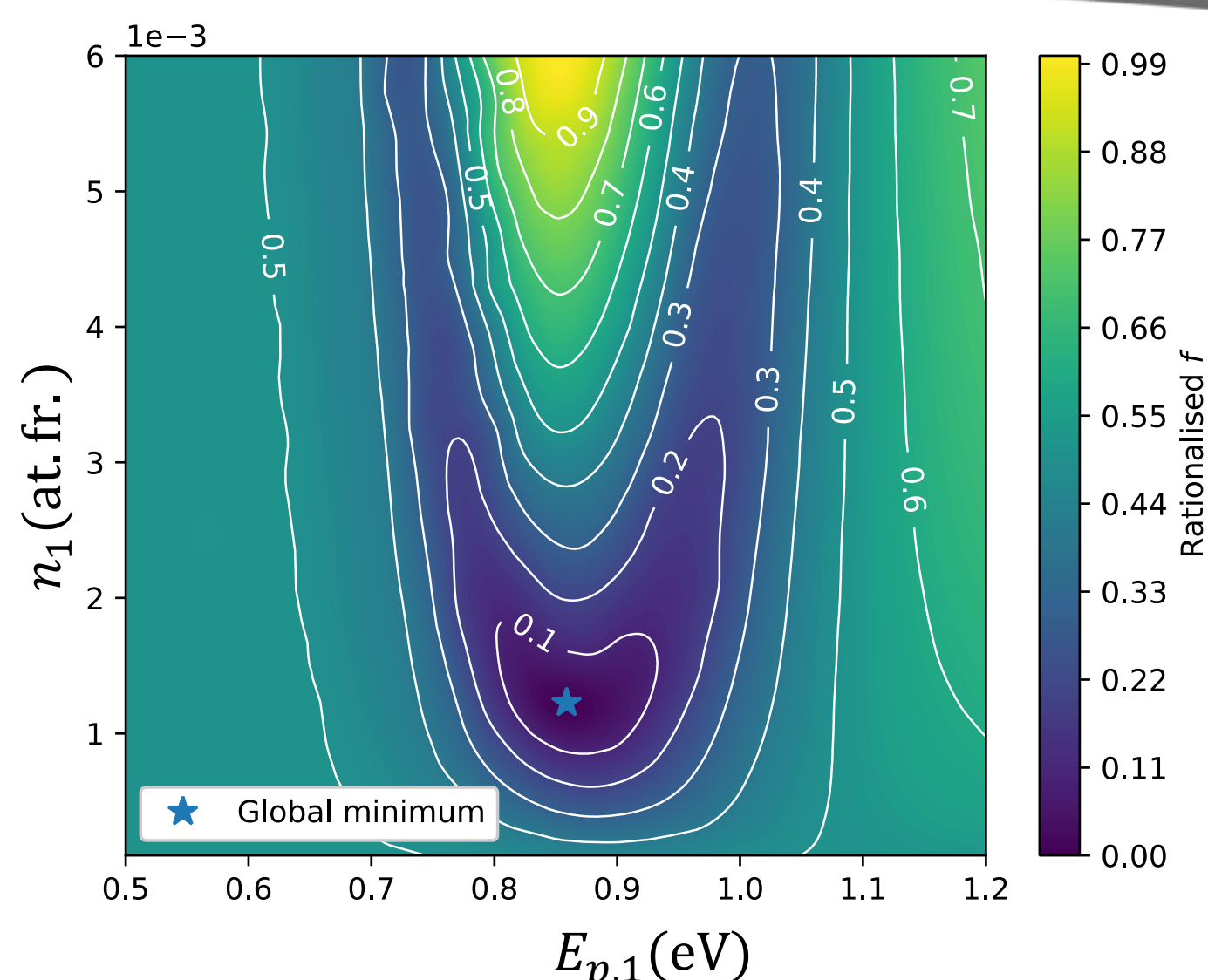
Example cost function

- Error function based on W TDS spectrum

$$f(\mathbf{x}) = \frac{\sum_i \alpha_i |d_i - d_{sim}|}{\sum_i \alpha_i}$$

- α_i : weights
- d_i : experimental data
- d_{sim} : simulated data

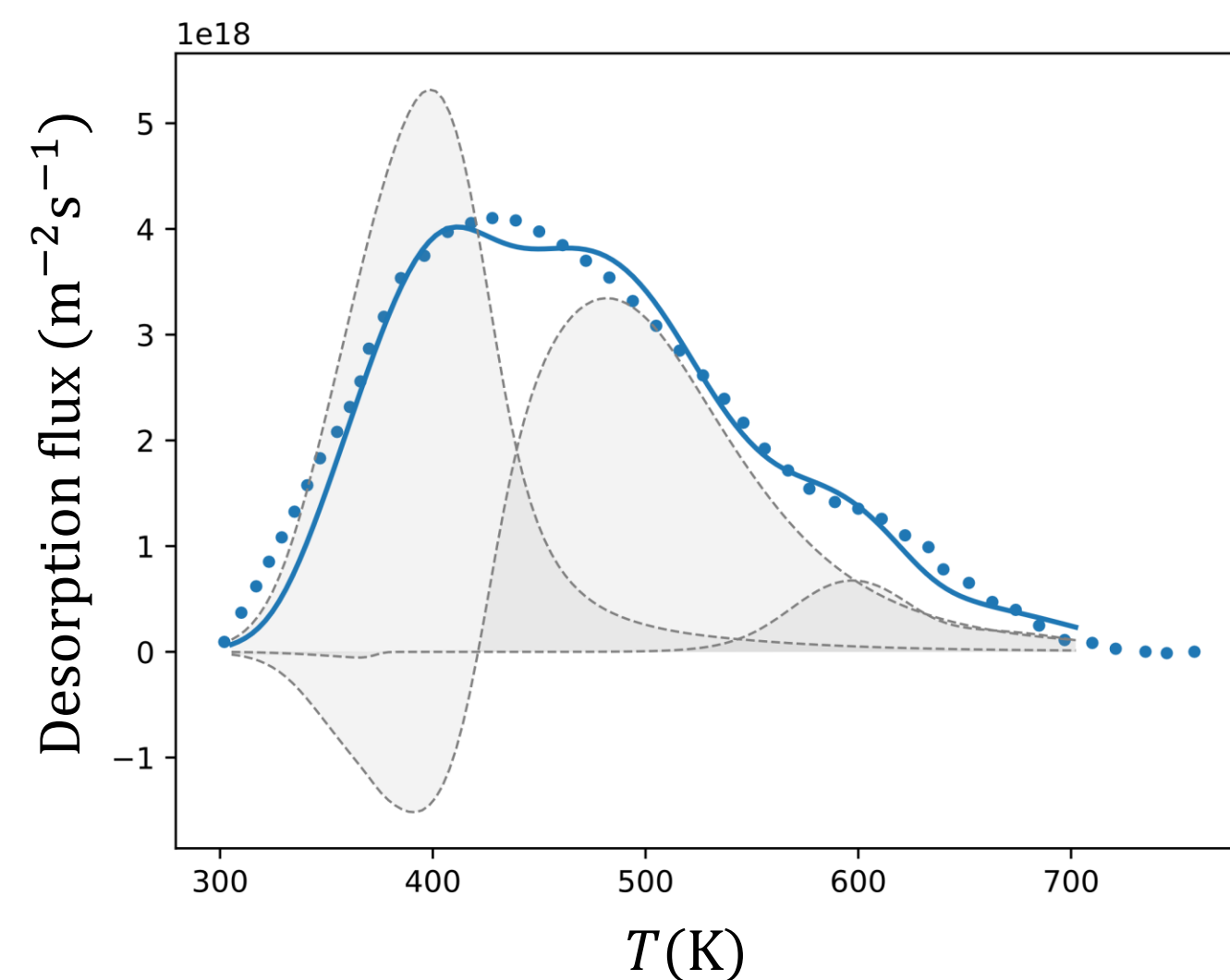
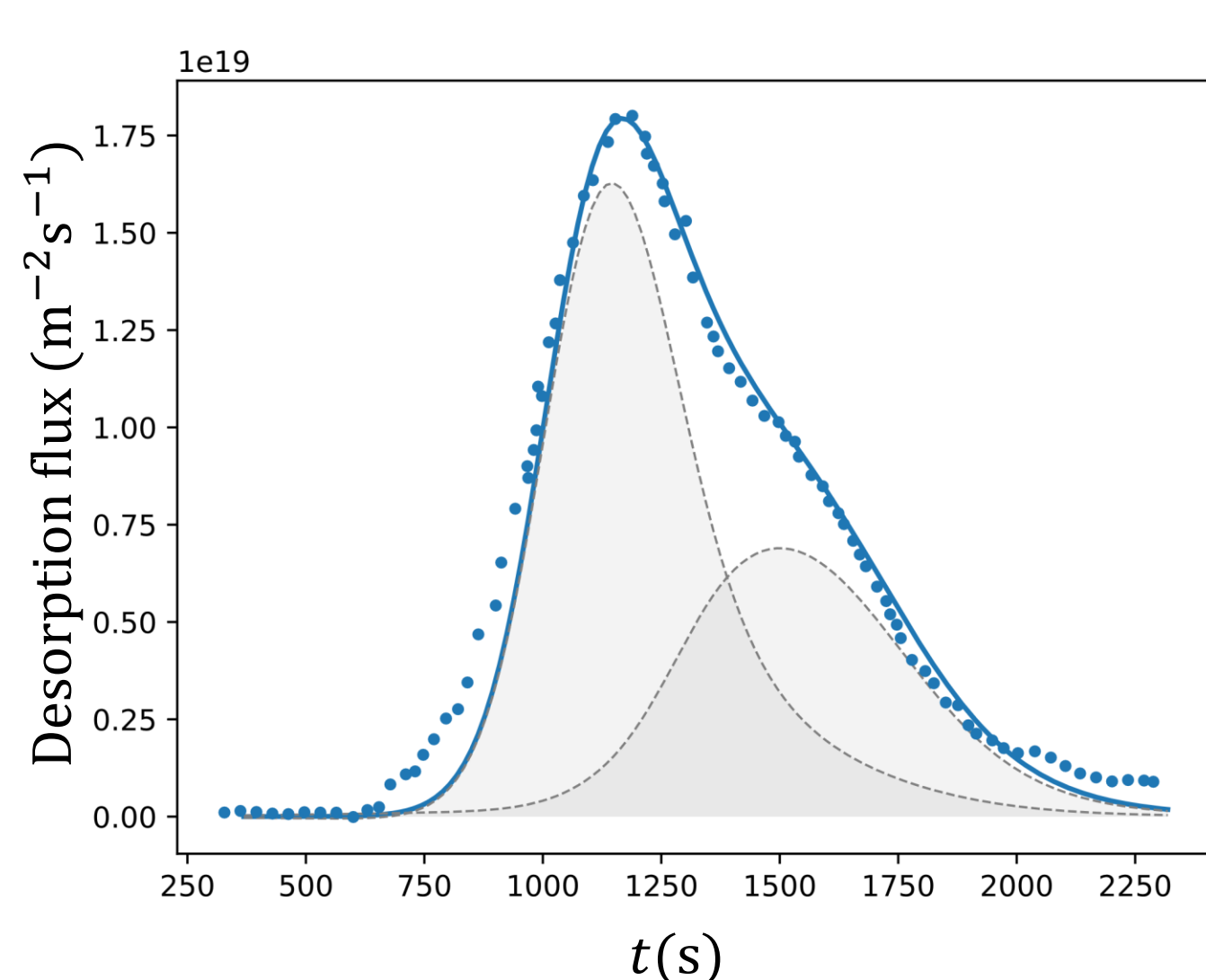
- Objective: find the minimum



Tungsten

- W under 200 eV D⁺ at 300K [2]
- 5D optimisation (3 energies, 4 densities)
 - $E_{p,1} = 0.83$ eV ; $E_{p,2} = 0.97$ eV
 - $E_{p,3} = 1.51$ eV
 - $n_1 = 10^{-3}$ at.fr. ;
 - $n_2 = 7 \times 10^{-4}$ at.fr.

→ Convergence reached in a few hours



Co-deposited Be-D

- Co-deposited 1μm-thick Be-D under at 330K [3]
- 6D optimisation (2 energies, 2 densities, 2 initial occupancies)
 - $E_{p,1} = 0.75$ eV ; $E_{p,2} = 0.93$ eV
 - $n_1 = 10^{-1}$ at.fr. ;
 - $n_2 = 4 \times 10^{-2}$ at.fr.
 - $f_1 = 0.73$; $f_2 = 0.28$

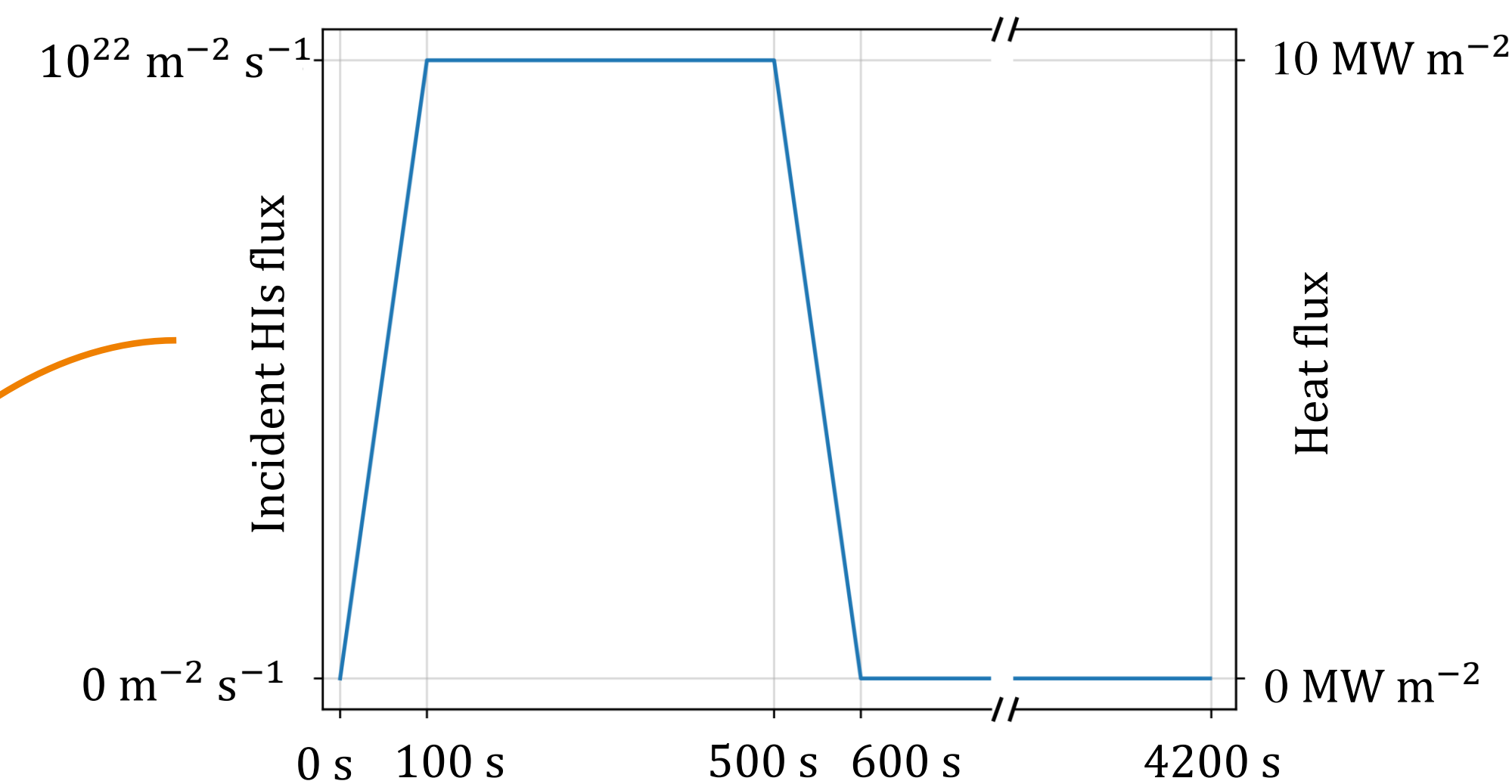
→ Convergence reached in a few minutes

APPLICATION: ITER MONOBLOCKS

Simulation parameters

- 2 traps in W
- 1 trap in CuCrZr

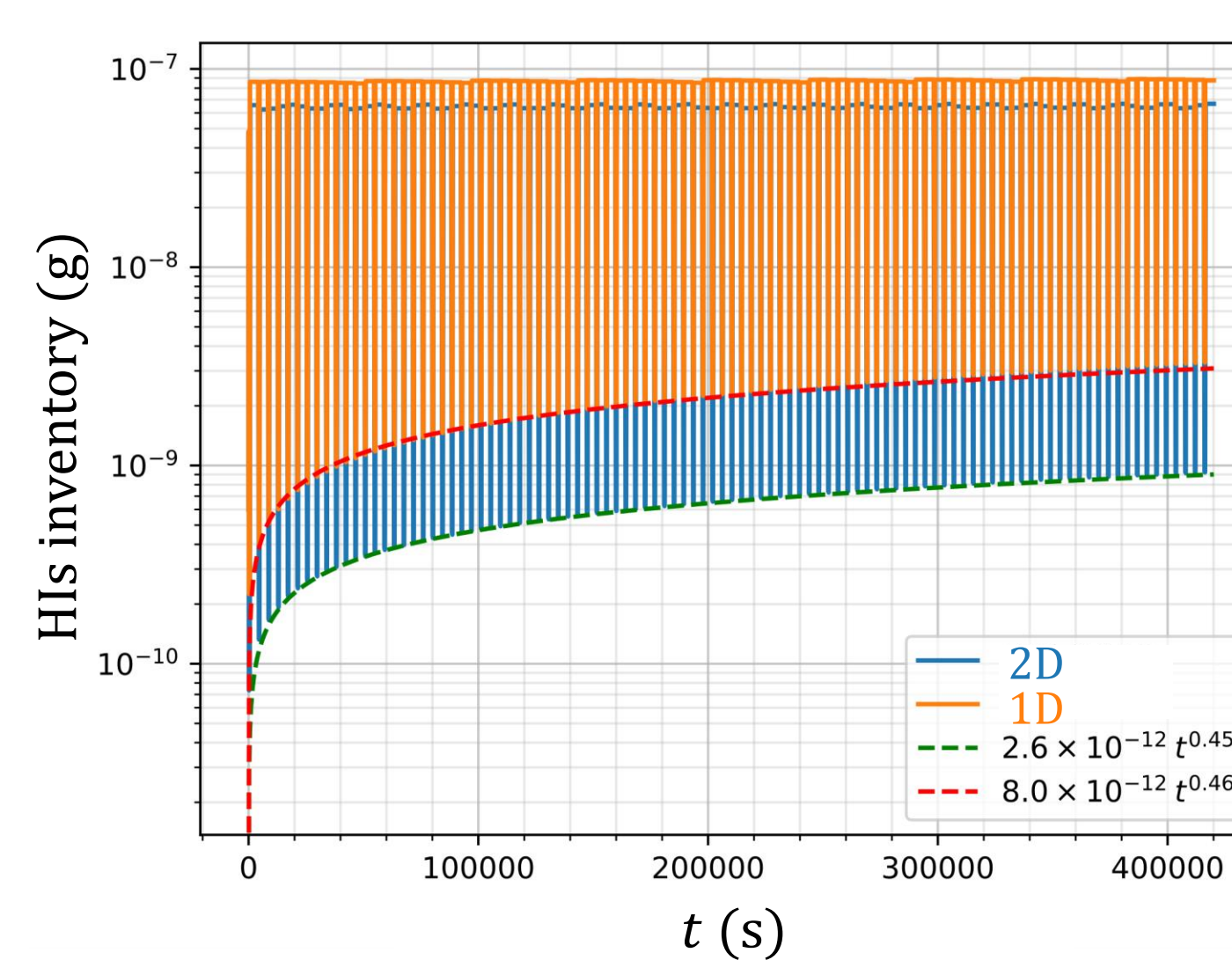
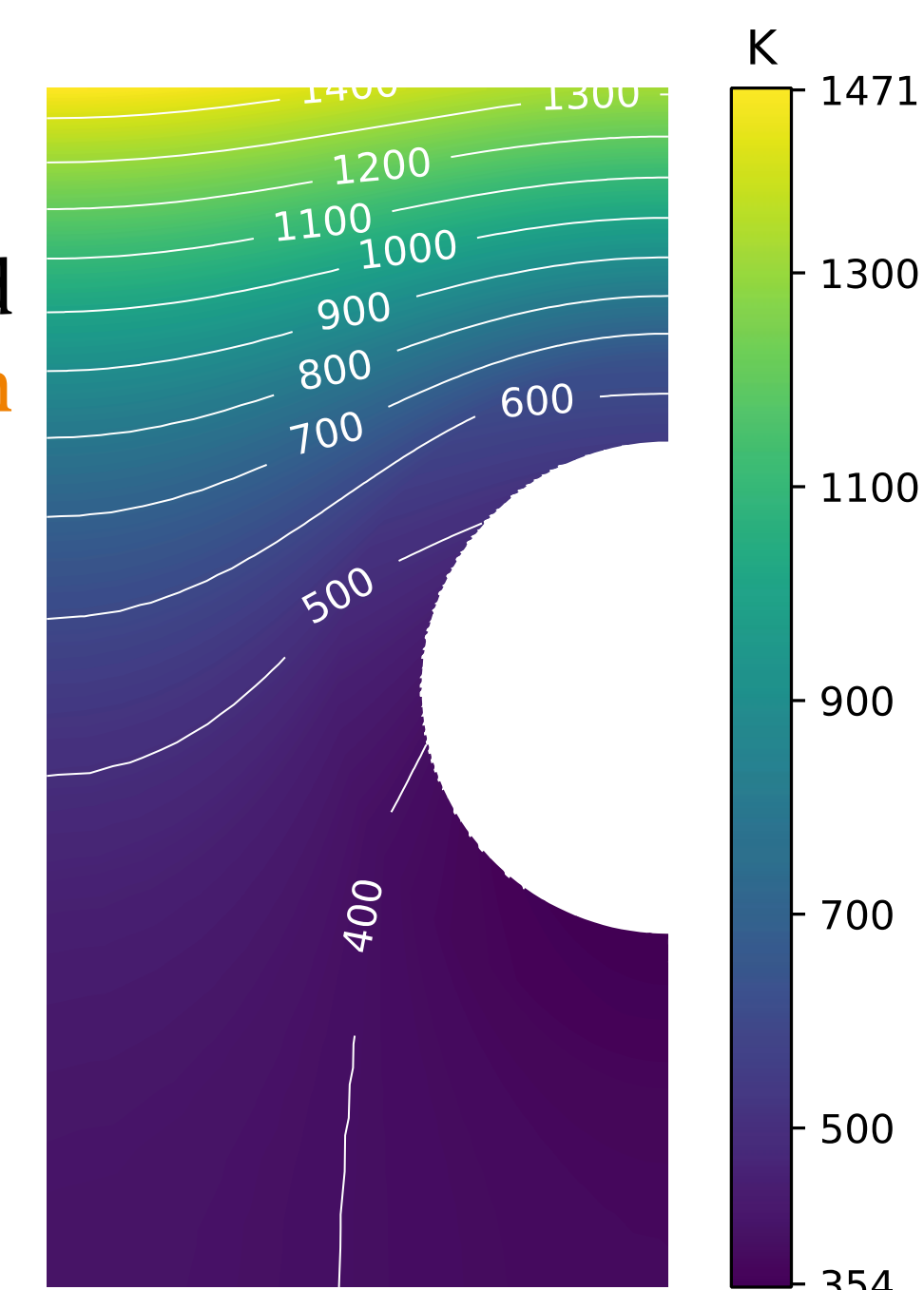
W
Cu
CuCrZr



- Convective exchange
- Recombination

Temperature field during implantation

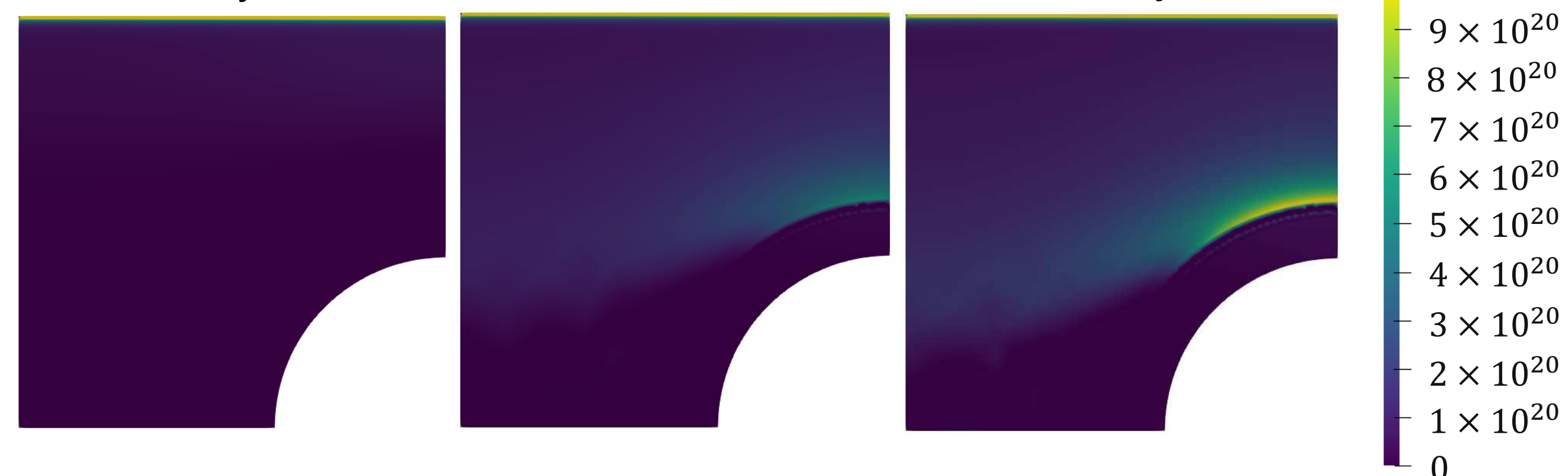
- Maximum surface temperature 1471 K
- Homogeneous temperature during rests



HIs Inventory over time

- Inventory limited by near surface retention zone
- Inventory during implantations **keeps increasing**
- Up to **95% error** between 1D and 2D

1st cycle 50th cycle 100th cycle



HIs retention field during resting phases

CONCLUSIONS

- FESTIM**: a modelling tool for hydrogen transport modelling
- Well suited for **high-dimensional optimisation**
- High inventory in ITER PFCs during resting phases
- 1D** modelling is **not sufficient** for **quantitative estimation** of PFC inventory

References:

- Delaporte-Mathurin et al. (NME, 2019)
- Ogorodnikova et al. (JNM, 2003)
- Baldwin, Schwarz-Selinger, and Doerner (Nucl. Fusion, 2014)
- Hollingsworth et al. (Nucl. Fusion, 2019)