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





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CuCrZr

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

$$\frac{dc_{\rm m}}{dt} = \nabla(D\nabla c_{\rm m}) + S - \sum_{i} \frac{dc_{\rm t,i}}{dt}$$

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

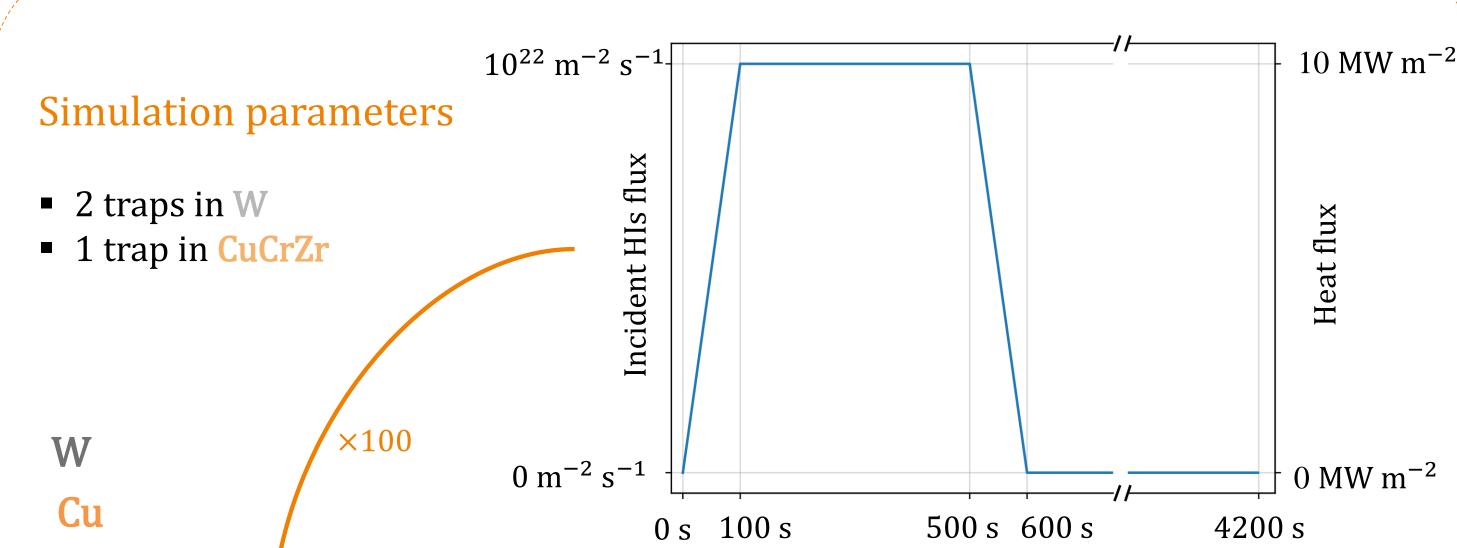
$$\frac{dc_{\rm t,i}}{dt} = k c_{\rm m} (n_{i} - c_{\rm t,i}) - p c_{\rm t,i}$$

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

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

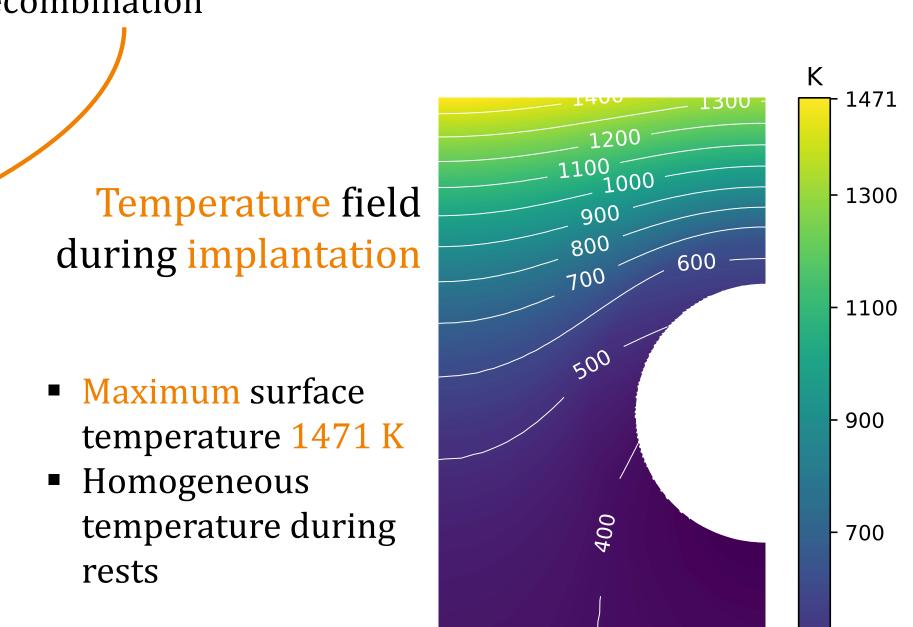


Heat transfer



ITER MONOBLOCKS

- Convective exchange
- Recombination



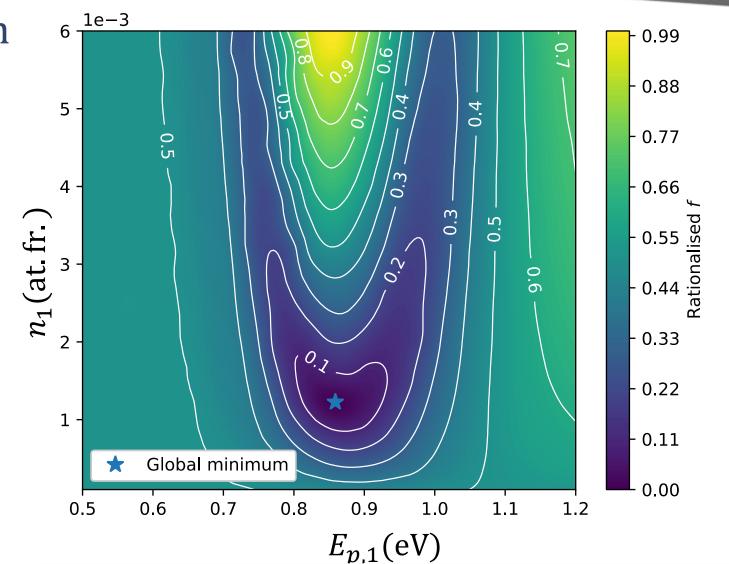
PROPERTIES IDENTIFICATION

Example cost function

Error function based on W TDS spectrum

$$f(x) = \frac{\sum_{i} \alpha_{i} |d_{i} - d_{\text{sim}}|}{\sum_{i} \alpha_{i}}$$

- α_i : weights
- d_i : experimental data
- d_{sim} : simulated data
- Objective: find the minimum







 W under 200 eV D⁺ at 300K [2] ■ 5D optimisation (3 energies, 4 densities)

•
$$E_{p,1} = 0.83 \text{ eV}$$
; $E_{p,2} = 0.97 \text{ eV}$
• $E_{p,3} = 1.51 \text{ eV}$

1000 1250 1500 1750 2000 2250

t(s)

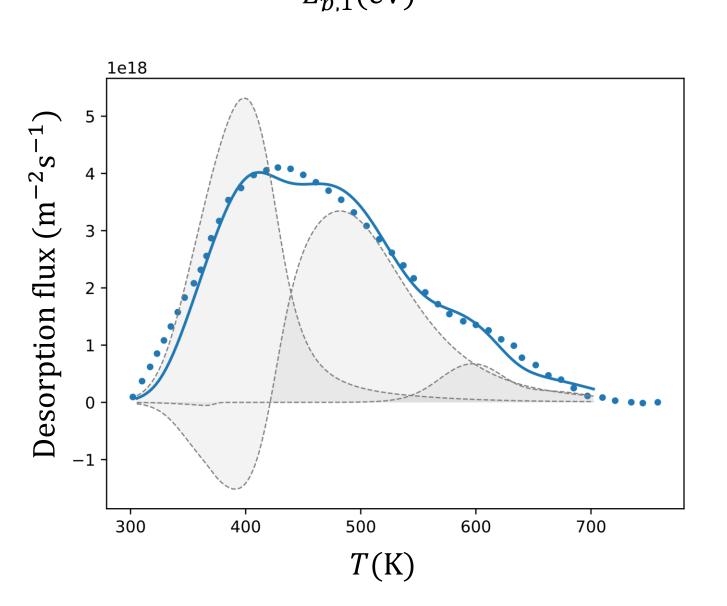
- $n_1 = 10^{-3}$ at. fr.;
- $n_2 = 7 \times 10^{-4}$ at. fr.

1e19

1.25

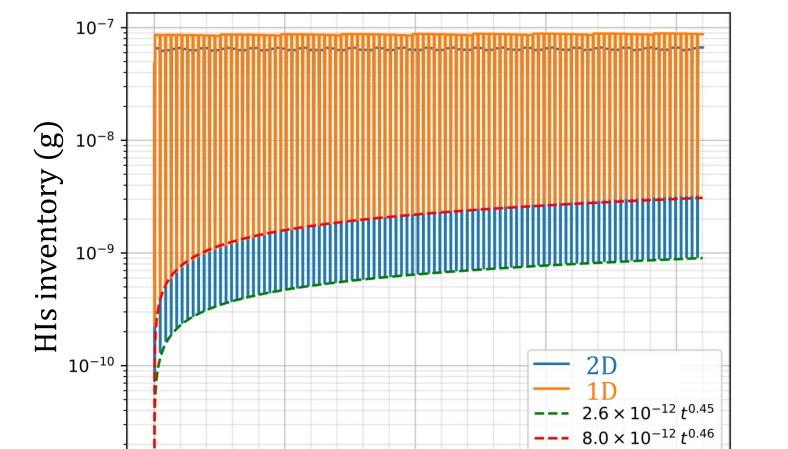
Desorption flux (

→ 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)
 - $E_{p,1} = 0.75 \text{ eV}$; $E_{p,2} = 0.93 \text{ eV}$
 - $n_1 = 10^{-1}$ at. fr. ;
 - $n_2 = 4 \times 10^{-2}$ at. fr.
 - $f_1 = 0.73$; $f_2 = 0.28$
- → Convergence reached in a few minutes



200000

t (s)

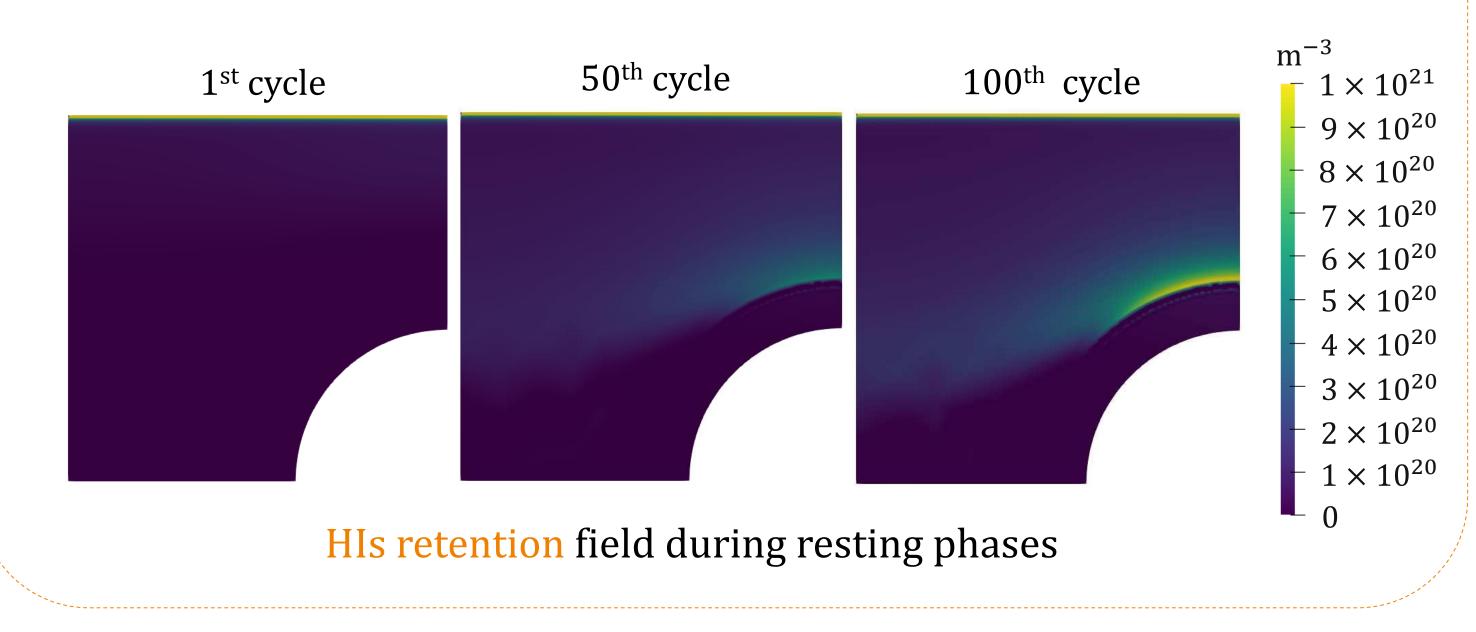
100000

1 cm

HIs Inventory over time

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

500



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:

- [1] Delaporte-Mathurin et al. (NME, 2019)
- [2] Ogorodnikova et al. (JNM, 2003)
- [3] Baldwin, Schwarz-Selinger, and Doerner (Nucl. Fusion, 2014)
- [4] Hollingsworth et al. (Nucl. Fusion, 2019)