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

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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

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

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

Heat transfer

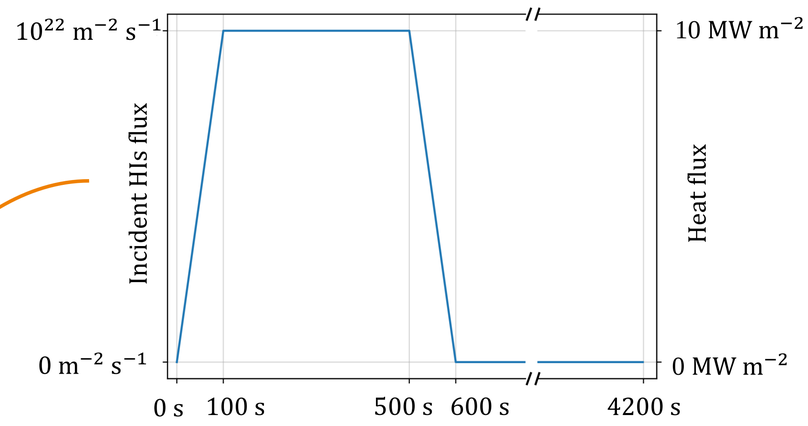
$$\rho C_p \frac{dT}{dt} = \nabla(\lambda \nabla T) + Q$$

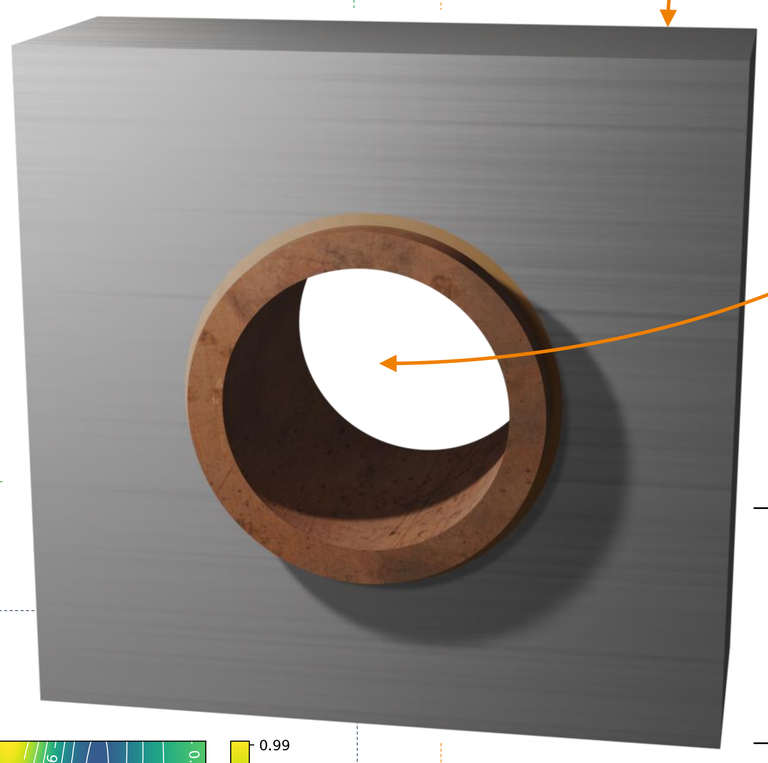
- Finite Element Methods
- FEniCS backend
- FESTIM code [1]

APPLICATION: ITER MONOBLOCKS

Simulation parameters

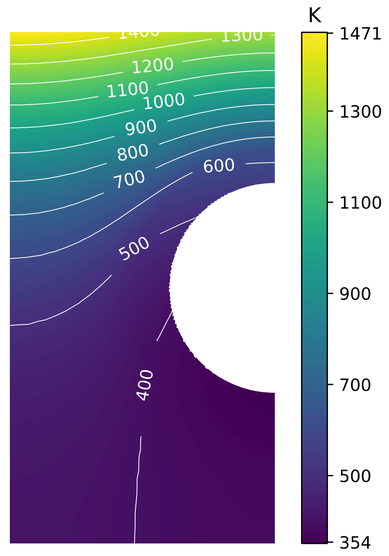
- 2 traps in W
- 1 trap in CuCrZr





- Convective exchange
- Recombination

Temperature field during implantation

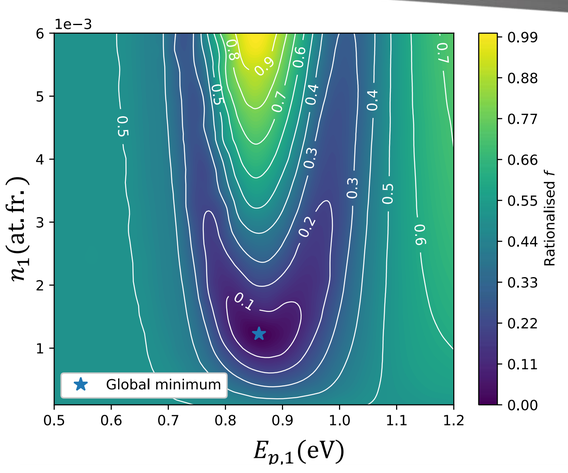


- Maximum surface temperature 1471 K
- Homogeneous temperature during rests

PROPERTIES IDENTIFICATION

Example cost function

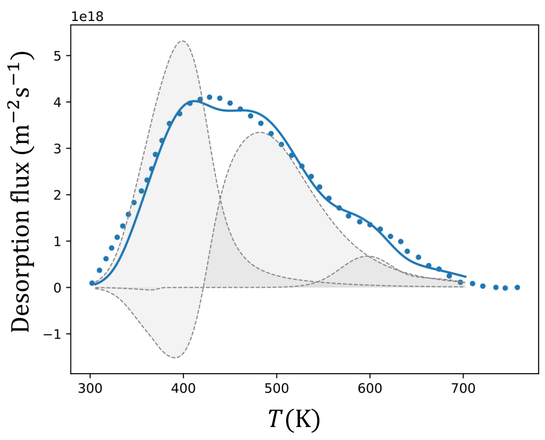
- Error function based on W TDS spectrum
- $f(\boldsymbol{x}) = \frac{\sum_i \alpha_i \, |d_i - d_{\text{sim}}|}{\sum_i \alpha_i}$
  - α_i: weights
  - d_i: experimental data
  - d_{sim}: simulated data
- Objective: find the minimum

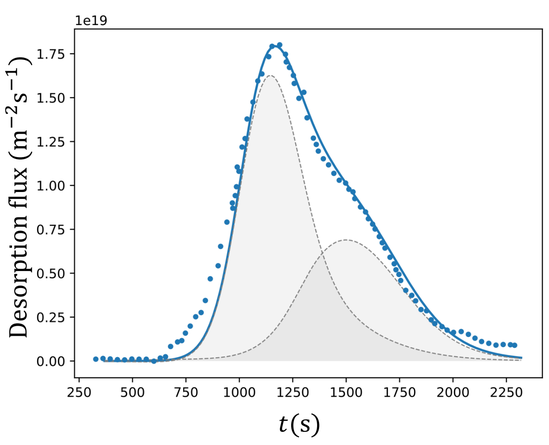


Tungsten

- 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

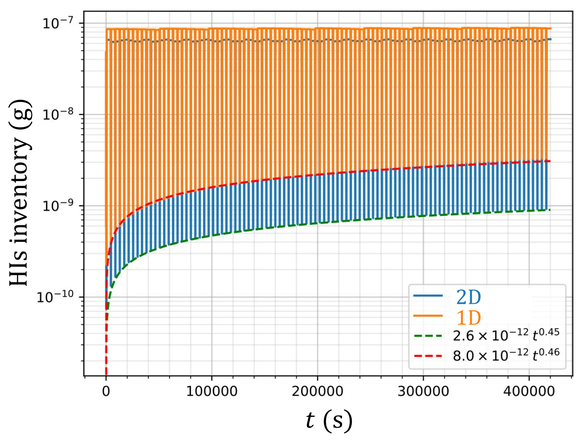




Co-deposited Be-D

- 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.
  - $f_1 = 0.73$; $f_2 = 0.28$

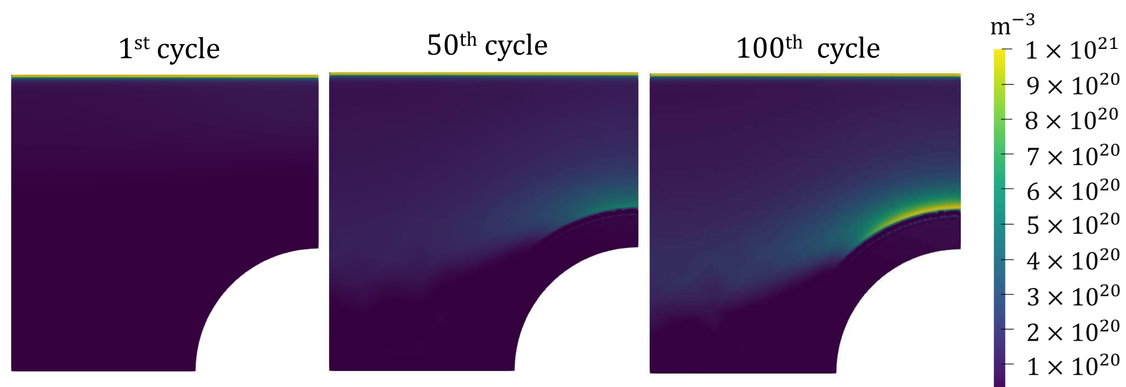
→ Convergence reached in a few minutes



HIs Inventory over time

- Inventory limited by near surface retention zone
- Inventory during implantations keeps increasing

→ Up to 95% error between 1D and 2D



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:
[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)

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