Introduction

How does PWI influence the fusion plasma

- Principle picture

- H (D, T) recycling (implantation & (out-diffusion)) determines the neutral particle dynamics in the SOL.
- Erosion produces plasma impurities that migrate and re-deposit
- Deposition and re-erosion changes impurity source distribution
- Need to include plasma to predict surface evolution

- Subdivide the first wall into N-tiles

- Plasma model [1]:
  - Plasma transport can be characterized by a re-deposition matrix:
    \[
    \frac{\partial n_{\text{ei}}}{\partial t} = \text{Fraction of eroded flux of element ei at charge state qi from wall tile wj that ends up on tile wk}
    \]
- Surface model [1,2]:
  - All erosion & deposition is assumed to occur homogeneously in the reaction zone:
    \[
    \frac{dN}{dt} = \text{Incident flux} \cdot \text{Reflection} \cdot \text{Eroded Flux} \cdot \text{Bulk exchange}
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The WallDYN concept

Linking impurity migration and surface evolution

How does PWI influence the fusion plasma

- Partial erosion yield \( Y_{\text{er}} \)
- Incident particle spectrum \( \Gamma_{\text{in}}(E) \)
- Reflection yield \( R_{\text{refl}} \)
- Incident flux of \( \Gamma_{\text{in}}(E) \)

Surface composition \( \delta_i \) changes due to ero/dep by incident particle spectrum

Changes source distribution

Changes incident spectrum

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- How does PWI influence the fusion plasma

Linking impurity migration and surface evolution

- The WallDYN concept
  - Example: Be migration in JET-ILW

A different view on hydrogen diffusion / trapping in metals

- Fill level dependent trapping: From DFT to lab experiments
- Example: Isotope exchange at ambient temperatures

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Linking impurity migration and surface evolution
The WallDYN concept

- Main features
  - Non iterative merge of global impurity transport (DIVIMP) with surface models (Sputtering, Chemical erosion, Sublimation, Seeding...)
  - Includes re-erosion of deposited material
  - Maintains a strict global material balance

- Implementation
  - Use continuous description of surface and plasma flux evolution using ODE's and AE's
  - Yields a DAE system that allows to truly couple different physical processes
  - Solved using an implicit BDF solver

- Advantage over iteratively coupling MC, MD or DFT codes
  - Iterative coupling occurs on different time scales
  - Error propagation during iterative coupling
  - Sampling artefacts in MC-based codes
  - Last but not least: Computation time

Linking impurity migration and surface evolution
Example: Be migration in JET-ILW [2]

- Be influx and deposition during L-Mode divertor phase JET-ILW 80295
  - WallDYN calculates evolution of Be influx and Be deposition
  - Be deposition pattern in excellent agreement with literature [1]
  - Be influx does not mean deposition
    - Erosion source strength + plasma transport are not enough to predict deposition
    - Need to include the entire transport chain

Linking impurity migration and surface evolution
Example: Be migration in JET-ILW

- H-Mode JET-C
    - O/X ratios based on post mortem analysis
      - Must include long term outgassing
        - JET-ILW:
          - Outgassing was measured
          - C-JET:
            - Gas balance/post mortem = 1/5
          - JET-ILW:
            - O/Be at tile 1, Apron 3 to 4%
            - O/Be in remote areas 40%
            - C-JET:
              - O/C = 40% at base temp.
              - O/C = 5% at high temp.

- WallDYN matches experiment if long term outgassing is taken into account

Linking impurity migration and surface evolution
The WallDYN concept

- Input into the WallDYN surface model:
  - Mixed material sputter yields \( Y_{i,j,k} = \left\{ \frac{d}{dt} N_{i,k} \right\} \)
    - Depends on all elements in the mixture, Energy, angle and temperature
    - Taken from SDTRIM.SP parameter scan, Experiment, MD...
  - Reflection yield of projectiles from mixed materials \( R_{i,j,k} \)
    - Depends on all elements in the mixture, Energy, angle
    - Taken from dynamic TRIM, Experiment, MD...

- WallDYN is a non iterative continuous code
  - Analytic expression required
  - Fit scaling laws to reflection and sputter yield data

- Example Be data for a Be, C, W mixture
  - Reasonable fit to database

Linking impurity migration and surface evolution
The WallDYN concept

- Input into the WallDYN plasma migration model:
  - Redistribution matrix
    \( \phi_{ijk} = \text{Fraction of eroded flux of element } i \text{ at charge state } j \text{ from wall tile } vj \text{ that ends up on tile } wk \)
    - Calculated by trace impurity code DIVIMP
  - Example: charge state integrated Be redistribution matrix
    - Diagonal points towards strong local re-dep
    - Plasma flows point towards inner divertor
    - Strong deposition on baffles
A different view on hydrogen diffusion / trapping in metals

Fill level dependent trapping: From DFT to lab experiments

- Classic diffusion/trapping picture of H in metals
- Two populations:
  - Solute
  - Trapped at trap type 1
- H is transported via solute diffusion
- Traps have single occupancy & fixed de-trapping energy
- At low temperature the traps are frozen
- Once all traps are filled they no longer interact with the solute at low T

![Diagram showing energy levels and trapping](image)

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A different view on hydrogen diffusion / trapping in metals

Fill level dependent trapping: From DFT to lab experiments

- The classic diffusion trapping picture fails to explain low temperature isotope exchange experiments
  - The initial D implantation is well reproduced by the classic model
  - BUT since all traps are frozen there is no isotope exchange in the classic model
- Apparently the classic model does not correctly describe the trapping/detrapping dynamics

![Diagram showing experimental data](image)

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A different view on hydrogen diffusion / trapping in metals

Fill level dependent trapping: From DFT to lab experiments

- DFT (e.g. 1) predicts that defects can store multiple H atoms (e.g. 6 in one mono-vacancy)
  - The de-trapping energy depends on the fill level of the trap
  - (De-) trapping changes the trap energy for all H in a trap
  - (De-) trapping of one H can modify the binding energy of many other H

![Diagram showing trapping energy changes](image)

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A different view on hydrogen diffusion / trapping in metals

Fill level dependent trapping: From DFT to lab experiments

- Isotope exchange with fill level dependent trapping: Experiment vs. New Model
  - With DFT data for mono vacancies isotope exchange "too efficient"
  - BUT model can in principle match data
  - Ad-Hoc fit with two, two level trap types
    - Trap type 1: D flux (m-2s-1)
    - Trap type 2: D flux (m-2s-1)
    - Trap type 1: D flux (m-2s-1)
    - Trap type 2: D flux (m-2s-1)

![Diagram showing isotope exchange](image)

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Summary

- WallDYN allows to couple surface process data from different source to plasma transport
- WallDYN calculates global impurity migration, erosion, layer deposition and co-deposition
- WallDYN tracks the entire erosion/migration/deposition/re-erosion chain
  - Main input: mixed material sputter and reflection yields
  - Currently taken from dynamic TRIM (calculations)
- The classic Diff./Trapp. model does not correctly describe the trapping/detrapping dynamics
- DFT predicted fill level dependence can explain low temperature isotope exchange
- New rate equation model allows to test DFT predictions against experimental data
- Classic Diff./Trapp & fill level dependent model indiscernable in mono-isotopic case
  - Main input: fill level dependent detrapping energies
  - Currently only available for monovacancies from DFT
  - Maybe use MD for extended defects?

Discussion slides

Isotope exchange case

- Depth profiles at t = 100sec (End of Iso-A implantation)
- Depth profiles at t = 900sec (Just before Iso-B implantation)
Isotope exchange case

Depth profiles at $t = 1000\text{sec}$ (Start of Iso-B implantation)

- Occ. Dep.
- Classic.

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Depth profiles at $t = 1100\text{sec}$ (100 sec of Iso-B implantation)

- Occ. Dep.
- Classic.

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Depth profiles at $t = 2000\text{sec}$ (1000 sec of Iso-B implantation)

- Occ. Dep.
- Classic.

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<th>Time (sec)</th>
<th>Total amount (μm$^{-2}$)</th>
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<tr>
<td>10000</td>
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</tr>
</tbody>
</table>

Factor ~0.8

Factor ~10

Depends on trap energies!

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