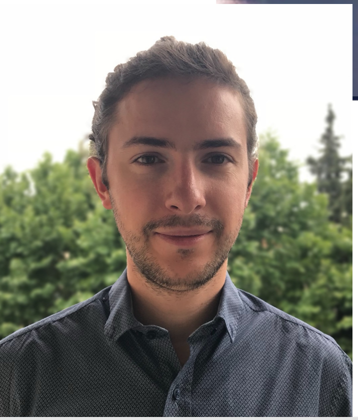
The Dynamics of Wall Elements (DWE) code: a recycling model for SolEdge-EIRENE

TSVV5 meeting
June 06, 2025



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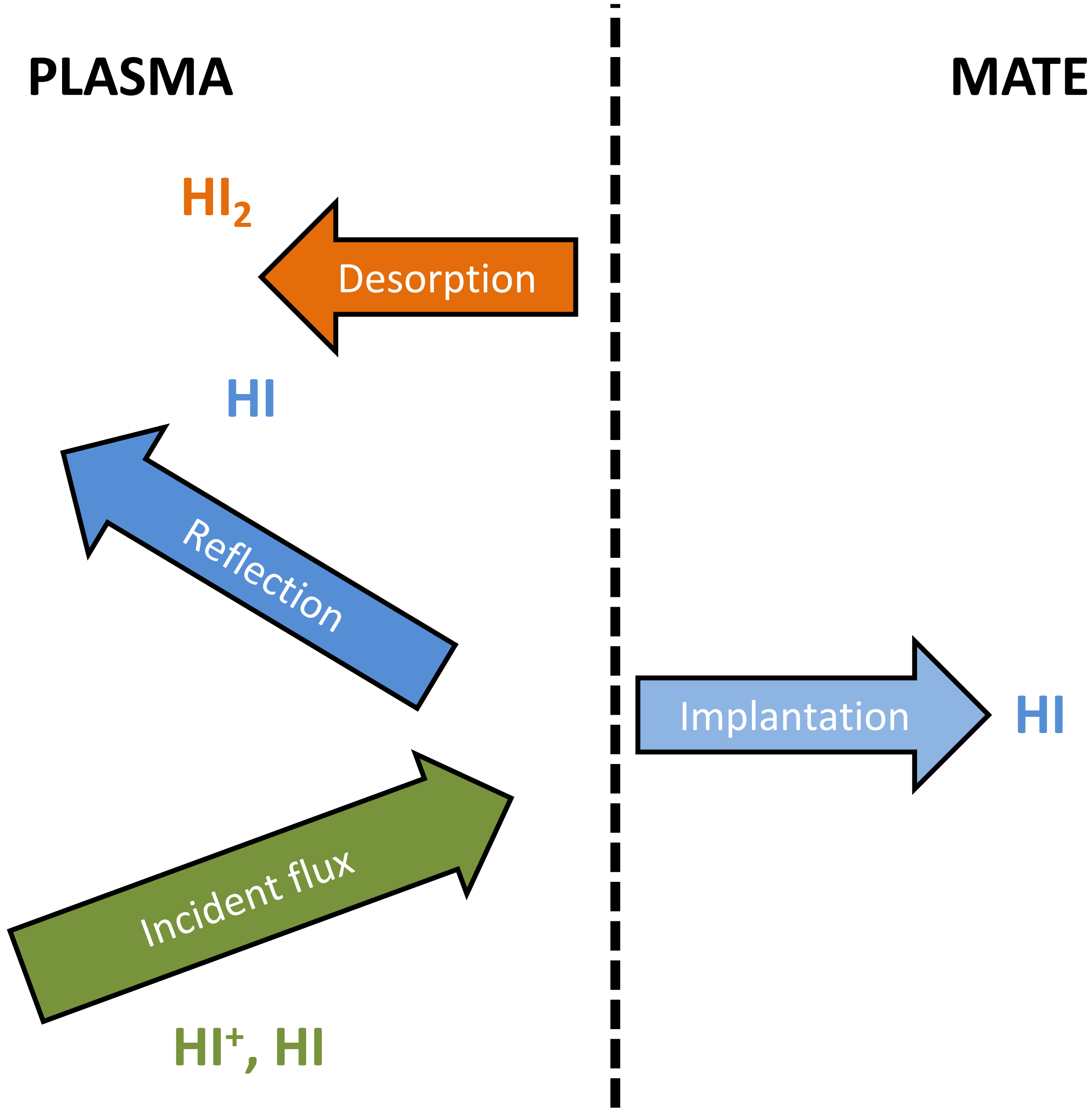
Recycling in SolEdge-EIRENE



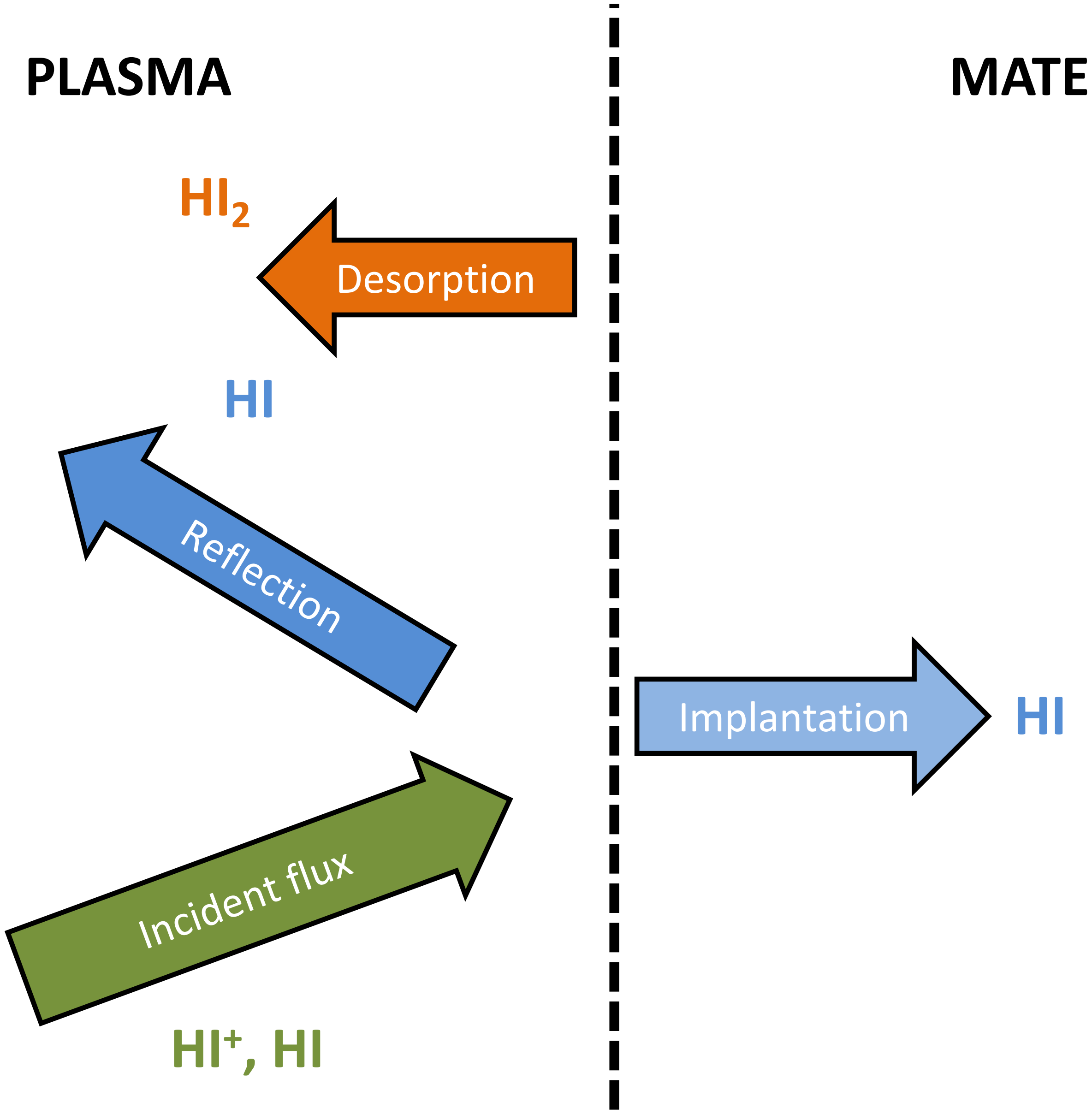
Recycling handled in **EIRENE**:

$$RECYCT = R_n + (1 - R_n)R_m$$

- **Reflection**: $R_n = \frac{\Gamma_{ref}}{\Gamma_{inc}}$
  calculated self-consistently with tabulated **TRIM** tables

- **Desorption**: $R_m = \frac{\Gamma_{out}}{\Gamma_{imp}^{i+} + \Gamma_{imp}^{at}}$
  set **ad-hoc** by the user
  often = 1 ➔ force particle conservation
  or < 1 ➔ wall pumping

Recycling in SolEdge-EIRENE



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- **Reflection**: $R_n = \frac{\Gamma_{ref}}{\Gamma_{inc}}$
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- **Desorption**: $R_m(t) = \frac{\Gamma_{out}(t)}{\Gamma_{imp}^{i+}(t) + \Gamma_{imp}^{at}(t)}$
  ~~set **ad-hoc** by the user~~
  ~~often = 1 ➔ force particle conservation~~
  ~~or < 1 ➔ wall pumping~~

Outline

1) The Dynamics of Wall Elements (DWE) code
2) Wall initialisation with the DWE code (before coupled plasma-wall simulation)
3) Reduced model for hydrogen retention as a tool for DWE simulation analysis
4) Conclusions

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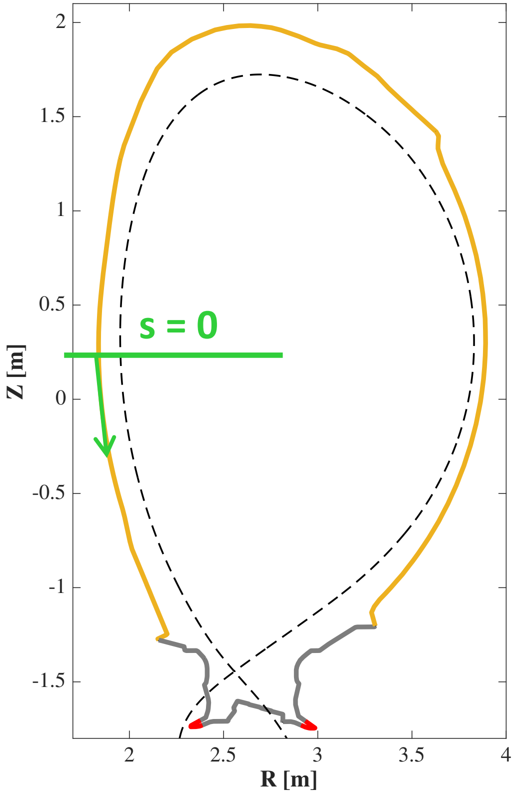
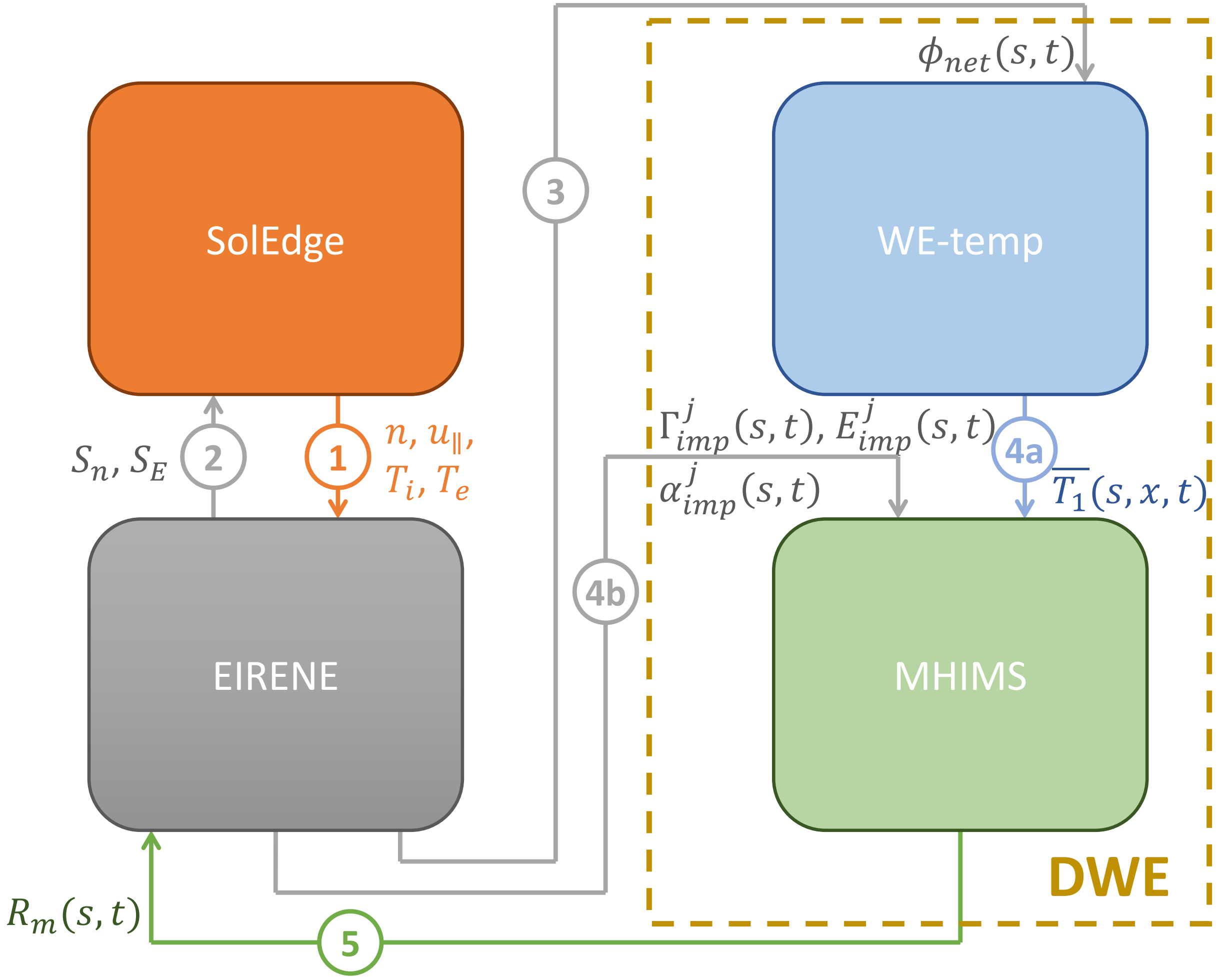
The Dynamics of Wall Elements (DWE) code

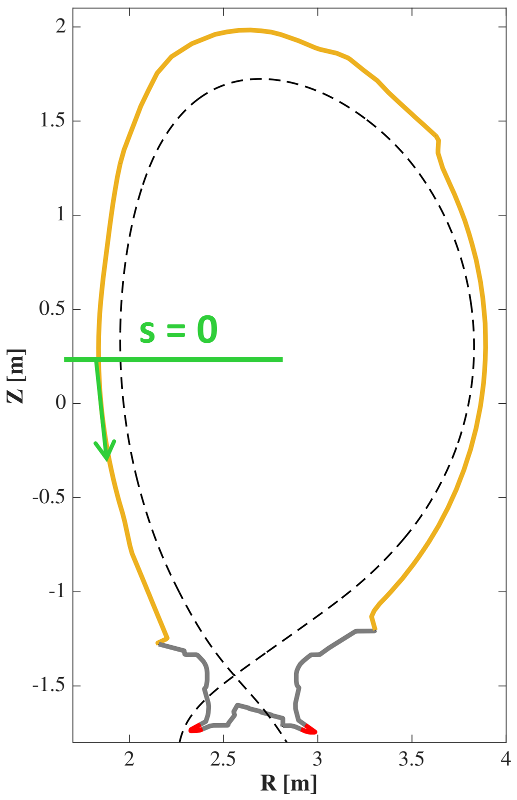


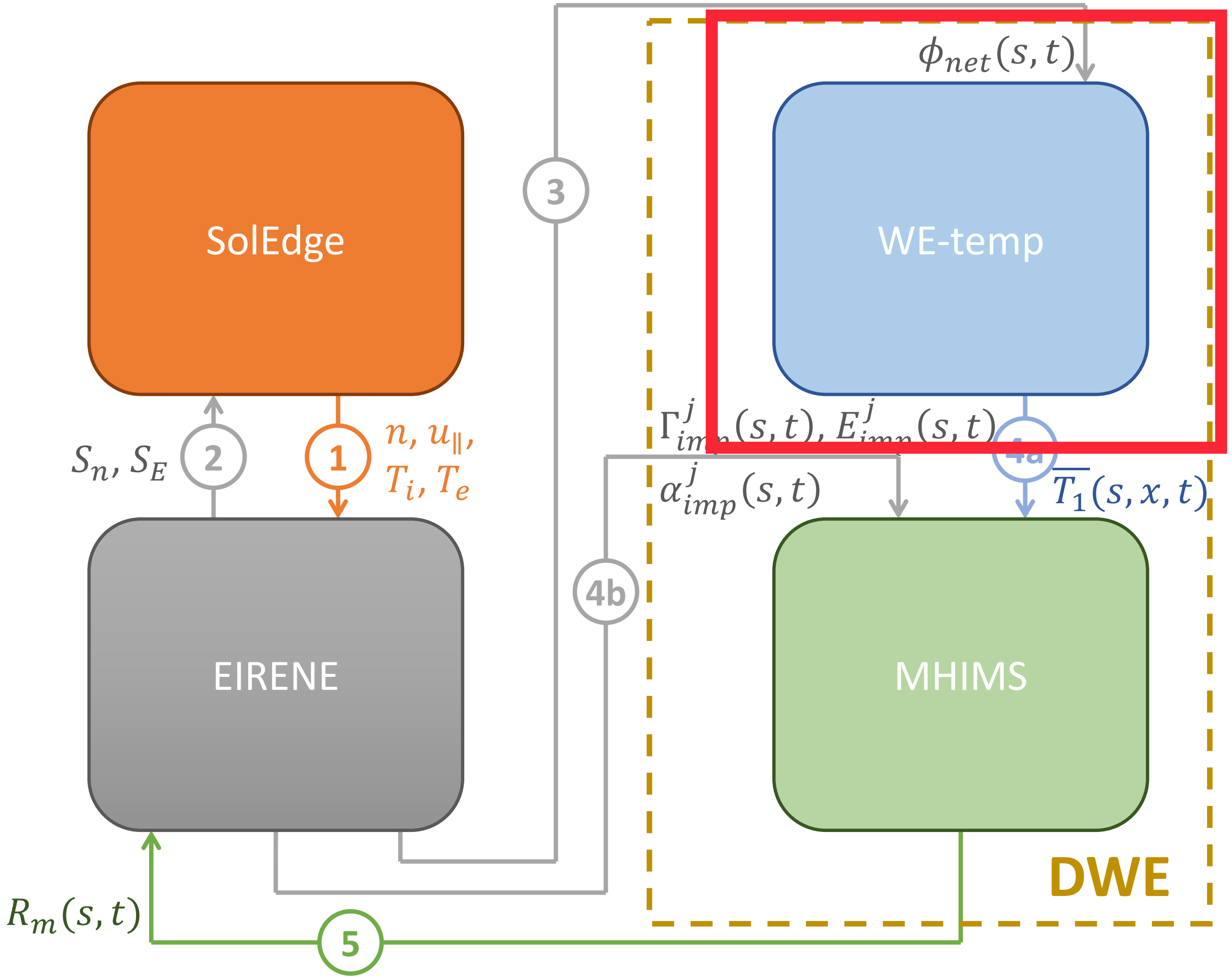


J. Denis et al., *Nuclear Materials and Energy Fusion, 19 (2019)*

J. Denis et al., *PhD thesis (2020)*

The Dynamics of Wall Elements (DWE) code





Wall temperature heat equation

J. Denis et al., Nuclear Materials and Energy Fusion, 19 (2019)
J. Denis et al., PhD thesis (2020)

The Dynamics of Wall Elements (DWE) code

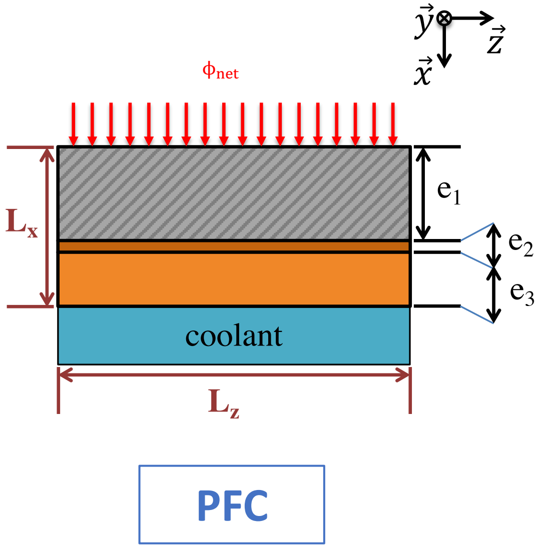
WE-temp: Wall Element temperature

- Temperature profile in thin layer of surface material (< 1 mm)
- Handle different PFC technologies (inertial, actively-cooled) and design (materials)
- Handle steady-state and transient heat loads

→ 1D linear heat equation solved using superposition theorem

$$\phi_{net}(t) = \sum_{k=1}^{N_\phi(t)} \Delta\phi_k \, \mathcal{H}(t - t_k)$$

$$\Delta \boldsymbol{T}_1(\boldsymbol{x}, \boldsymbol{t}) = \bar{T}_1(x,t) - T(0) = \sum_{k=1}^{N_\phi(t)} \Delta\phi_k \, T_1^{step}(x, t - t_k)$$



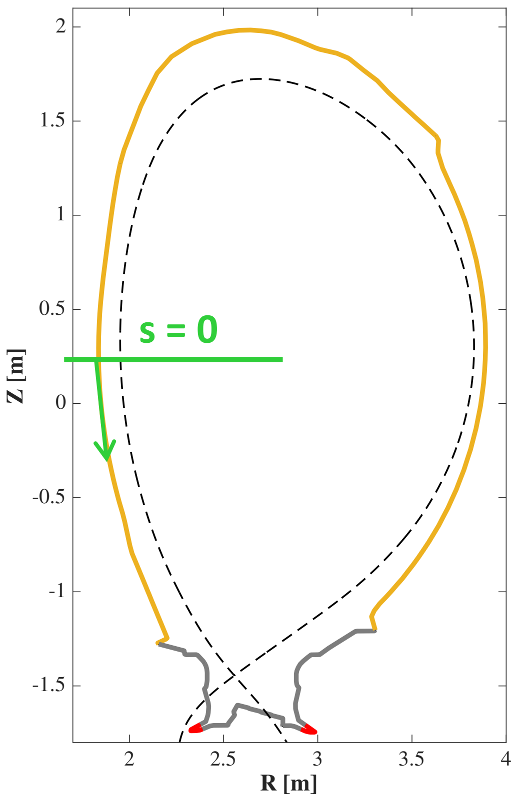
PFC step response

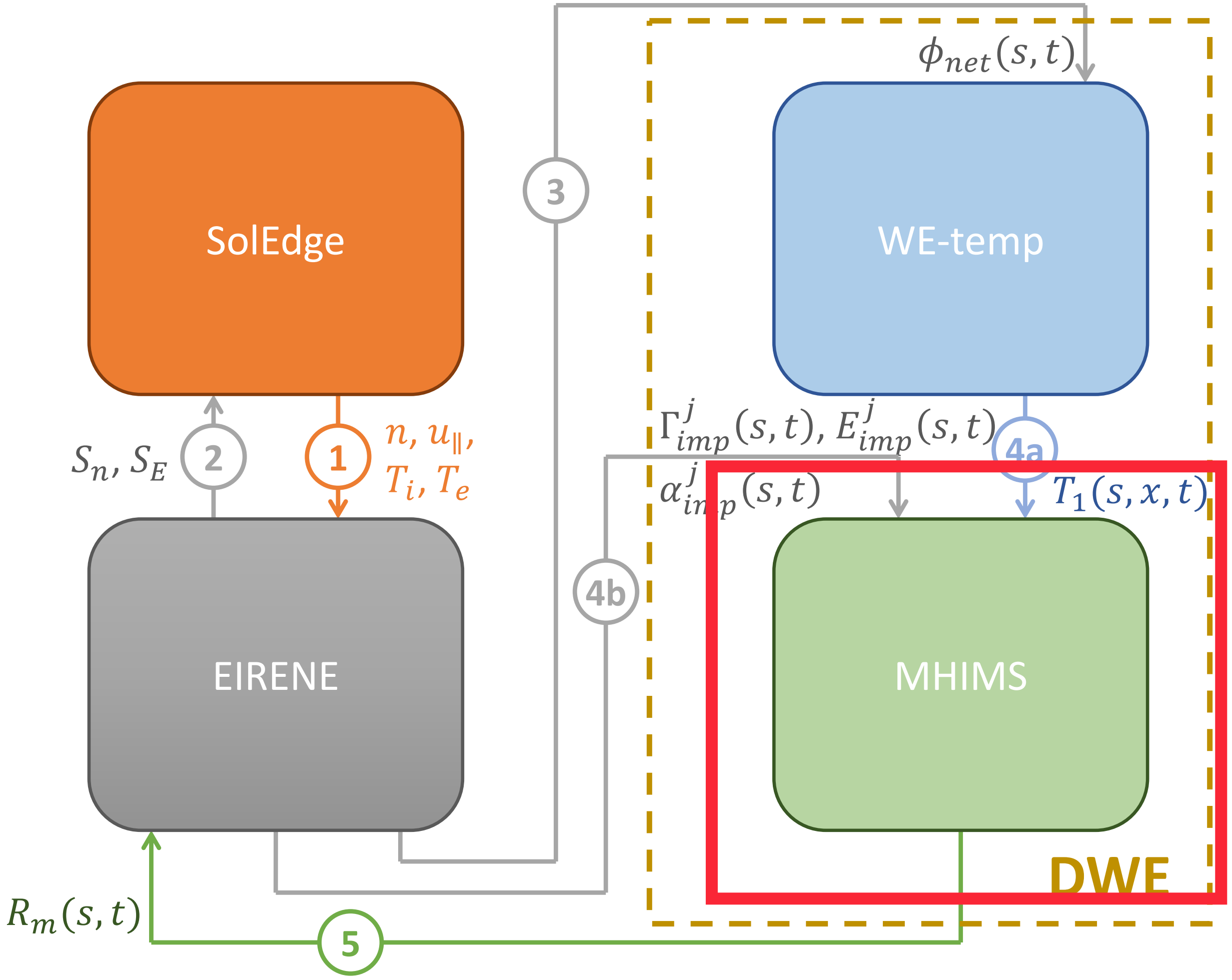
⇒ calculated using quadrupole method

+ numerical or analytical inverse Laplace transform

J. Denis et al., PhD thesis (2020)

The Dynamics of Wall Elements (DWE) code





Hydrogen-material interaction via Reaction-Diffusion equations

= CRDS or TESSIM code

J. Denis et al., Nuclear Materials and Energy Fusion, 19 (2019)
J. Denis et al., PhD thesis (2020)

The Dynamics of Wall Elements (DWE) code

MHIMS: Migration of Hydrogen Isotopes in MaterialS

$$\frac{\partial\, n_m(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(D(T)\cdot\frac{\partial n_m}{\partial x}\right) - \sum_{i=1}^{N_{trap}} \frac{\partial n_{t,i}}{\partial t} + S_{ext}^{i+}(x,t) + S_{ext}^{at}(x,t)$$

$$\frac{\partial n_{t,i}(x,t)}{\partial t} = \nu_{t,i}^{*}(T)\cdot\frac{n_i(x) - n_{t,i}}{n_{IS}} n_m - \nu_{dt,i}(T)\cdot n_{t,i}$$

$$\text{B.C. at } x = 0\text{: } n_m(0,t) = 0$$

$$\text{B.C. at } x = L\text{: } \left| \begin{array}{l} n_m(L,t) = 0 \\ \qquad\quad \text{or} \\ D(T)\cdot\dfrac{\partial n_m\,(L,t)}{\partial x} = 0 \end{array} \right.$$

Particles divided in 2 populations :

- Mobile particles (diffusion): $\boldsymbol{n_{\mathrm{m}}(x,t)}$
- Trapped particles: $\boldsymbol{n_{t,i}(x,t)}$

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diffusion equation for mobile

$$\frac{\partial n_{t,i}(x,t)}{\partial t} = \nu_{t,i}^{*}(T)\cdot\frac{n_i(x) - n_{t,i}}{n_{IS}} n_m - \nu_{dt,i}(T)\cdot n_{t,i}$$

B.C. at $x = 0$: $n_m(0,t) = 0$

B.C. at $x = L$: $n_m(L,t) = 0$ or $D(T)\cdot\frac{\partial n_m(L,t)}{\partial x} = 0$

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reaction between mobile HI and free trap:

$$[\mathrm{HI}]_{\mathrm{m}} + \mathrm{Trap}_{\mathrm{free}} \leftrightarrow [\mathrm{HI}]_{\mathrm{t}}$$

$$\mathrm{B.C.\ at}\ x=0:\ n_m(0,t)=0$$

$$\mathrm{B.C.\ at}\ x=L:\ \left|\begin{array}{l} n_m(L,t)=0 \\ \qquad \text{or} \\ D(T)\cdot\dfrac{\partial n_m\,(L,t)}{\partial x} = 0 \end{array}\right.$$

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B.C. at $x = 0$: $n_m(0,t) = 0$ ← surface processes not rate-limiting

B.C. at $x = L$: $n_m(L,t) = 0$ or $D(T)\cdot\frac{\partial n_m(L,t)}{\partial x} = 0$

$$\Gamma_{out} = D(T)\cdot\frac{\partial n_m}{\partial x}(x=0)$$

$$R_m(t) = \frac{\Gamma_{out}(t)}{\Gamma_{imp}^{i+}(t) + \Gamma_{imp}^{at}(t)}$$

$$R_m(t\to\infty)\to 1$$

Particles divided in 2 populations :

- Mobile particles (diffusion): $n_m(x,t)$
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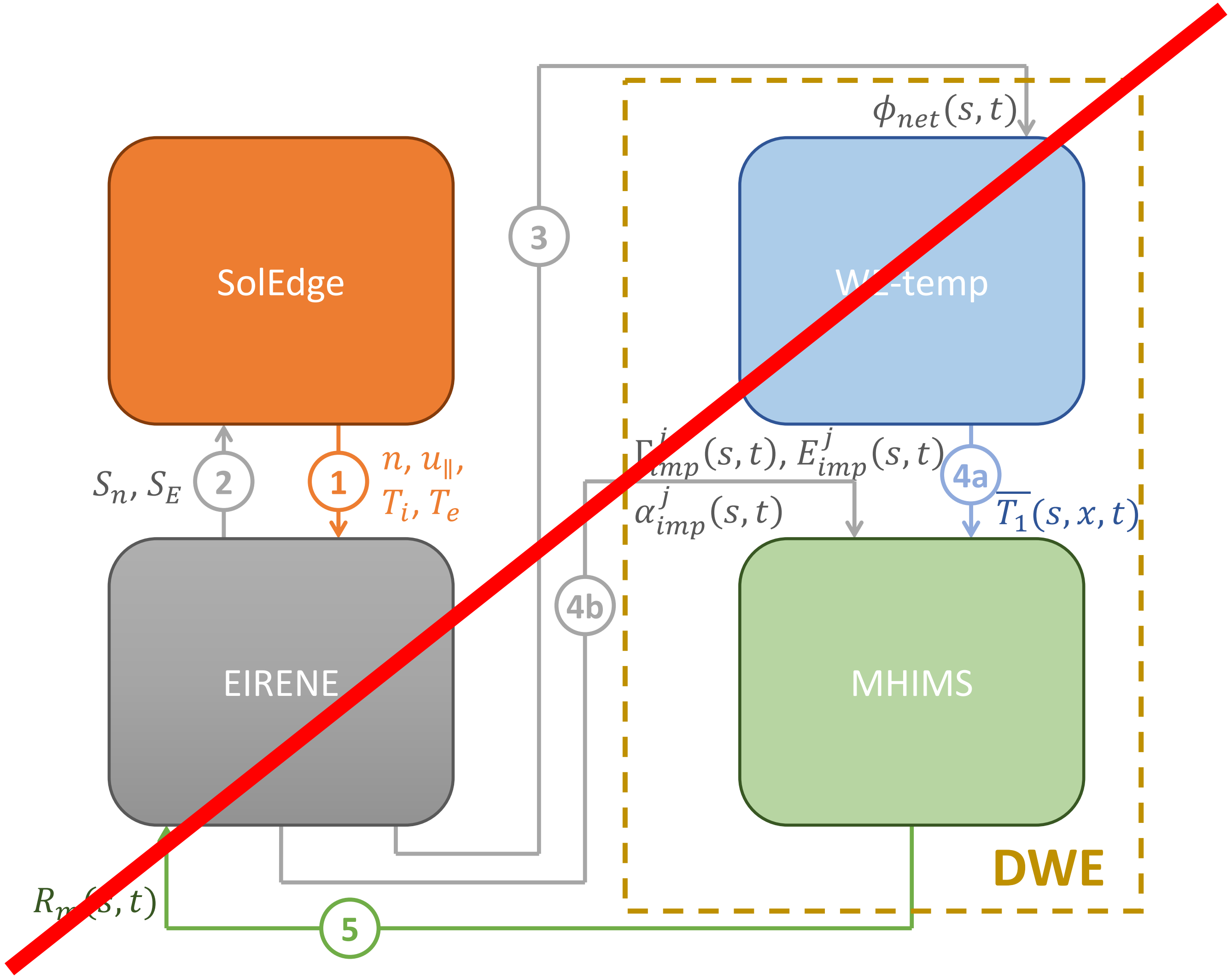
- HI diffusion coefficient: $D(T) = D_0 \cdot e^{-\frac{E_{diff}}{k_B \cdot T}}$
- Trapping frequency: $\nu_{t,i}^{*}(T)\ [s^{-1}] \propto D(T)$
- Detrapping frequency: $\nu_{dt,i}(T) = \nu_{dt,i}^{0} \cdot e^{-\frac{E_{dt,i}}{k_B \cdot T}}$
- Interstitial site density: n_{IS}
- Trap density: $n_i(x)$
- Implantation sources: $S_{ext}^{j}(x,t) \Longrightarrow \int S_{ext}^{j}(x,t).\,dx = \Gamma_{imp}^{j}(t)$

(Material + HI) parameters

→ From simulation: DFT, KMC

→ From fitting of implantation experiments or post-mortem analysis

But the direct coupling with SolEdge3X-EIRENE is not operational



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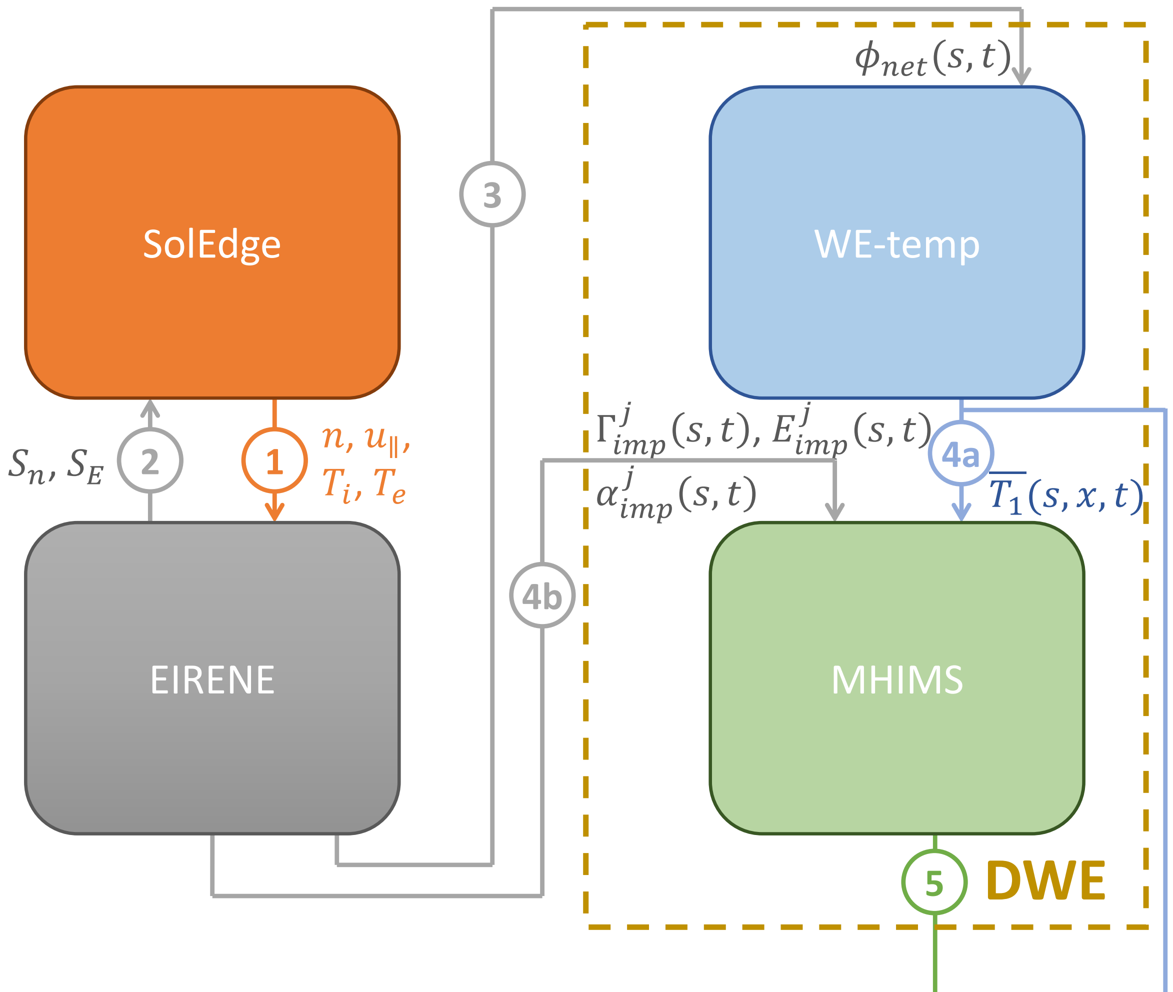
Indirect coupling of SolEdge-EIRENE and DWE for wall initialisation



DWE outputs:

- Density of mobile hydrogen isotopes [m^{-3}]: $n_m(s,x,t)$
- Density of trapped hydrogen isotopes [m^{-3}]: $n_{t,i}(s,x,t)$
- Outgassing flux density [m^{-2}.s^{-1}]: $\Gamma_{out}(s,t)$
- Wall temperature [°C]: $\overline{T_1}(s,x,t)$

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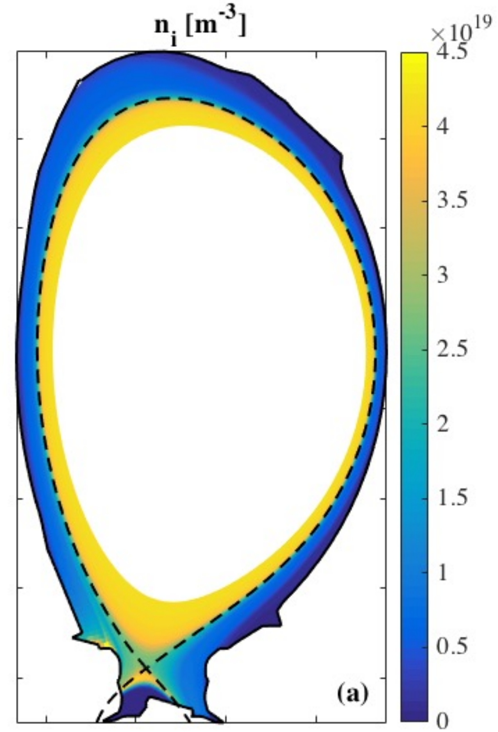
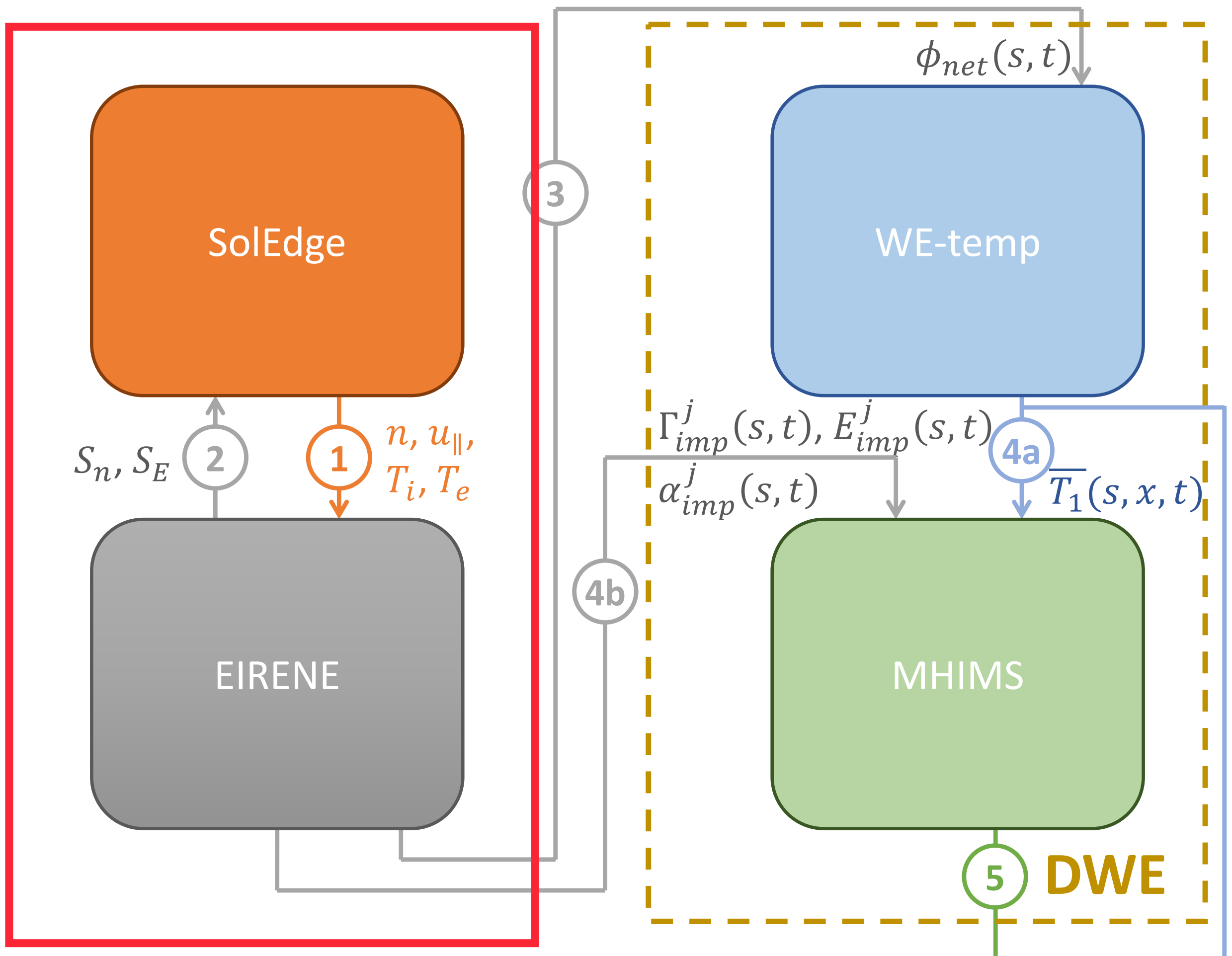


Plasma backgrounds



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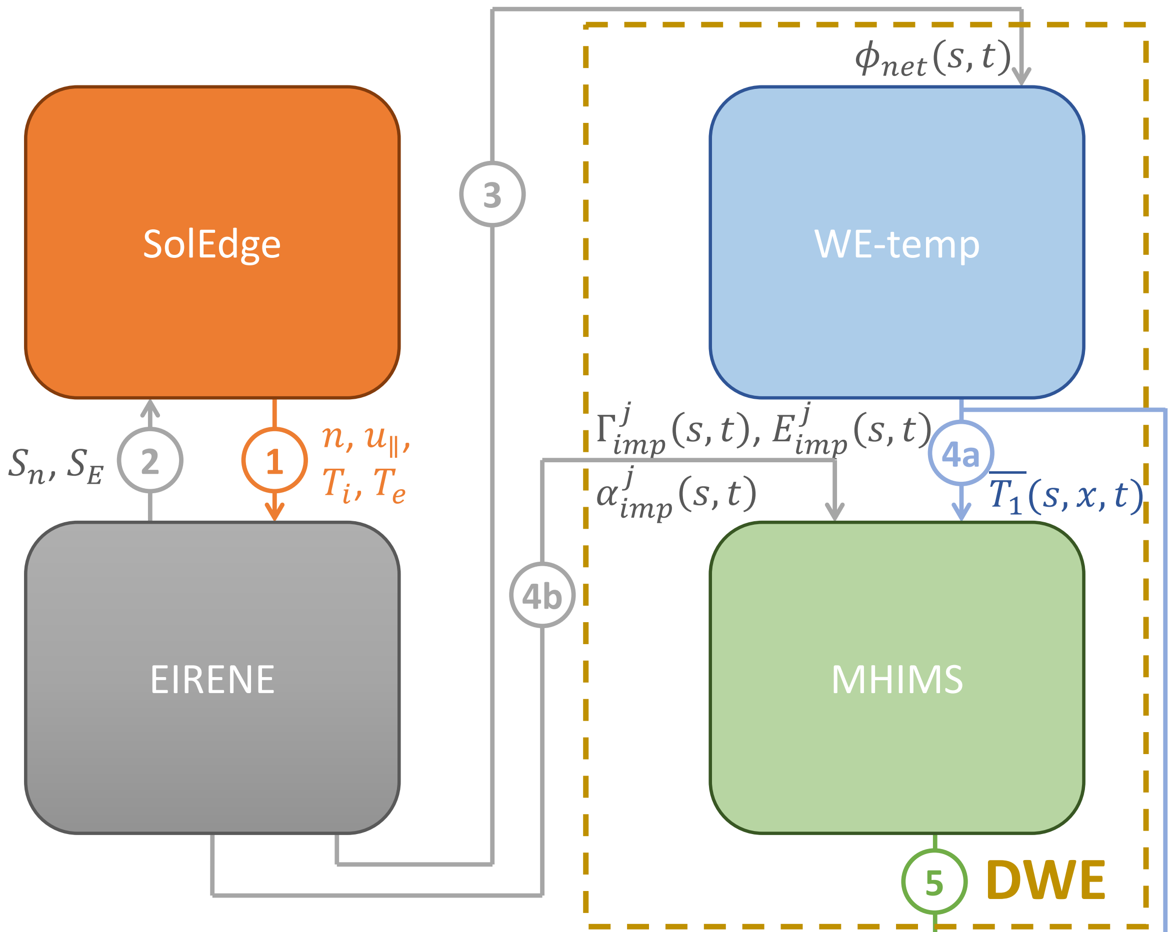

Hydrogen inventory

DWE outputs:

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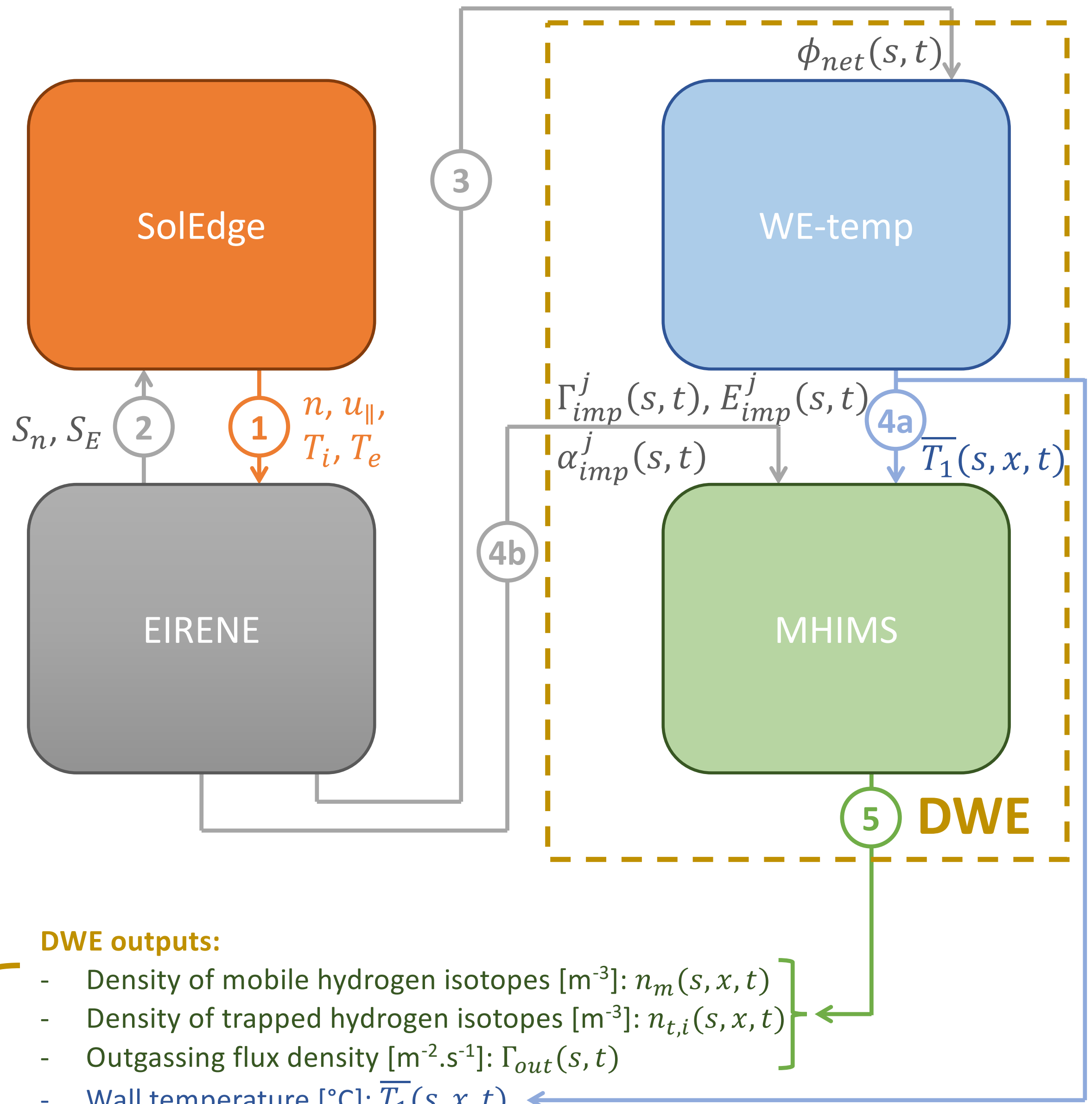
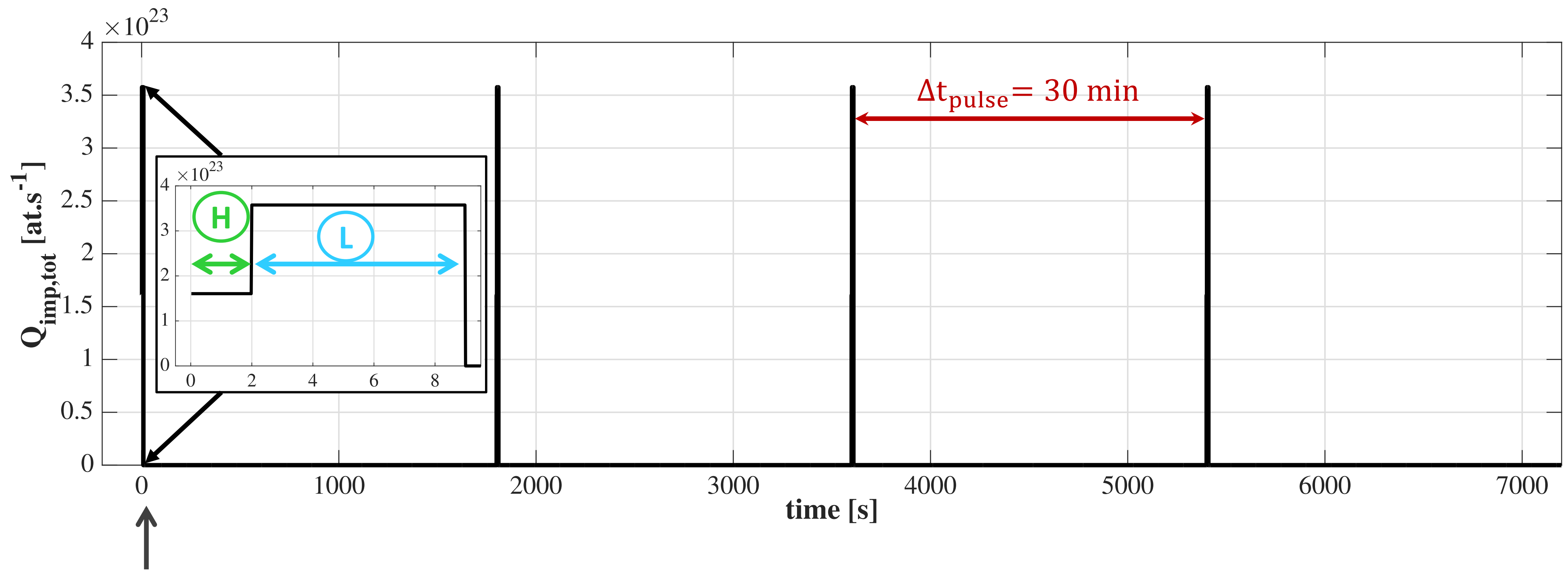


DWE outputs:

During and between discharges

- Density of mobile hydrogen isotopes [m^{-3}]: $n_m(s,x,t)$
- Density of trapped hydrogen isotopes [m^{-3}]: $n_{t,i}(s,x,t)$
- Outgassing flux density [m^{-2}.s^{-1}]: $\Gamma_{out}(s,t)$
- Wall temperature [°C]: $\overline{T_1}(s,x,t)$

Simulation of similar discharges in full-W JET



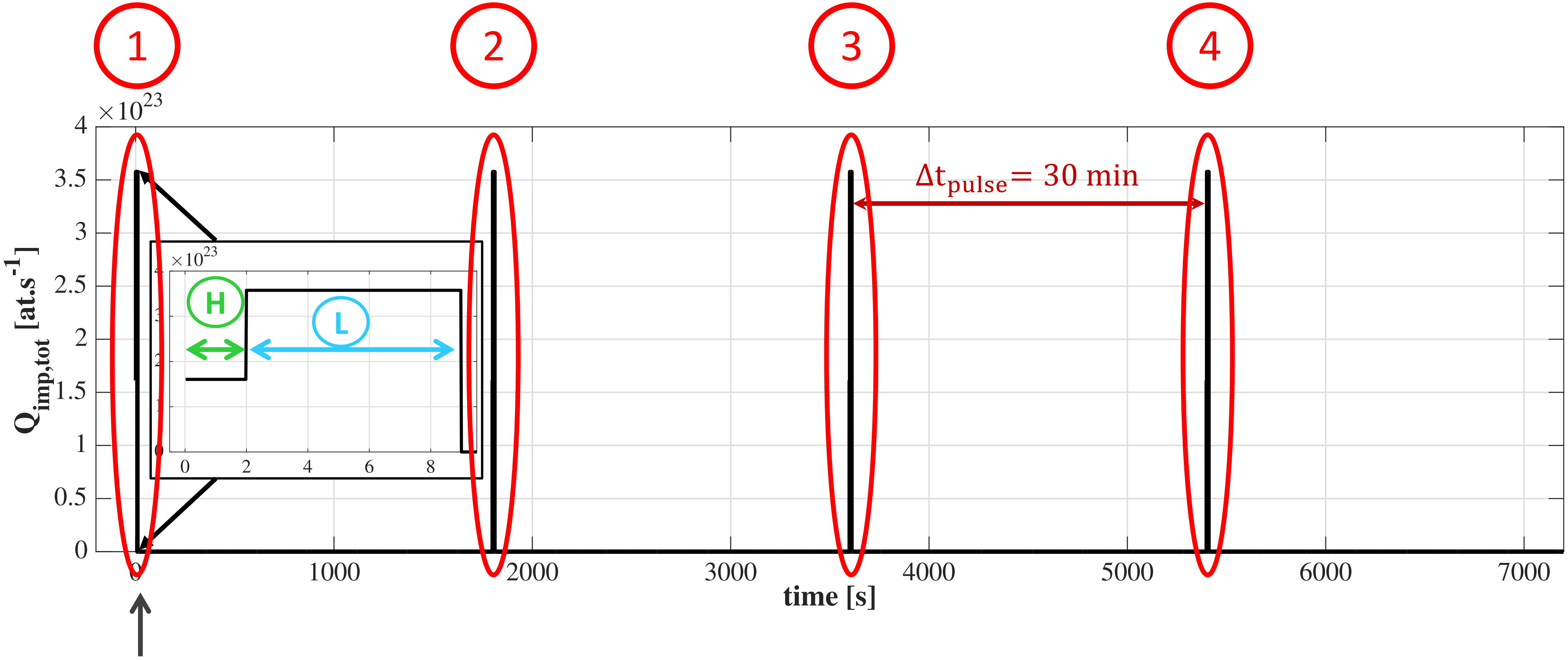
At t = 0 s: empty wall

Full-W wall with 3 traps:

- $E_{dt,1} = 0.85$ eV
- $E_{dt,2} = 1.00$ eV
- $E_{dt,3} = 1.5$ eV

J. Denis et al., Nuclear Materials and Energy Fusion, 19 (2019)
J. Denis et al., PhD thesis (2020)

Dynamic retention during discharges: retention rate



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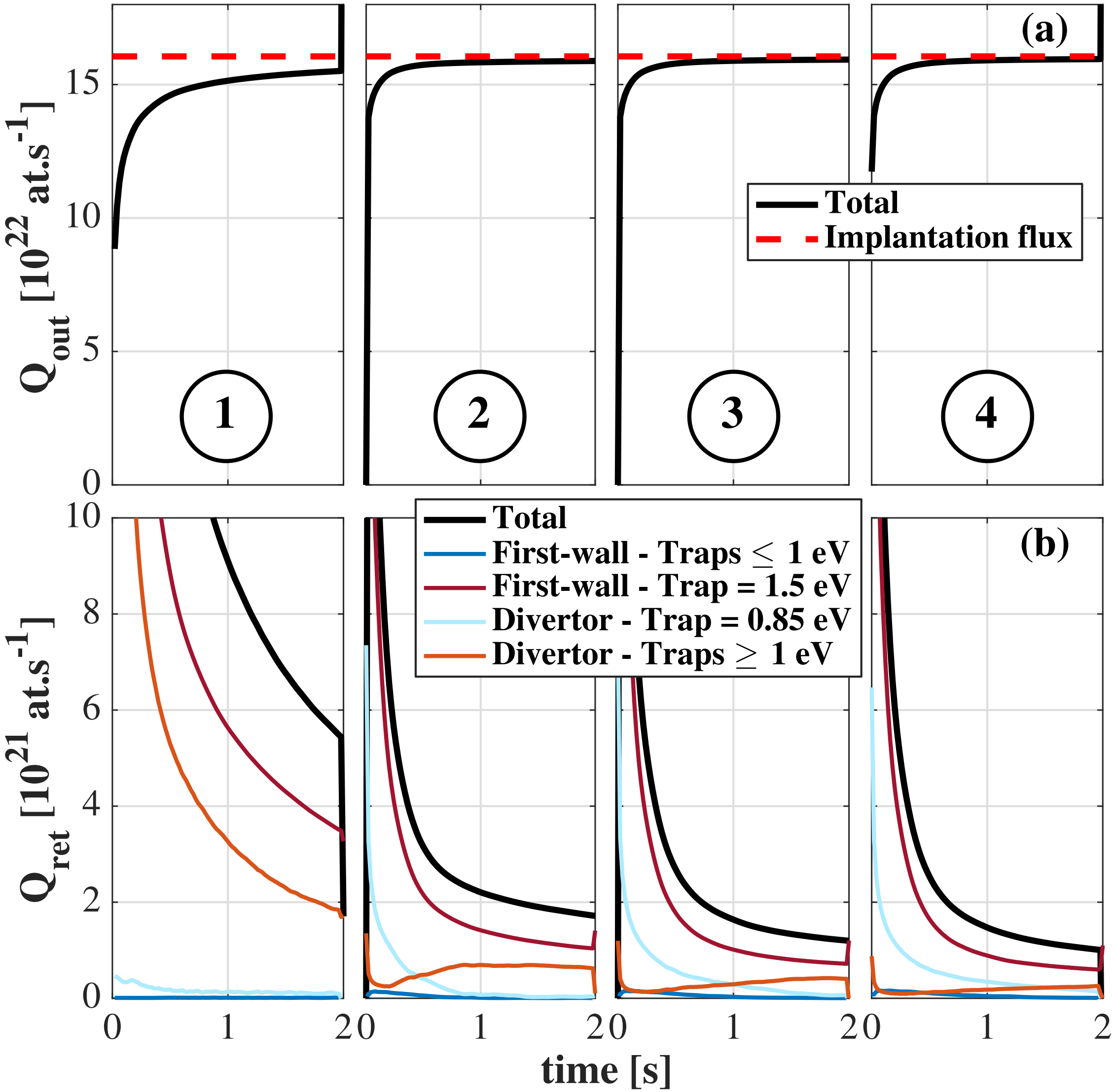
Dynamic retention during discharges: retention rate

H-mode



The retention rate is reproducible from the 3rd discharge

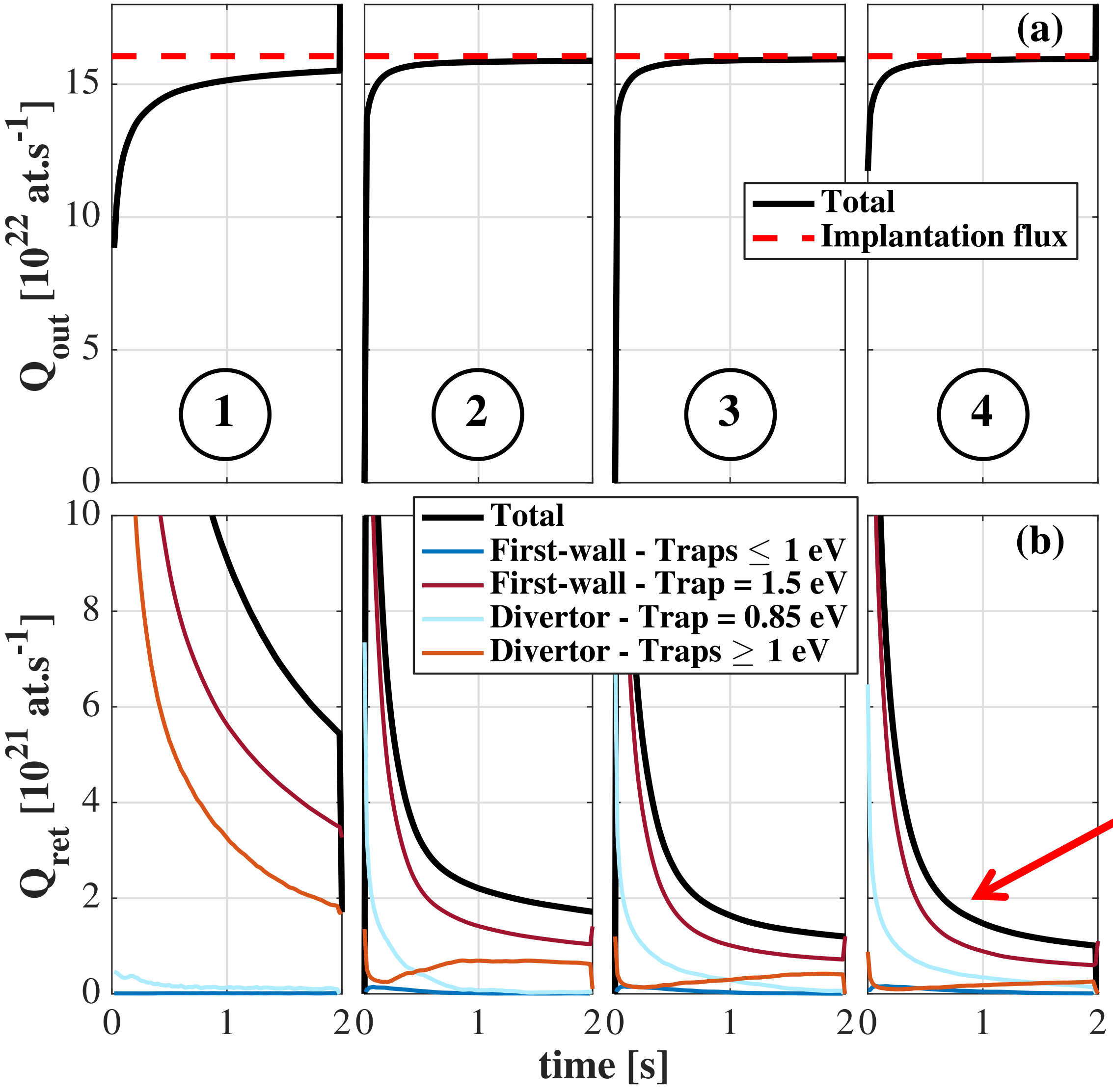
➔ the wall is initialised

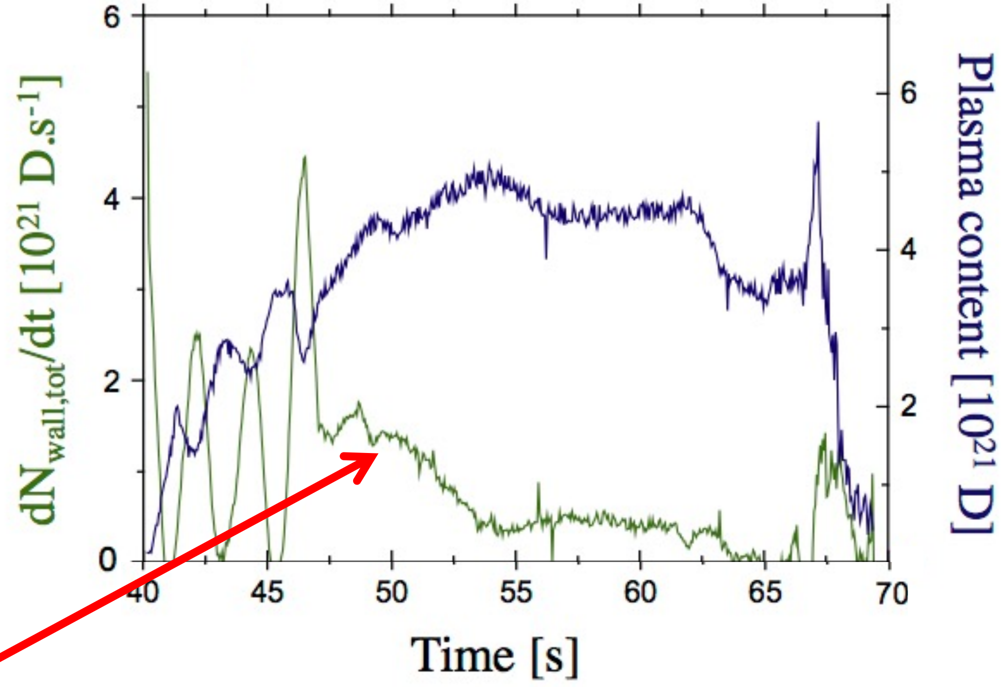
J. Denis et al., Nuclear Materials and Energy Fusion, 19 (2019)

J. Denis et al., PhD thesis (2020)

Retention rate in the simulation is consistent with experimental observations

H-mode





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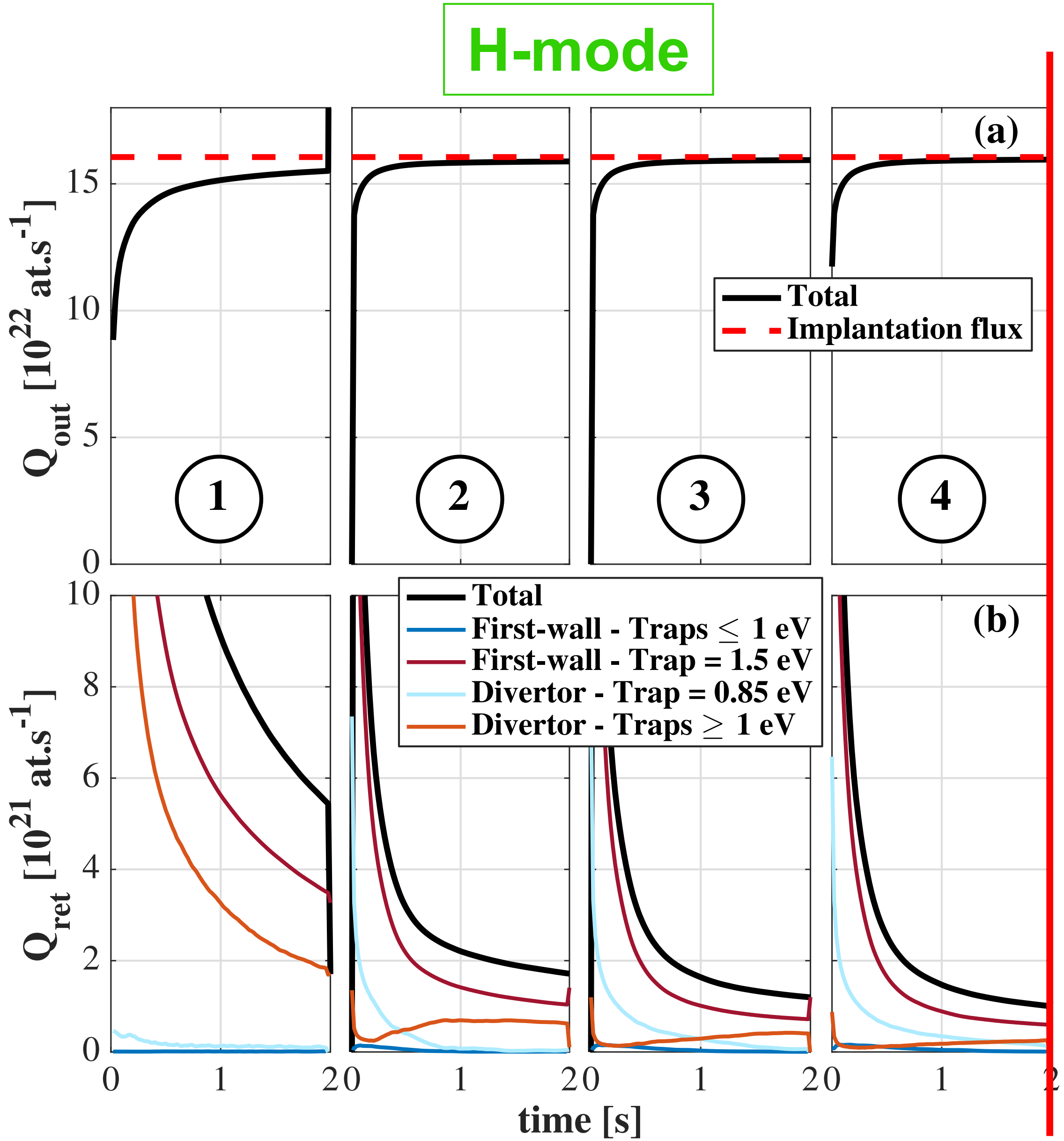
Recycling coefficient at t = 2 s



Recycling coefficient at t = 2 s?

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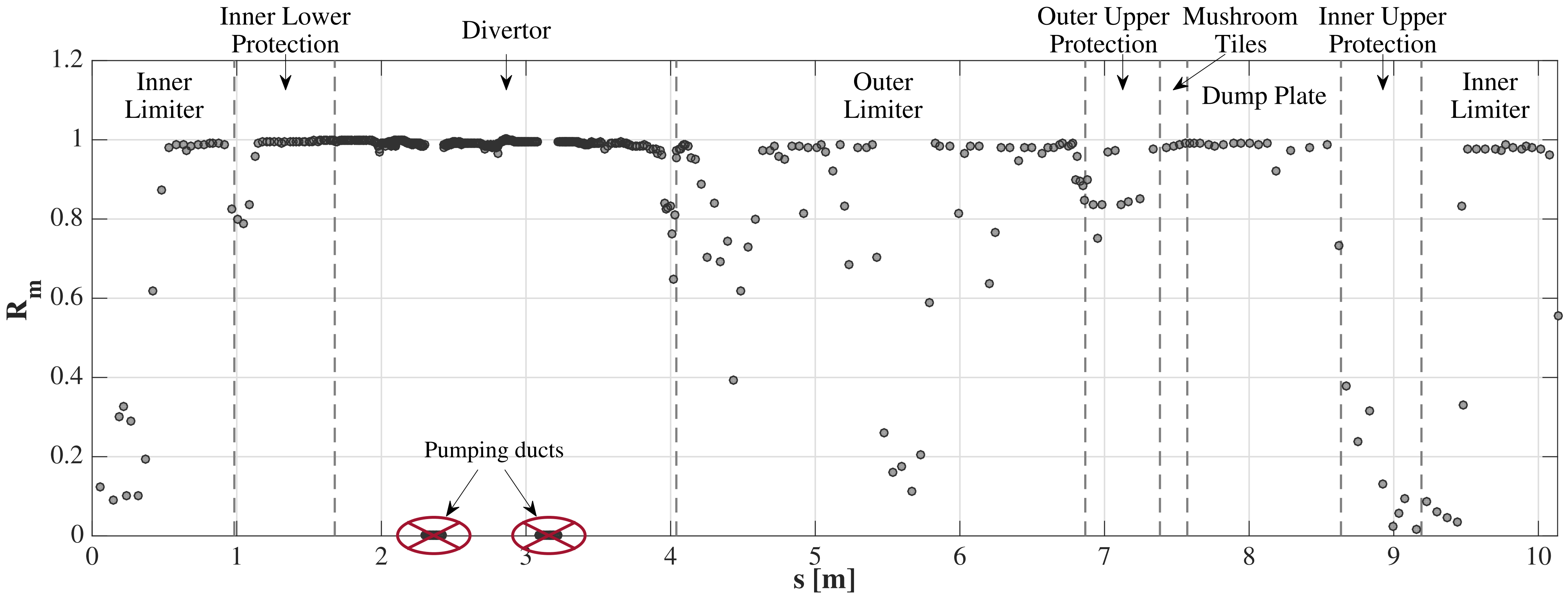
Recycling coefficient at t = 2 s



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Reduced model for hydrogen retention

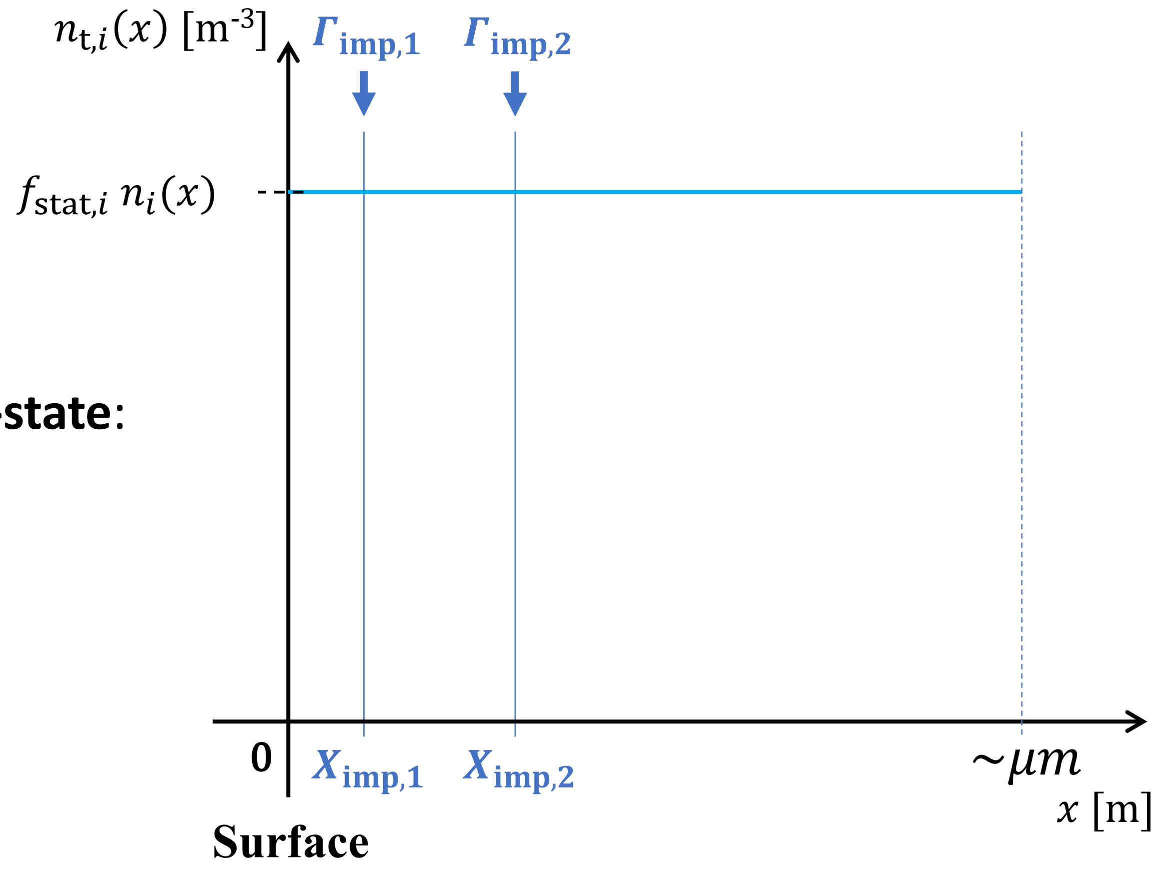
Hypothesis:

(1) Fixed implantation conditions : flux $\Gamma_{\mathrm{imp},j}$, energy $E_{\mathrm{imp},j}$
(2) Two point sources : j = H⁺, H
(3) Wall temperature constant : T
(4) Steady-state

➔ Hydrogen **inventory dominated by traps**

➔ Density of **trapped H** in **subsurface layer** (µm) **at steady-state**:

$$n_{\mathrm{t},i}(x) = f_{\mathrm{stat},i}\, n_i(x)$$



Trap filling ratio:

$$\boldsymbol{f}_{\mathbf{stat},\boldsymbol{i}}(T, \Gamma_{\mathrm{imp},j}, E_{\mathrm{imp},j}) = \frac{1}{1 + \dfrac{\nu_{\mathrm{dt},i}(T)}{\nu_{\mathrm{t,stat}}(\Gamma_{\mathrm{imp},j}, E_{\mathrm{imp},j})}}$$

- when $\nu_{\mathrm{dt},i} \gg \nu_{\mathrm{t,stat}}$, $f_{\mathrm{stat},i} \to 0$ (empty traps)
- when $\nu_{\mathrm{dt},i} = \nu_{\mathrm{t,stat}}$, $f_{\mathrm{stat},i} = 0.5$
- when $\nu_{\mathrm{dt},i} \ll \nu_{\mathrm{t,stat}}$, $f_{\mathrm{stat},i} \to 1$ (saturated traps)

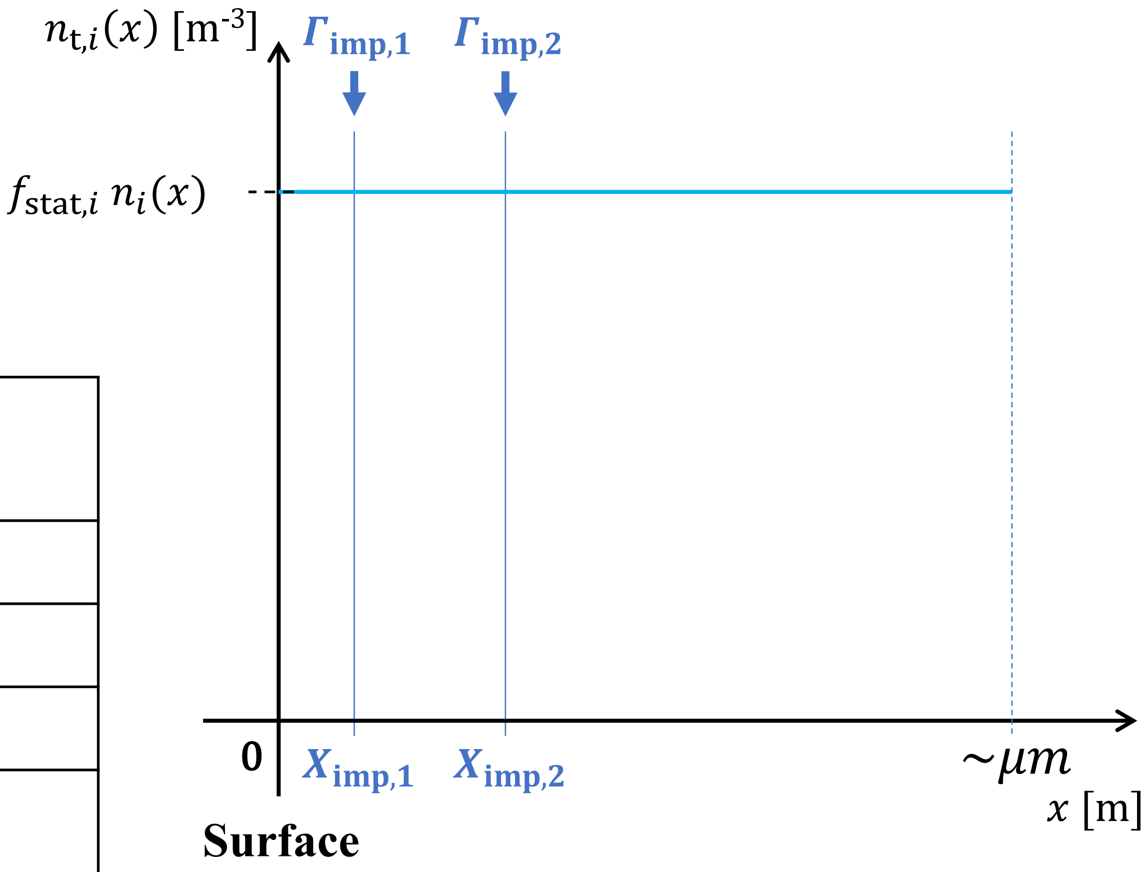
J. Denis et al., Journal of Nuclear Materials 570 (2022)

Reduced model for hydrogen retention: wall dynamics w.r.t. plasma

Trap filling ratio:

$$f_{\mathrm{stat},i} = \frac{1}{1 + \frac{\nu_{\mathrm{dt},i}(T)}{\nu_{\mathrm{t,stat}}(\Gamma_{\mathrm{imp},j}, E_{\mathrm{imp},j})}}$$

Constant implantation $\nu_{\mathrm{t,stat}} = constant$	$\nearrow T$	$\searrow T$
$\nu_{\mathrm{dt},i}(T)$	$\nearrow$	$\searrow$
$f_{\mathrm{stat},i}$	$\searrow$	$\nearrow$
H inventory	$\searrow$	$\nearrow$
Wall dynamics w.r.t. plasma	Fuelling	Pumping



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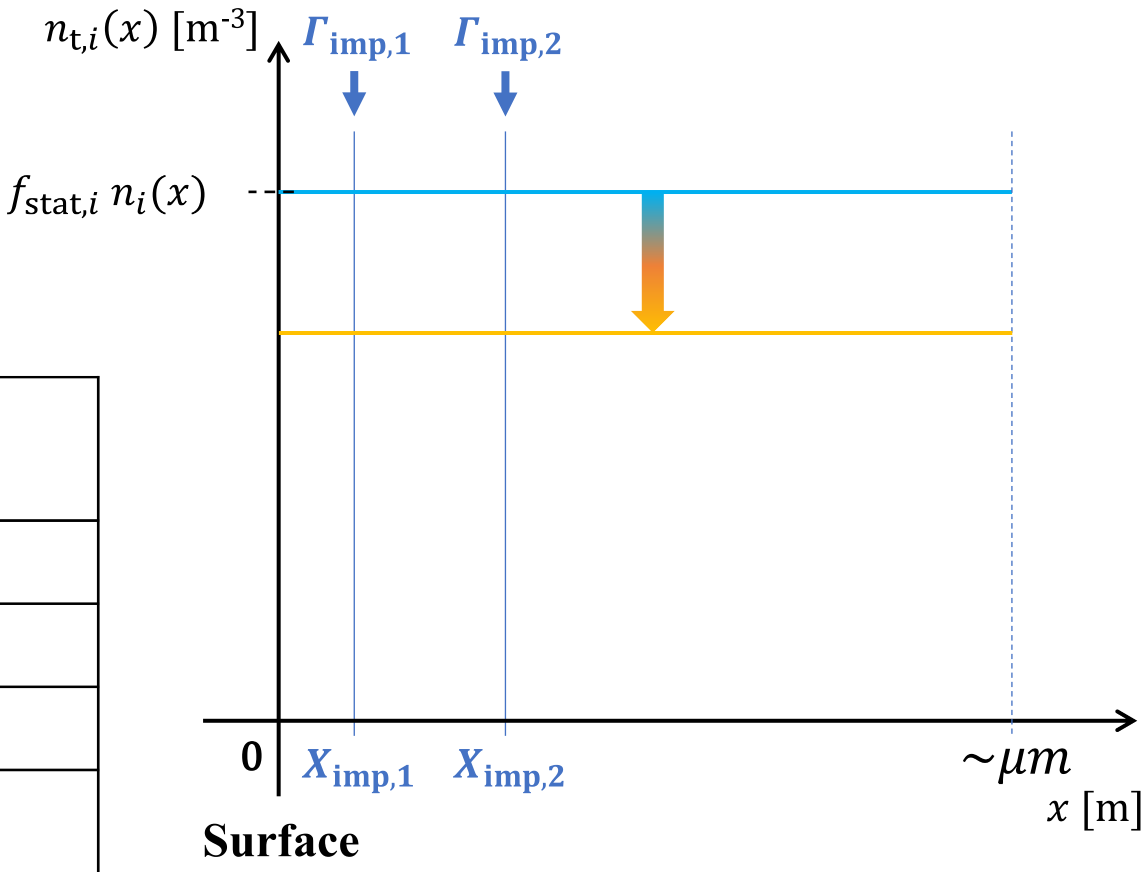

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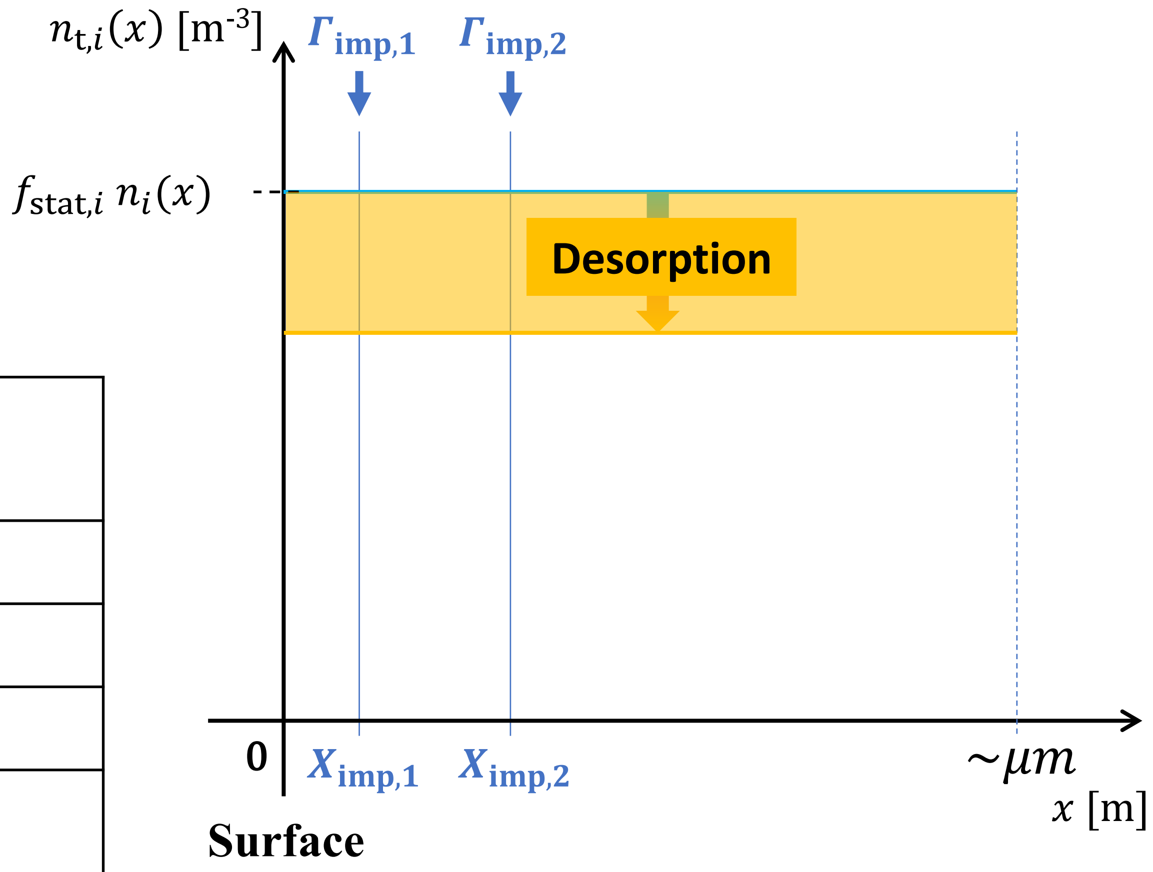

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Trap filling ratio:

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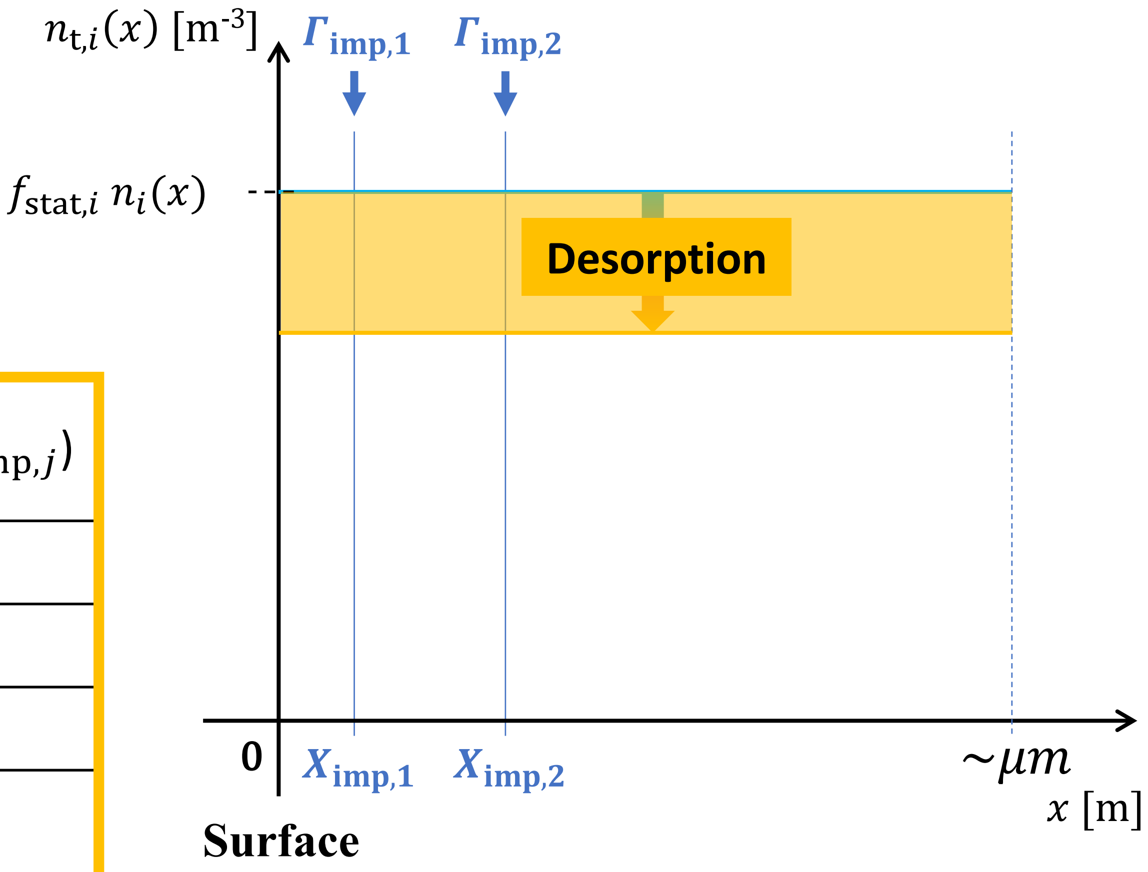
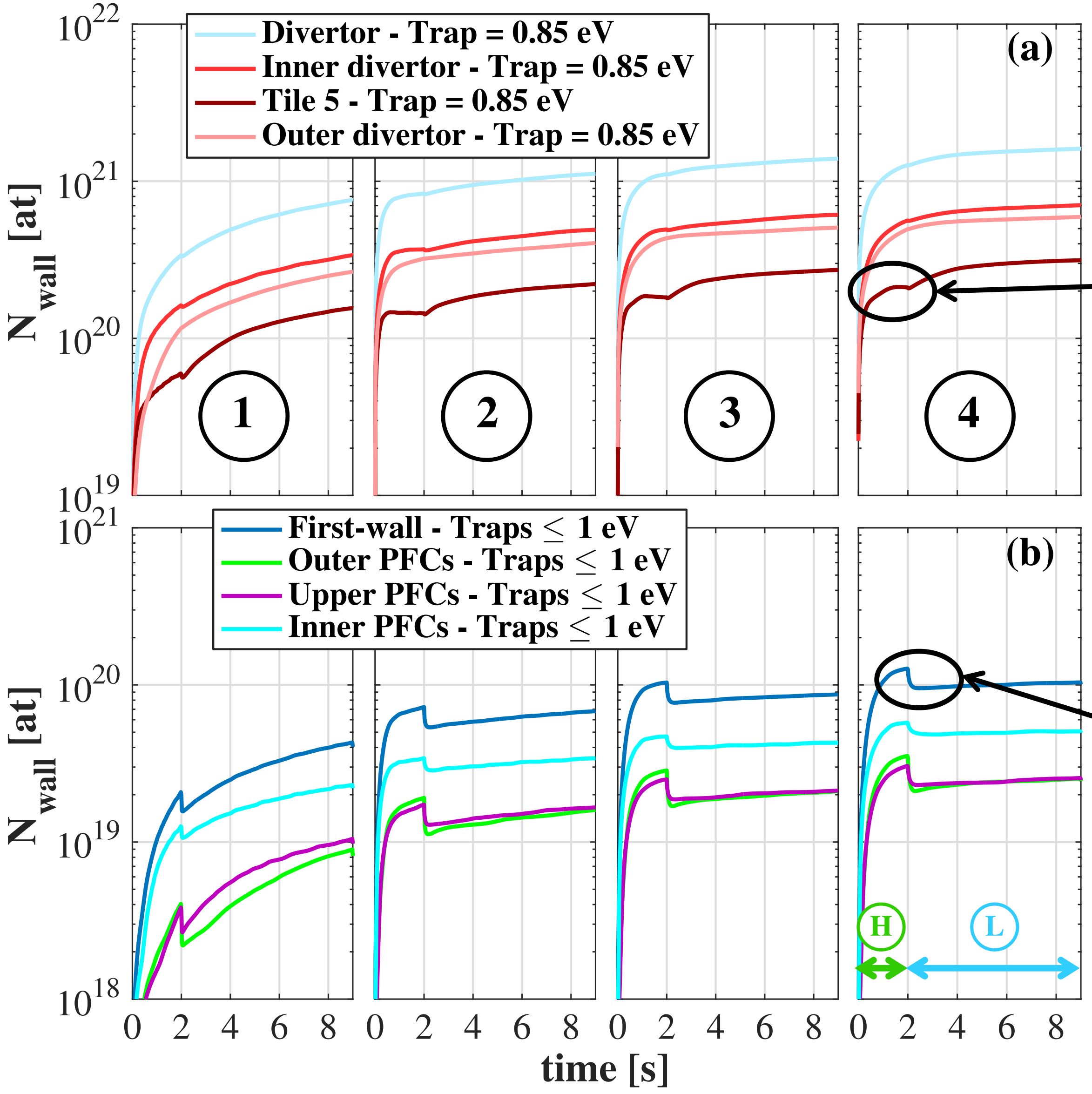
Constant wall temperature $\nu_{\text{dt},i} = constant$	$\nearrow (\Gamma_{\text{imp},j} \,.\, X_{\text{imp},j})$	$\searrow (\Gamma_{\text{imp},j} \,.\, X_{\text{imp},j})$
$\nu_{\text{t,stat}}(\Gamma_{\text{imp},j}, E_{\text{imp},j})$	$\nearrow$	$\searrow$
$f_{\text{stat},i}$	$\nearrow$	$\searrow$
H inventory	$\nearrow$	$\searrow$
Wall dynamics w.r.t. plasma	Pumping	Fuelling



Retention dynamics in low-energy traps during transition H-mode → L-mode



DIVERTOR

H-mode phase:
Decrease in inventory in strike-points tiles

FIRST-WALL

H → L transition:
Decrease in inventory in all first-wall

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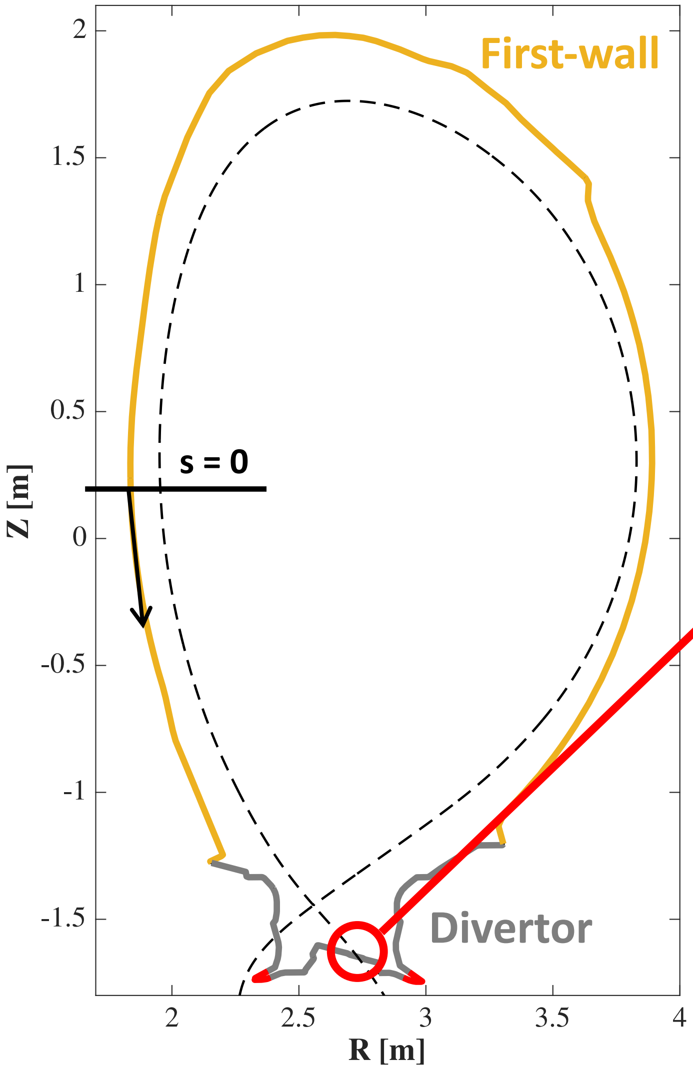
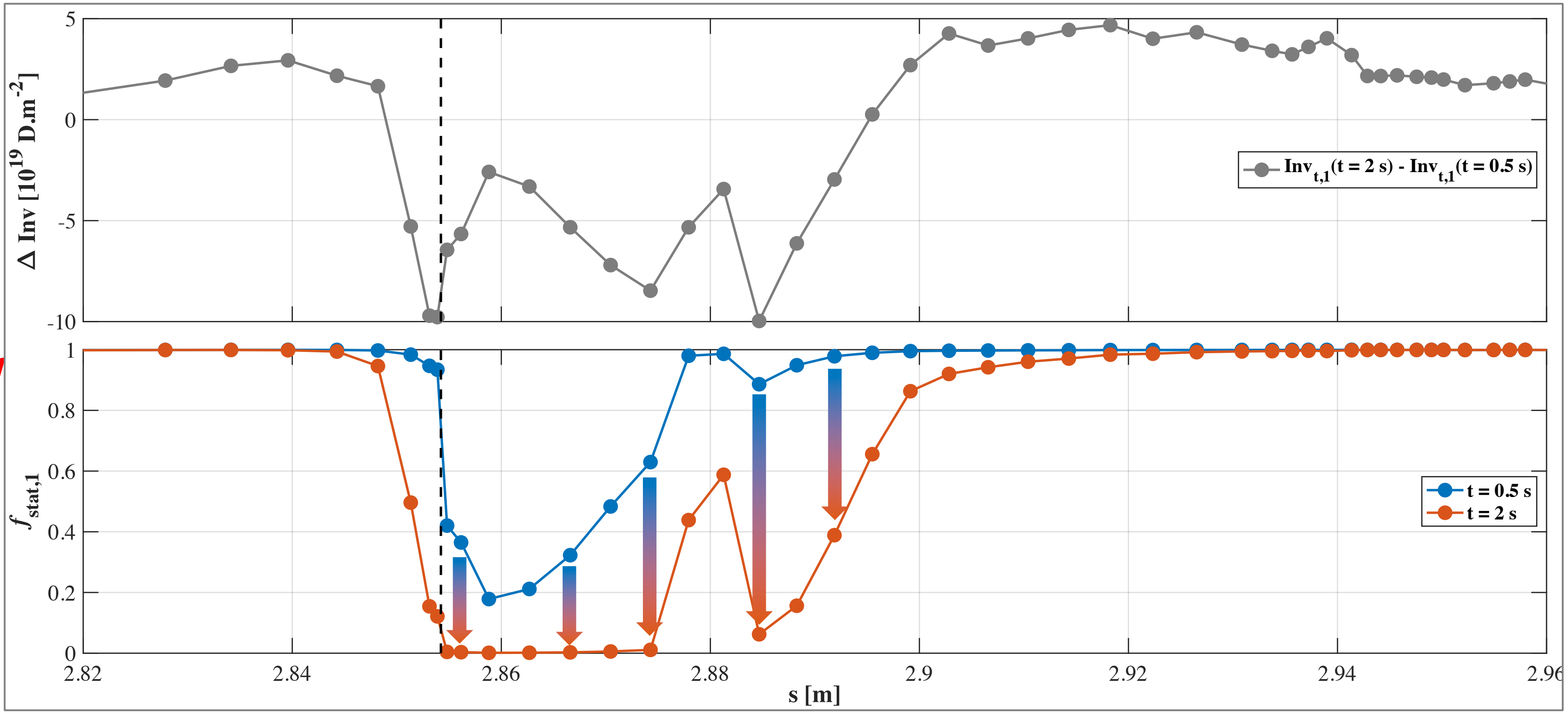
Reduced model as a tool to explain inventory variation during discharges



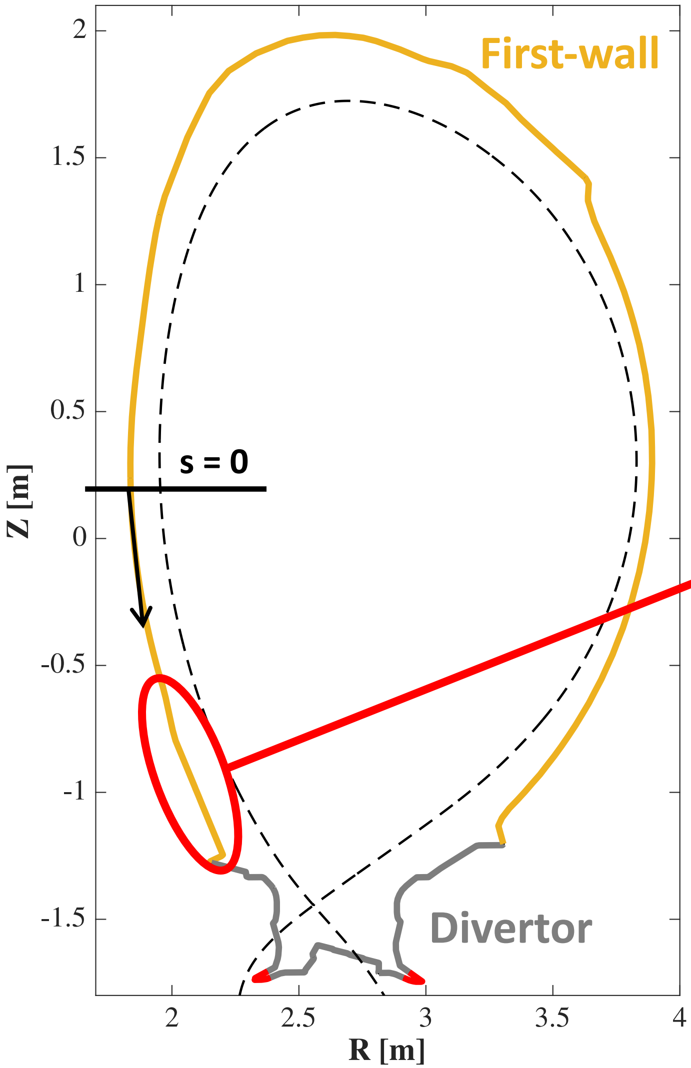
Divertor – outer strike-point

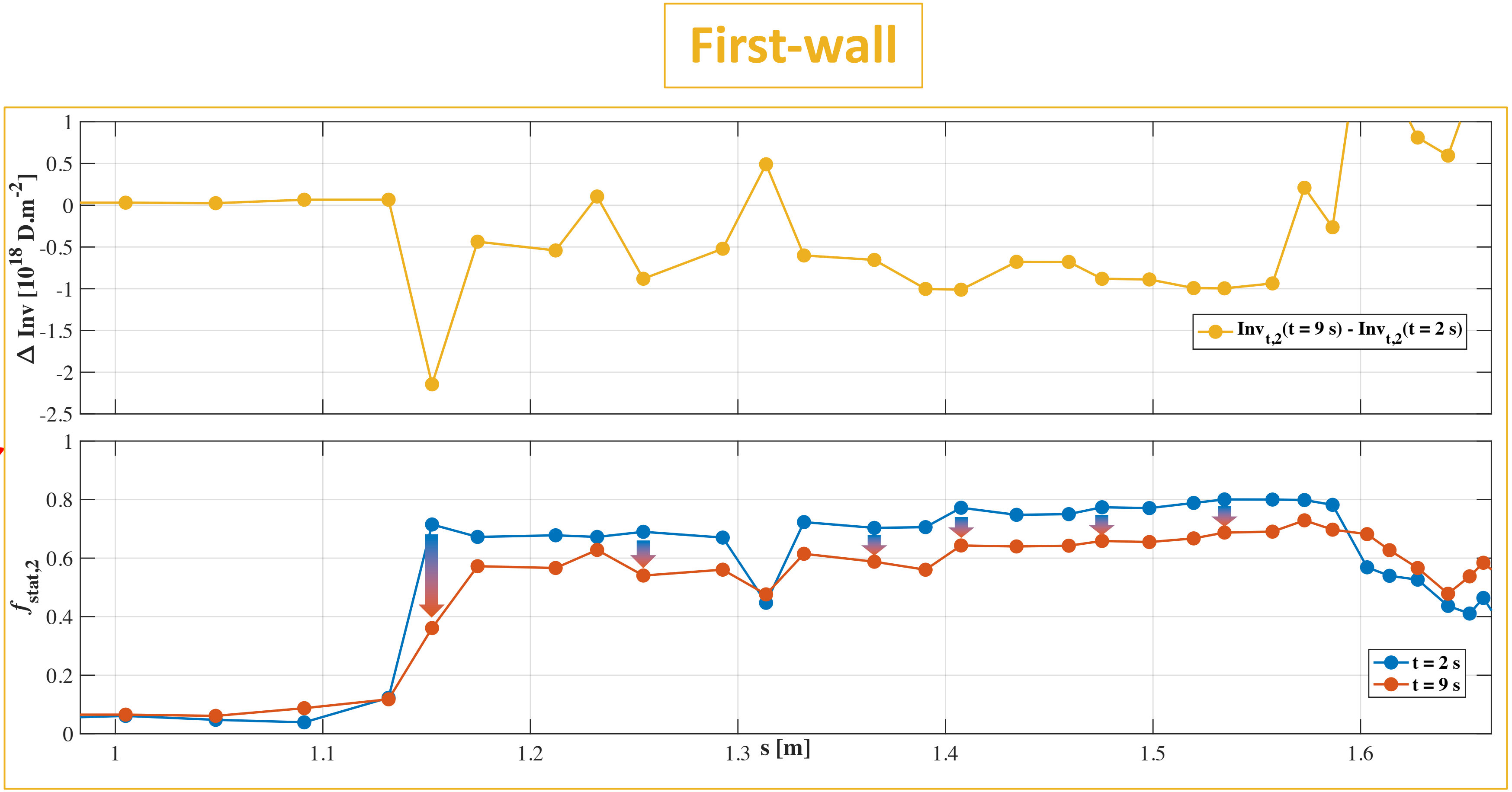


Decrease in inventory due to temperature increase

J. Denis et al., to be submitted

Reduced model as a tool to explain inventory variation during discharges





Decrease in inventory due to decrease in impact energy

J. Denis et al., to be submitted

Outline

1) The Dynamics of Wall Elements (DWE) code
2) Wall initialisation with the DWE code (before coupled plasma-wall simulation)
3) Reduced model for hydrogen retention as a tool for DWE simulation analysis
4) Conclusions