Plasma-neutral interaction processes in ITER from SOLEDGE3X full-vessel boundary plasma simulations

4th Technical Meeting on Divertor Concepts, 7–10 nov. 2022, Vienna

DE LA RECHERCHE À L'INDUSTRIE

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Outline

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- 1. Context and motivation
- 2. Impact of throughput
- 3. Impact of enhanced far-SOL transport (shoulder formation)
- 4. Summary

Key driver of divertor performance: Plasma-Neutral Interact°

Performance of the Divertor…

- Heat flux dissipation
- Pumping efficiency
- Impurity confinement
- Erosion resilience

Key driver: plasma-neutral interactions

… and also of the First Wall:

- FW erosion (CX atoms)
- Impurity plasma contamination
- Main chamber recycling

Plasma-neutral interactions also contribute

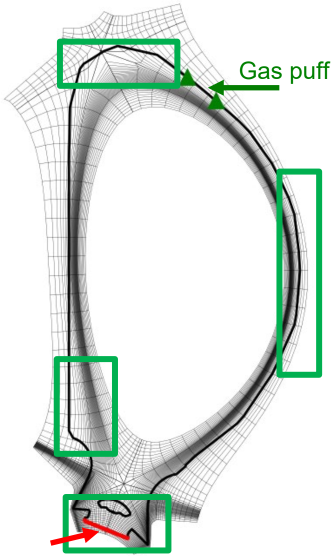
To project divertor solutions to DEMO: better understanding of the details of plasma-neutral interaction processes is needed

This talk focus: Contributions analysis from simulations

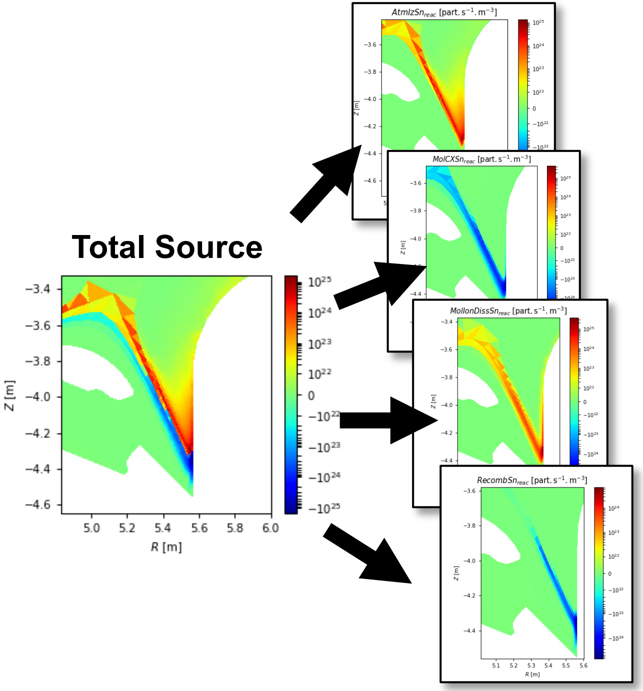
Goal of this talk:

- **From full domain ITER simulations** with **SOLEDGE3X**…
  - Divertor
  - Main chamber & FW
- …**impact analyses of 2 parameters**…
  1. Throughput (also validated against SOLPS-ITER)
  2. Density shoulder formation
- … and first attempts at interpretation through description of involved **plasma-neutral processes** from **new code diagnostics**

SOLEDGE3X domain



New code output with each reaction's contribution to sources



Simulations setup

The SOLEDGE3X code and setup:

See talk by P.Tamain tomorrow

- **SOLEDGE3X:** Fluid multispecies (Zhdanov closure), 3D-turbulent or 2D-mean-field plasma solver coupled to kinetic neutrals from EIRENE or fluid neutrals

[H. Bufferand et al. 2021 Nucl. Fusion 61 116052]

- **Simulation setup:**
  - Based on SOLPS-ITER cases (#103027-#103030) [J.S. Park et al. 2021 Nucl. Fusion 61 016021]
  - 2D-mean-field (transport) mode, prescribed diff. coeffs.
  - **L-mode** transport
  - Pure H
  - **20MW** (PFPO-1)
  - No fluid drifts
  - **Advanced options in EIRENE** (elastic ion col., MAR, neutral-neutral col.)

Sensitivity analyses of 2 parameters:

1. **Throughput**
2. **Formation of shoulders**

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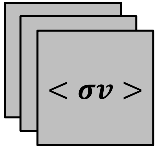
2. Impact of throughput :
Plasma-Neutral Interaction (PNI) model reaction set

Plasma-Neutral Interaction (PNI) **model** (→and so detachement model) driven by **reaction set**



Databases

- AMJUEL
- HYDHEL
- ADAS

Plasma-Neutral Interaction (PNI) model reaction set

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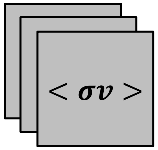
H_2^+ source



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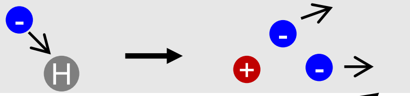
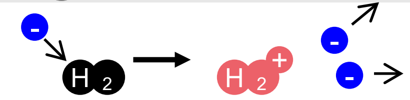
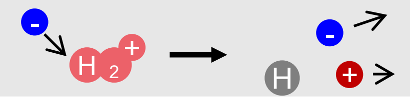
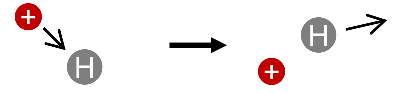
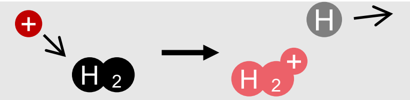
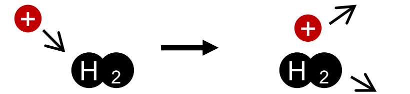
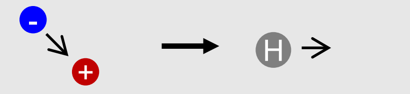
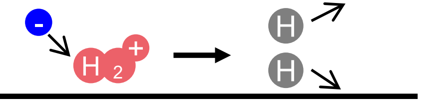
H_2^+ source

Legend:
- H Atom
- H_2 Molecule
- H_2^+ Molecular Ion
- Electron
- H^+ ion

Most important reactions (exerpt from full set):

Name (Abbrev.)	**Reaction**	**Description**
Atom Ionization (AtmIz)	$e^- + H° \rightarrow H^+ + 2e^-$	
Molecule Ionization (MolIz)	$e^- + H_2 \rightarrow H_2^+ + 2e^-$	
Molecular Ion Dissociation (MolIonDiss)	$e^- + H_2^+ \rightarrow H^+ + H° + e^-$	
Atom Charge Exchange (AtmCX)	$H^+ + H° \rightarrow H° + H^+$	
Molecule Charge Exchange (MolCX)	$H^+ + H_2 \rightarrow H_2^+ + H°$	
Ion-Molecule Elastic Collision (MolEL)	$H^+ + H_2 \rightarrow H^+ + H_2$	
Electron-Ion Recombination (Recomb)	$e^- + H^+ \rightarrow H°$	
Molecular Ion Dissociative Recombination (MolIonDissRecomb)	$e^- + H_2^+ \rightarrow 2H°$	

« Molecule-Assisted » Processes involving the H_2^+ molecular ion

XP: [K. Verhaegh et al 2021 Nucl. Fusion 61 106014]

MA-processes: sequence of 2 processes: *1 H_2^+ creation process ➔ 1 H_2^+ break-up process*

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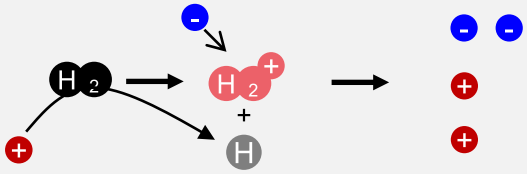
Molecule-Assisted Ionisation (MAI)

Molecule CX → **Molecular Ion Ionisation-Dissociation**



Net ion source = +1

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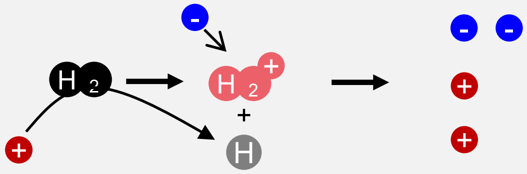

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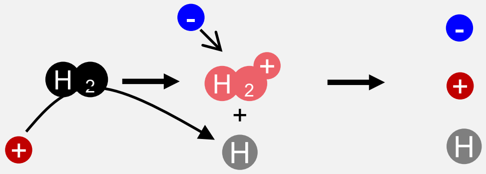
Molecule-Assisted Dissociation (MAD)

Molecule CX → **Molecular Ion Dissociation**



Net ion source = 0
But H° transport!

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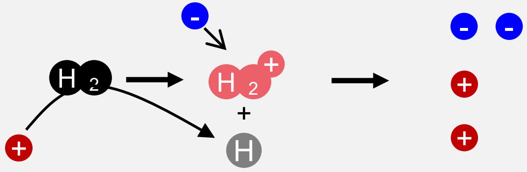
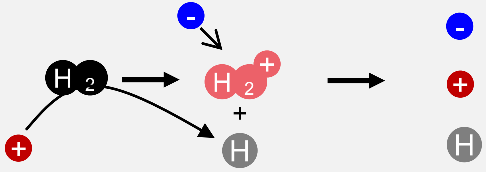


Net ion source = +1

Molecule-Assisted Dissociation (MAD)

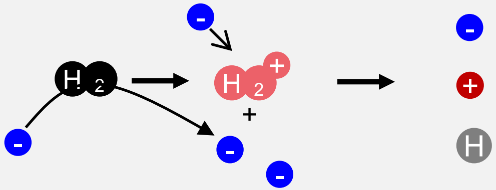
Molecule CX ➔ **Molecular Ion Dissociation**



Net ion source = 0 But H° transport!

Electron-Molecule-Assisted Dissociation (EMAD)

Molecule Ionization ➔ **Molecular Ion Dissociation**



Net ion source = +1

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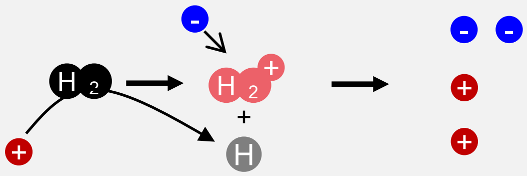
Molecule-Assisted Ionisation (MAI)

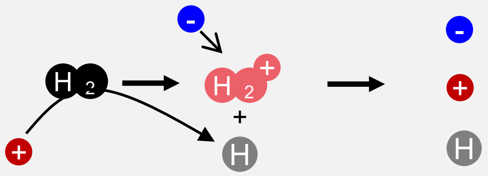
Molecule CX ➔ Molecular Ion Ionisation-Dissociation



Net ion source = +1

Molecule-Assisted Dissociation (MAD)

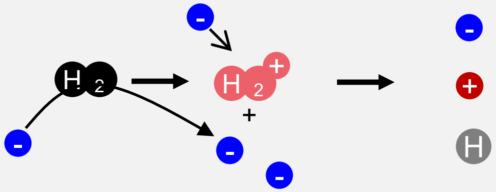
Molecule CX ➔ Molecular Ion Dissociation



Net ion source = 0
But H° transport!

Electron-Molecule-Assisted Dissociation (EMAD)

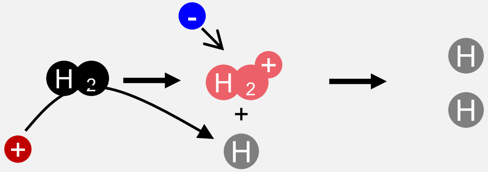
Molecule Ionization ➔ Molecular Ion Dissociation



Net ion source = +1

Molecule-Assisted Recombination (MAR)

Molecule CX ➔ Molecular Ion Dissociative Recombination



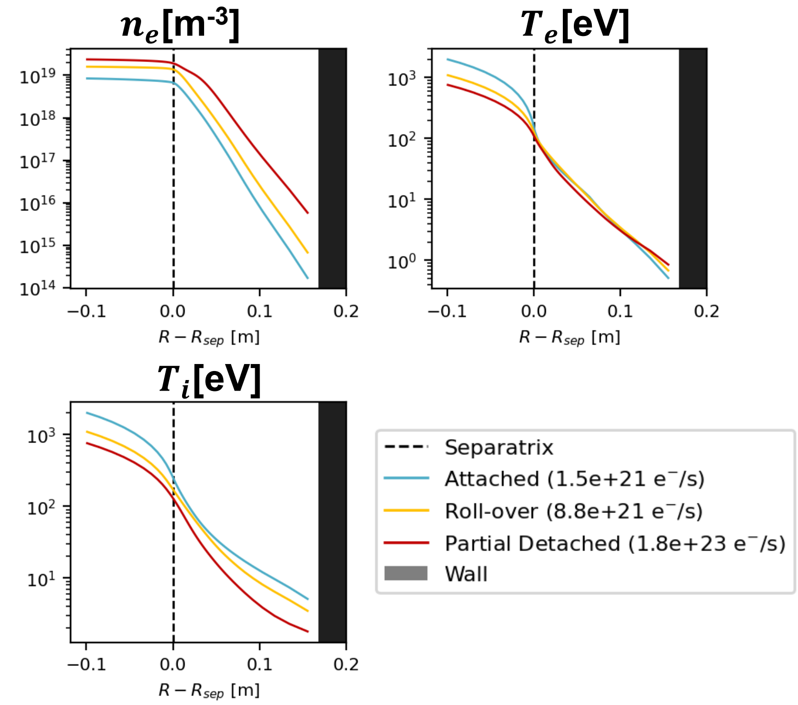
Net ion source = -1

3 representative cases: Attached, Rollover, Partial Detached

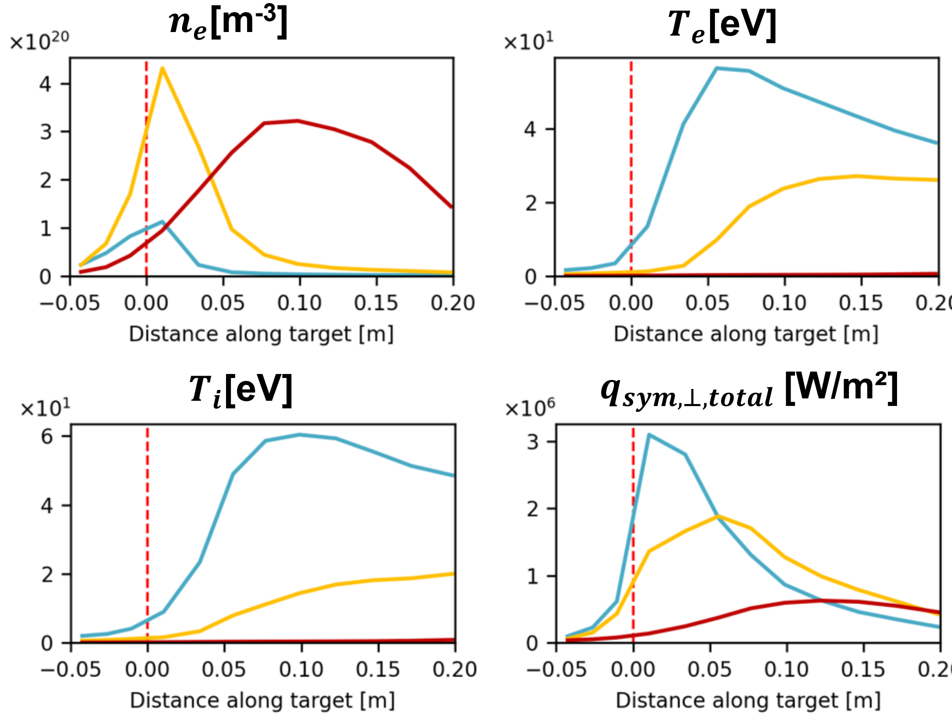
Throughput scan, 3 selected cases for analysis: from attached to partially detached at max throughput

(colors are different throughputs – blue: low → red: high)

Upstream (Outer midplane)

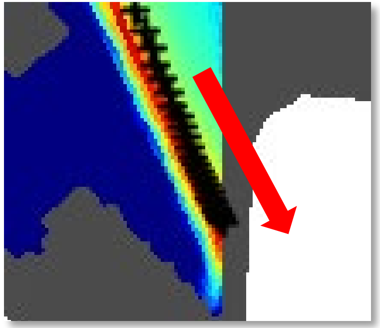


Outer Target



Analysis of cases: 1D field line plot @ Outer Target

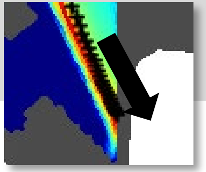
Plot along field line (black)**:**



4 quantities:

1. **Ion Particle Source**
2. **Number of Reactions**
3. **Ion Momentum Source**
4. **Ion Energy Source**
5. **Electron Energy Source**

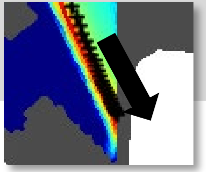
2. Impact of throughput :
Particle source (H^+ ion source)



Volume particle source [$s^{-1}.m^{-3}$]:

(plots include only significant major processes)

Particle source (H^+ ion source)



Volume particle source [$s^{-1}.m^{-3}$]:

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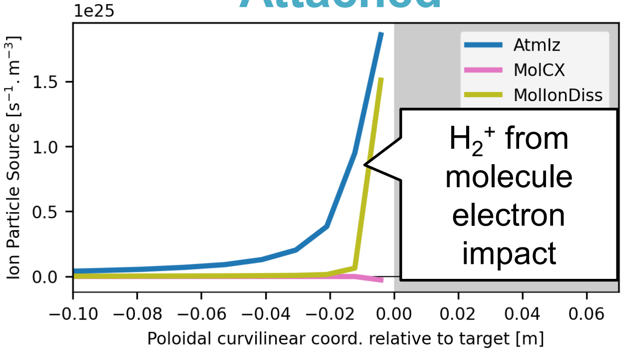
Attached



Dominant processes:

- AtmIz: $e^- + H^\circ \rightarrow H^+ + 2e^-$
- MolIz: $e^- + H_2 \rightarrow H_2^+ + 2e^-$!
- MolIonDiss: $e^- + H_2^+ \rightarrow H^+ + H^\circ + e^-$

EMAD

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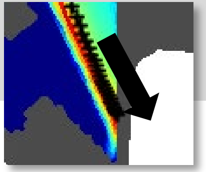

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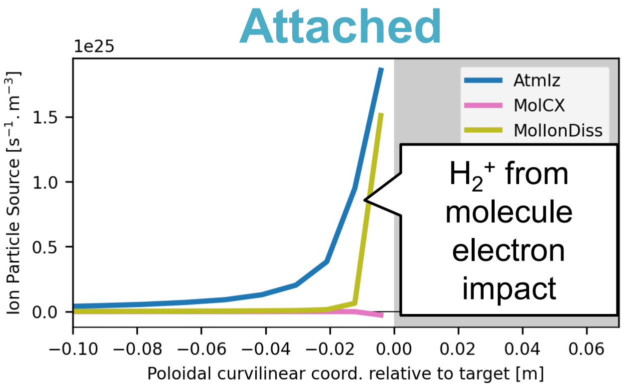

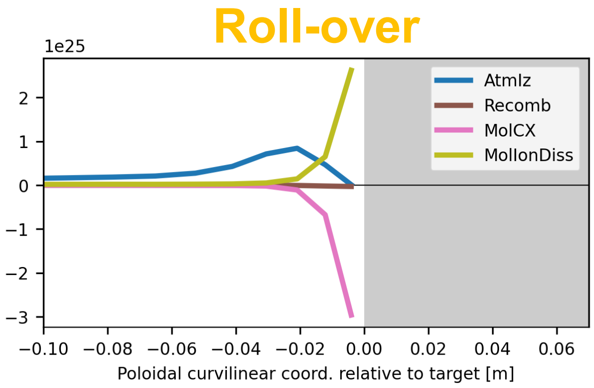

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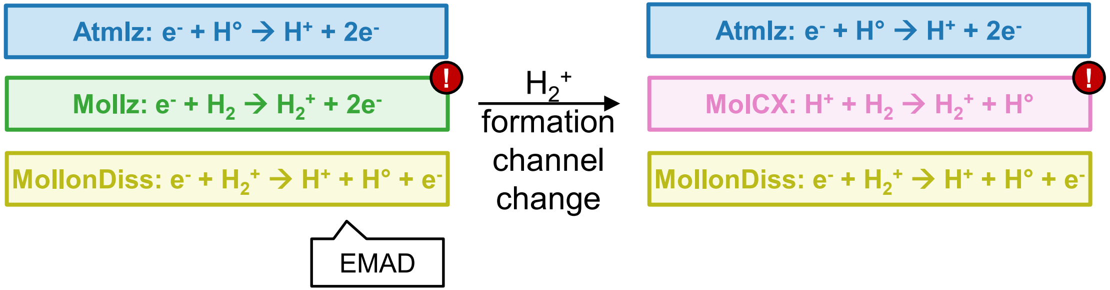
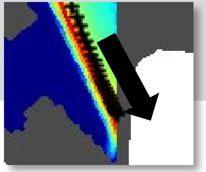


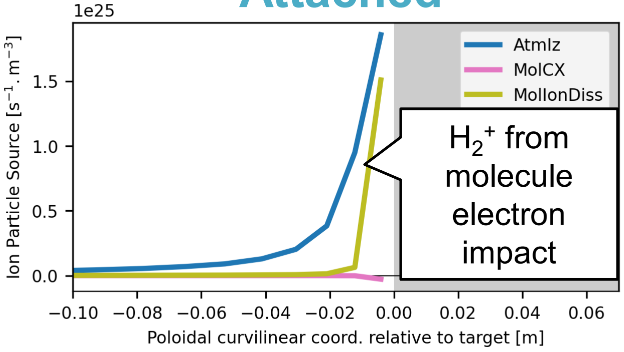
Particle source (H^+ ion source)



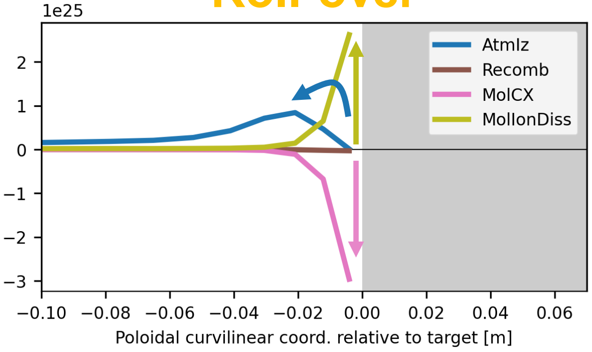
Volume particle source [$s^{-1}.m^{-3}$]:

(plots include only significant major processes)

Attached



Roll-over

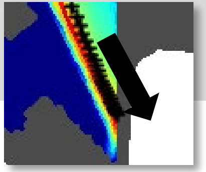


Dominant processes:

Attached		Roll-over
AtmIz: $e^- + H° \rightarrow H^+ + 2e^-$		AtmIz: $e^- + H° \rightarrow H^+ + 2e^-$
! MolIz: $e^- + H_2 \rightarrow H_2^+ + 2e^-$	H_2^+ formation channel change →	! MolCX: $H^+ + H_2 \rightarrow H_2^+ + H°$
MolIonDiss: $e^- + H_2^+ \rightarrow H^+ + H° + e^-$		MolIonDiss: $e^- + H_2^+ \rightarrow H^+ + H° + e^-$

EMAD

Particle source (H^+ ion source)



Volume particle source [$s^{-1}.m^{-3}$]:

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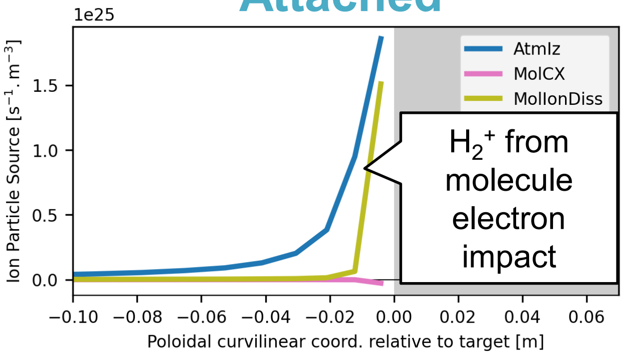

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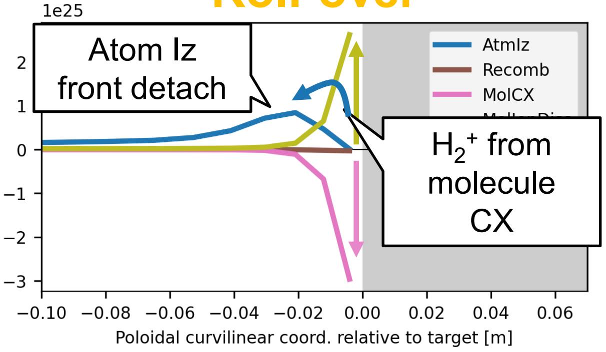

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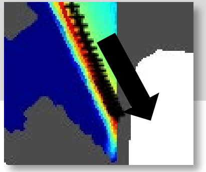
MolIonDiss: $e^- + H_2^+ \rightarrow H^+ + H° + e^-$		MolIonDiss: $e^- + H_2^+ \rightarrow H^+ + H° + e^-$
EMAD		MAD

Particle source (H^+ ion source)



Volume particle source [$s^{-1}.m^{-3}$]:

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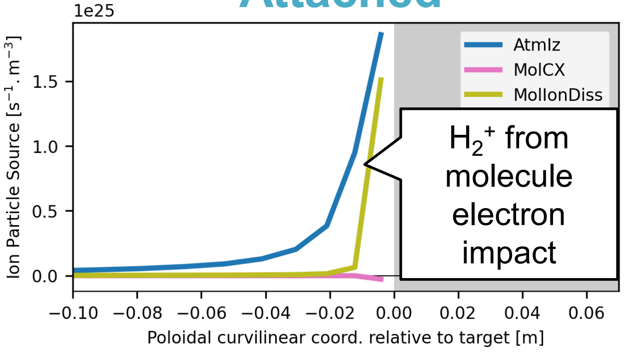
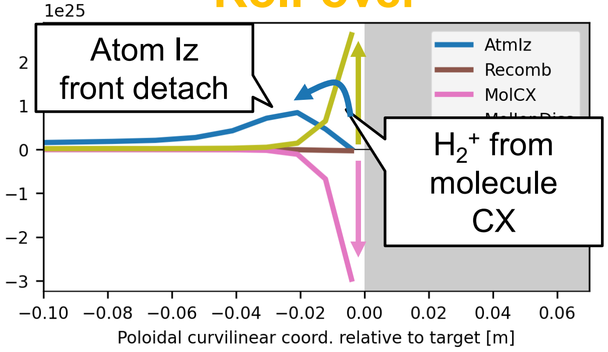
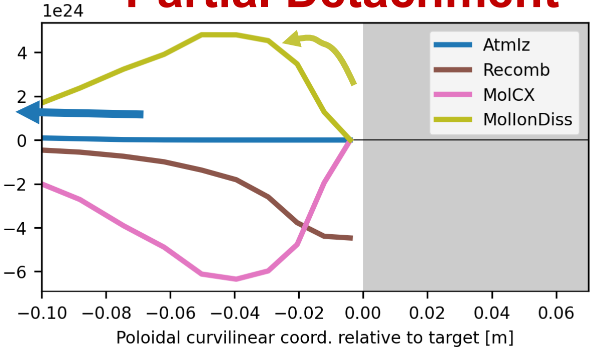
Attached



Roll-over



Partial Detachment



Dominant processes:

Attached:

- AtmIz: $e^- + H° \rightarrow H^+ + 2e^-$
- MolIz: $e^- + H_2 \rightarrow H_2^+ + 2e^-$ (!)
- MolIonDiss: $e^- + H_2^+ \rightarrow H^+ + H° + e^-$

EMAD

H_2^+ formation channel change →

Roll-over:

- AtmIz: $e^- + H° \rightarrow H^+ + 2e^-$
- MolCX: $H^+ + H_2 \rightarrow H_2^+ + H°$ (!)
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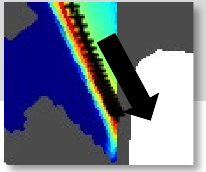
MAD

Partial Detachment:

- AtmIz: $e^- + H° \rightarrow H^+ + 2e^-$
- MolCX: $H^+ + H_2 \rightarrow H_2^+ + H°$
- MolIonDiss: $e^- + H_2^+ \rightarrow H^+ + H° + e^-$
- Recomb: $e^- + H^+ \rightarrow H°$ (!)

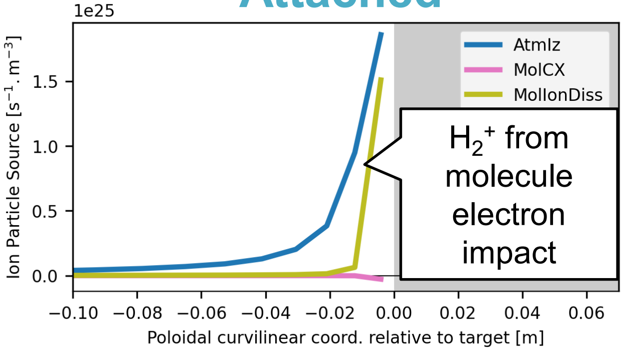
2. Impact of throughput :
Particle source (H^+ ion source)



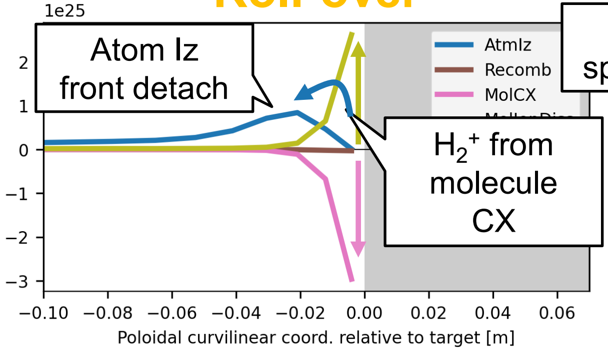
Volume particle source [$s^{-1}.m^{-3}$]:

(plots include only significant major processes)

Attached



Roll-over



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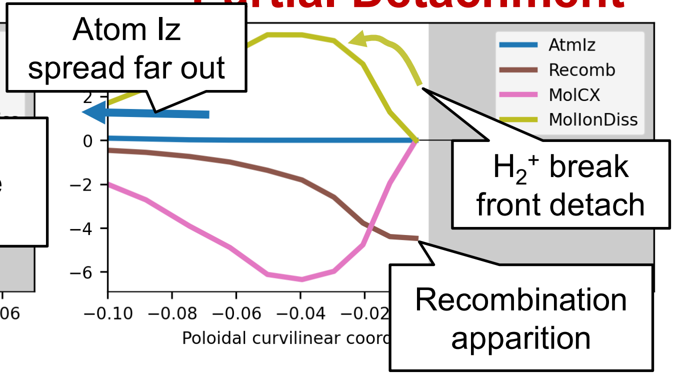

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EMAD

H_2^+ → formation channel change

Roll-over:

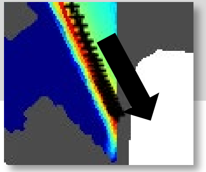
- AtmIz: $e^- + H° \rightarrow H^+ + 2e^-$
- MolCX: $H^+ + H_2 \rightarrow H_2^+ + H°$ (!)
- MolIonDiss: $e^- + H_2^+ \rightarrow H^+ + H° + e^-$

MAD

Partial Detachment:

- AtmIz: $e^- + H° \rightarrow H^+ + 2e^-$
- MolCX: $H^+ + H_2 \rightarrow H_2^+ + H°$
- MolIonDiss: $e^- + H_2^+ \rightarrow H^+ + H° + e^-$
- Recomb: $e^- + H^+ \rightarrow H°$ (!)

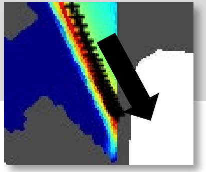
2. Impact of throughput : **Reaction counts**



Volume reaction rates [$s^{-1}.m^{-3}$]:

(plots include only significant major processes)

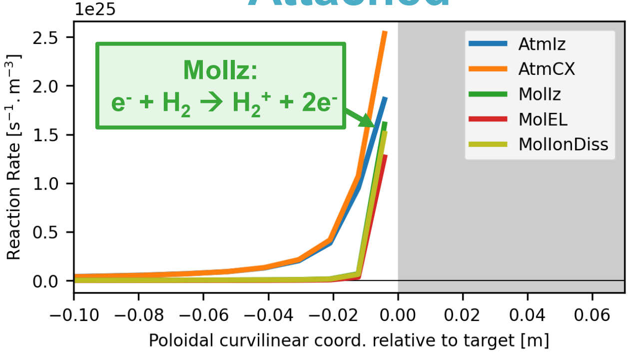
2. Impact of throughput : **Reaction counts**



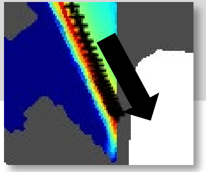
Volume reaction rates [$s^{-1}.m^{-3}$]:

(plots include only significant major processes)

Attached



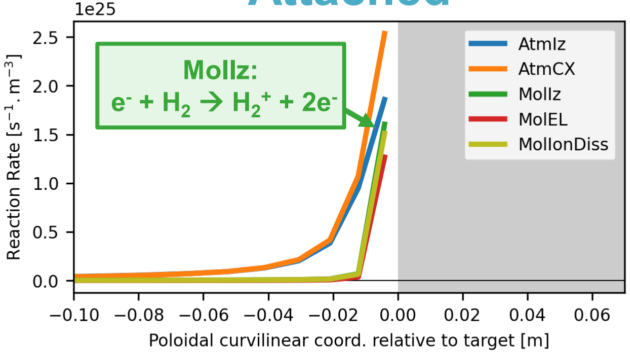
2. Impact of throughput :
Reaction counts



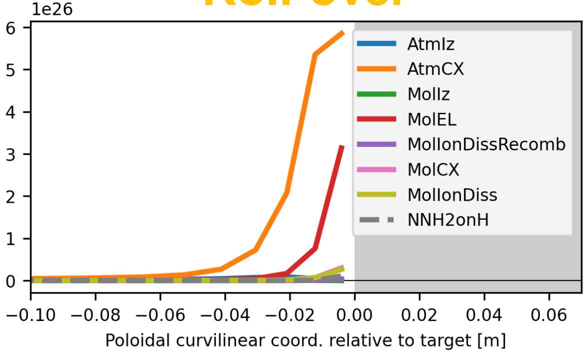
Volume reaction rates [$s^{-1}.m^{-3}$]:

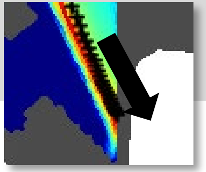
(plots include only significant major processes)

Attached



Roll-over

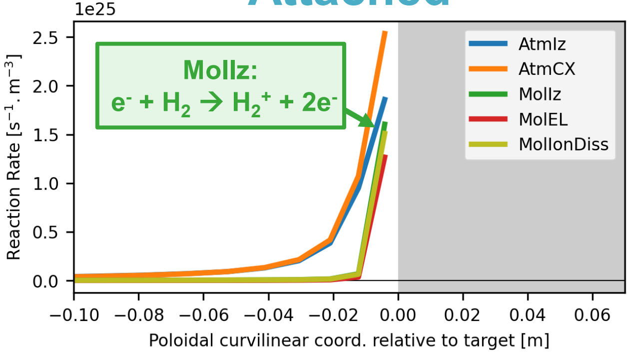




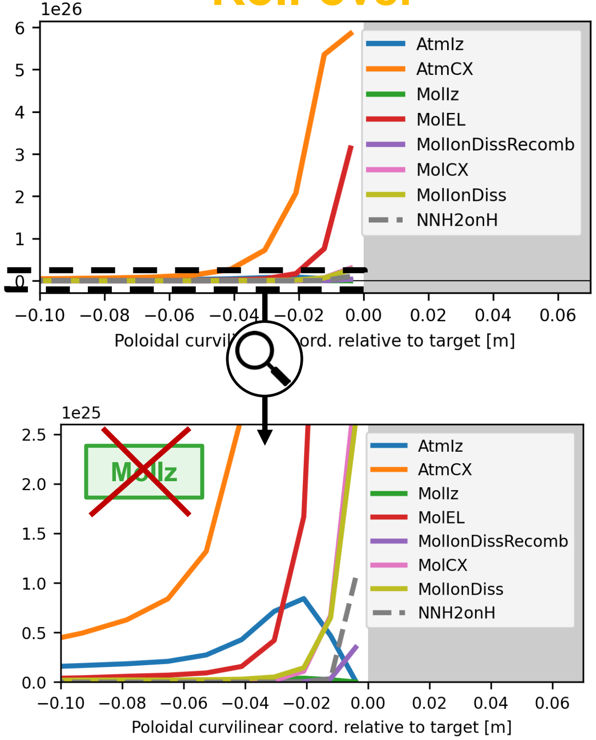
Volume reaction rates [$s^{-1}.m^{-3}$]:

(plots include only significant major processes)

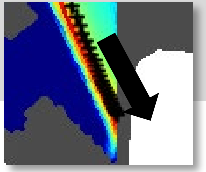
Attached



Roll-over



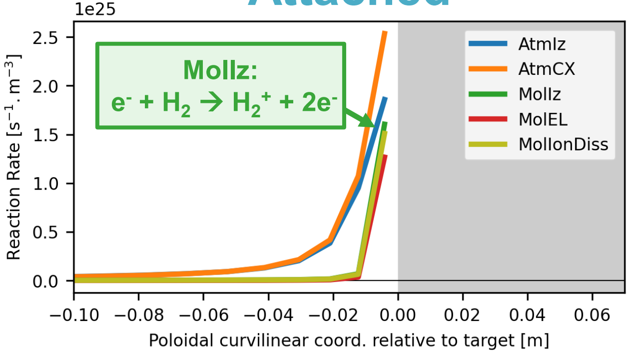
Reaction counts



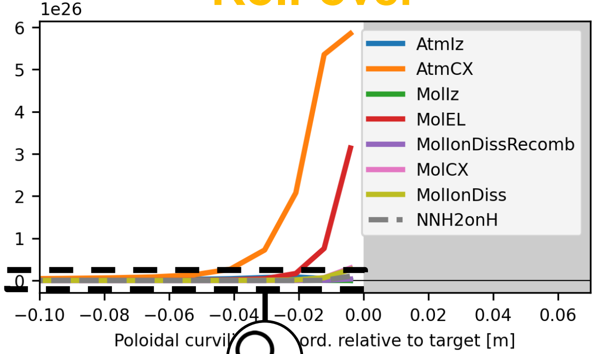
Volume reaction rates [$s^{-1}.m^{-3}$]:

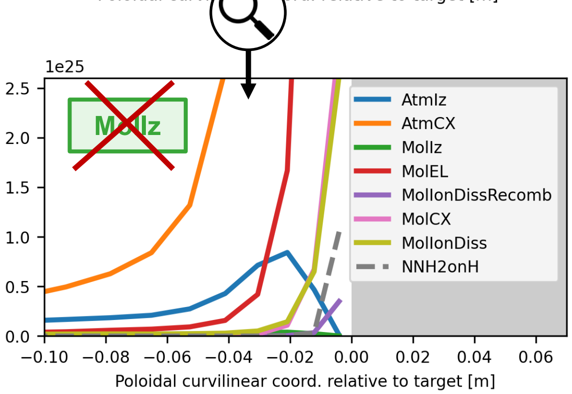
(plots include only significant major processes)

Attached

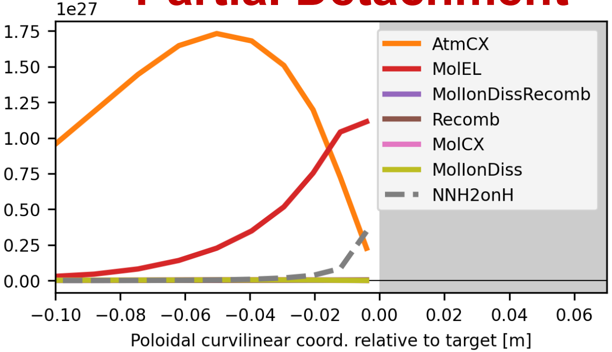


Roll-over

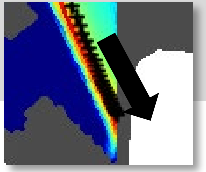




Partial Detachment

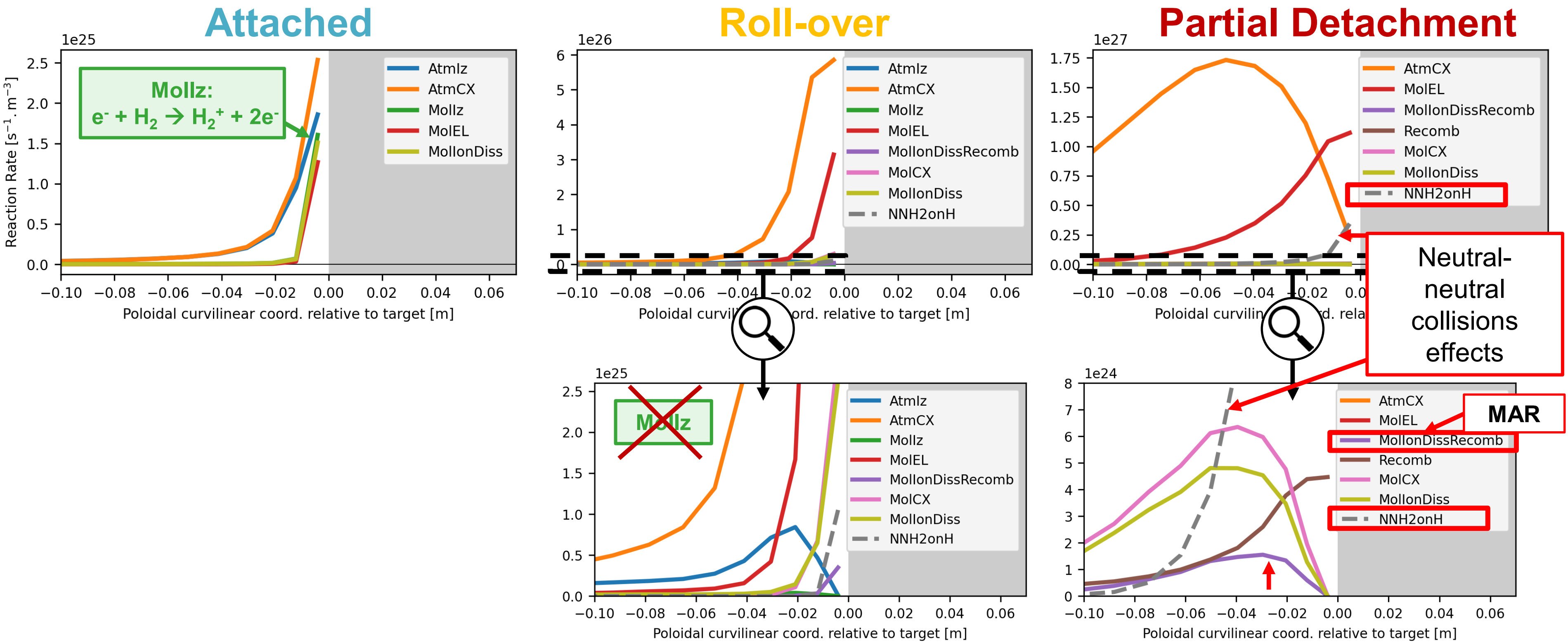


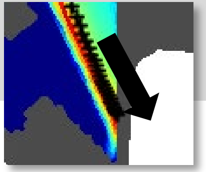
Reaction counts



Volume reaction rates [$s^{-1}.m^{-3}$]:

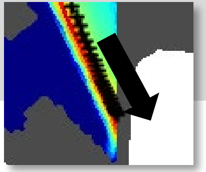
(plots include only significant major processes)





Volume momentum source [kg.s^{-2}.m^{-2}]:

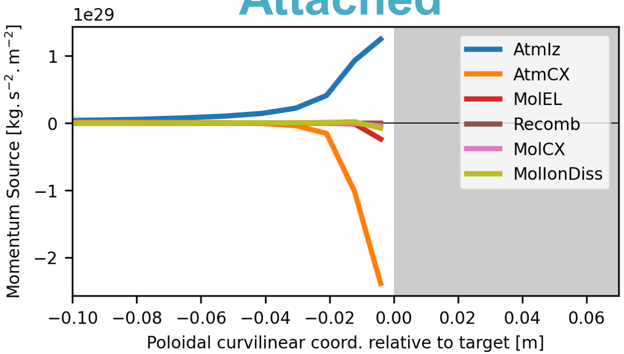
(plots include only significant major processes)



Volume momentum source [kg.s^{-2}.m^{-2}]:

(plots include only significant major processes)

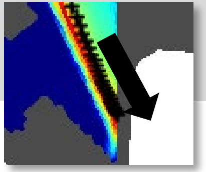
Attached



Dominant processes:

AtmCX: $H^+ + H^\circ \rightarrow H^\circ + H^+$

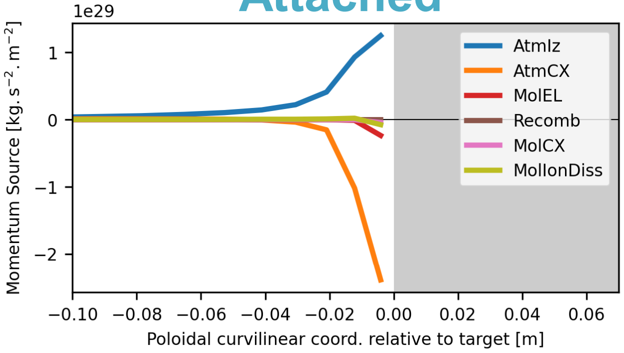
Momentum sources



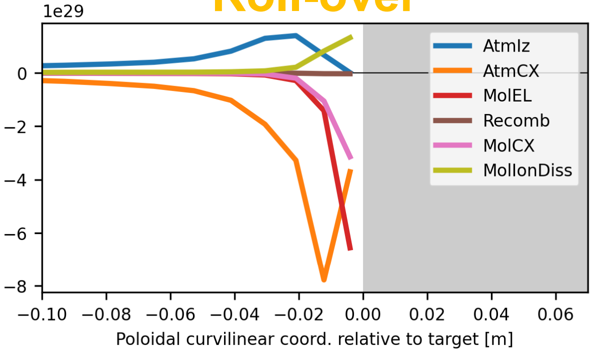
Volume momentum source [kg.s^{-2}.m^{-2}]:

(plots include only significant major processes)

Attached



Roll-over



Dominant processes:

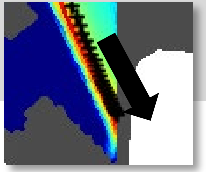
AtmCX: $H^+ + H^\circ \rightarrow H^\circ + H^+$

Roll-over:

AtmCX: $H^+ + H^\circ \rightarrow H^\circ + H^+$

MolElastic: $H^+ + H_2 \rightarrow H^+ + H_2$!

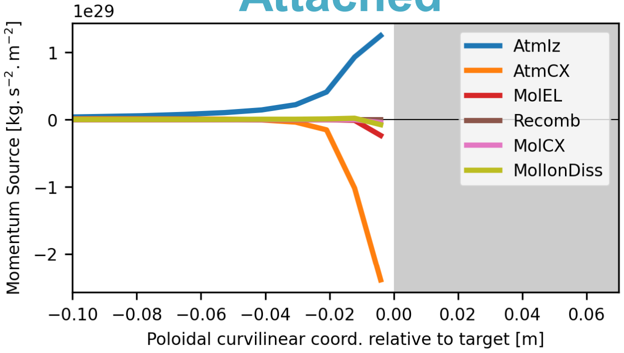
Momentum sources



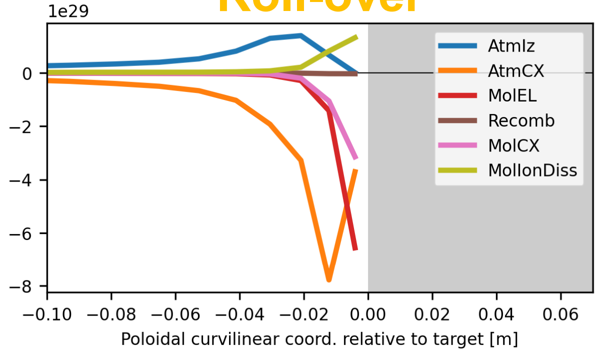
Volume momentum source [kg.s^{-2}.m^{-2}]:

(plots include only significant major processes)

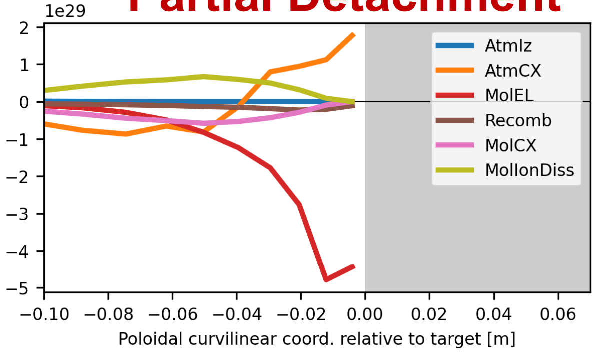
Attached



Roll-over



Partial Detachment



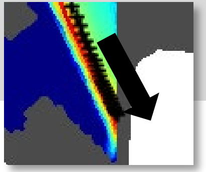
Dominant processes:

Attached:
- AtmCX: $H^+ + H° \rightarrow H° + H^+$

Roll-over:
- AtmCX: $H^+ + H° \rightarrow H° + H^+$
- MolElastic: $H^+ + H_2 \rightarrow H^+ + H_2$!

Partial Detachment:
- AtmCX: $H^+ + H° \rightarrow H° + H^+$!
- MolElastic: $H^+ + H_2 \rightarrow H^+ + H_2$

Momentum sources

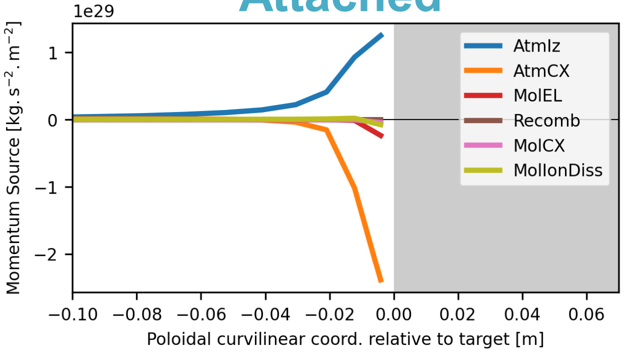


Volume momentum source [kg.s^{-2}.m^{-2}]:

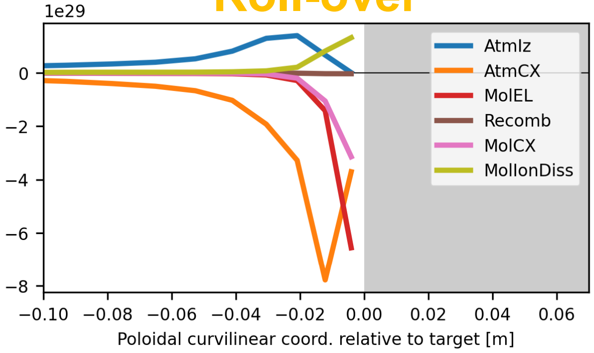
(plots include only significant major processes)

Atom CX source near Tgt

Attached



Roll-over



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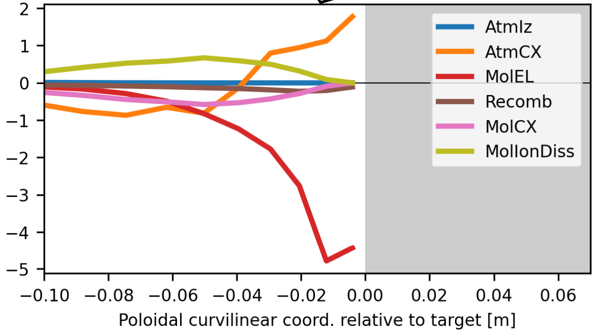


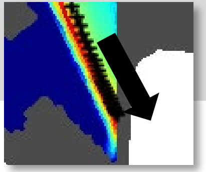
Dominant processes:

Attached:
- AtmCX: $H^+ + H° \rightarrow H° + H^+$

Roll-over:
- AtmCX: $H^+ + H° \rightarrow H° + H^+$
- MolElastic: $H^+ + H_2 \rightarrow H^+ + H_2$!

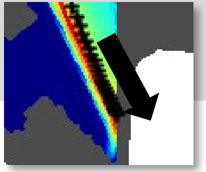
Partial Detachment:
- AtmCX: $H^+ + H° \rightarrow H° + H^+$!
- MolElastic: $H^+ + H_2 \rightarrow H^+ + H_2$

2. Impact of throughput : **Ion energy sources**



Volume ion energy source [W.m^{-3}]:

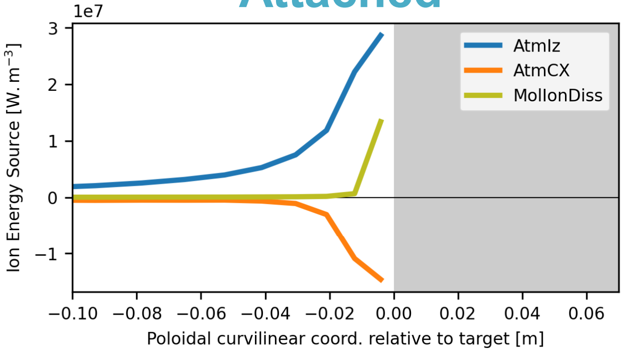
(plots include only significant major processes)



Volume ion energy source [W.m^{-3}]:

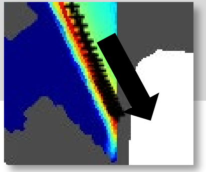
(plots include only significant major processes)

Attached



Dominant processes:

AtmCX: $H^+ + H° \rightarrow H° + H^+$



Volume ion energy source [W.m^{-3}]:

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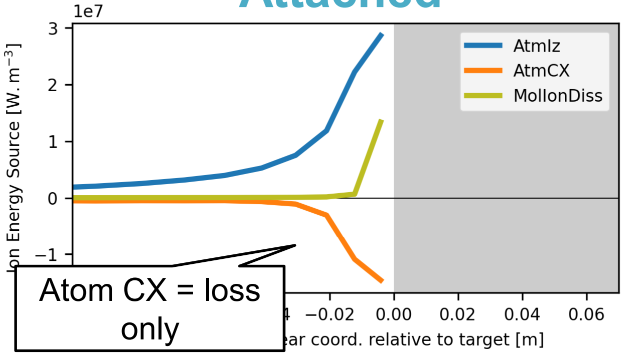
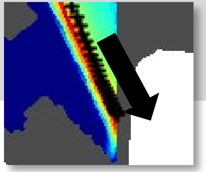


Dominant processes:

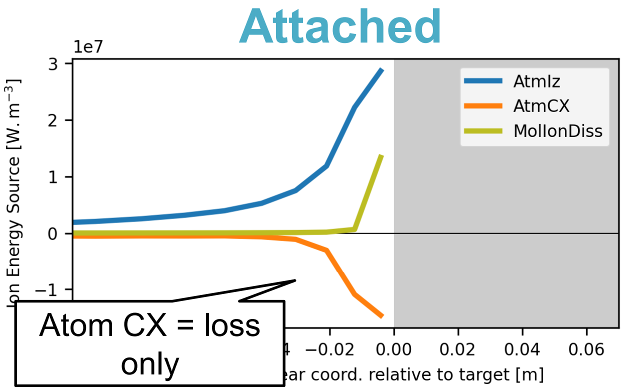
AtmCX: $H^+ + H° \rightarrow H° + H^+$

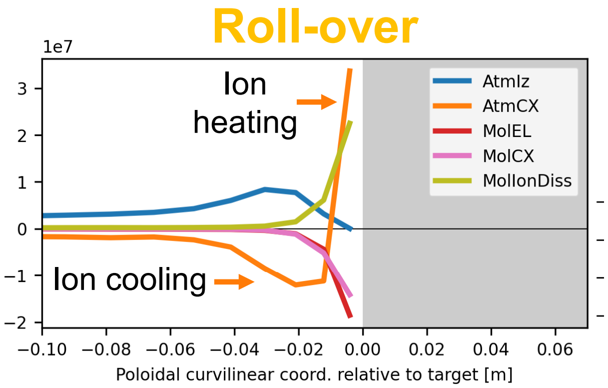
Ion energy sources



Volume ion energy source [W.m^{-3}]:

(plots include only significant major processes)





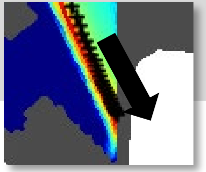
Dominant processes:

AtmCX: $H^+ + H^\circ \rightarrow H^\circ + H^+$

! **AtmCX: $H^+ + H^\circ \rightarrow H^\circ + H^+$**

! **MolElastic: $H^+ + H_2 \rightarrow H^+ + H_2$**

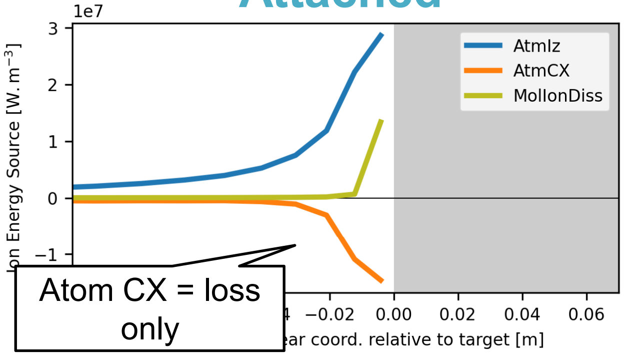
2. Impact of throughput :
Ion energy sources



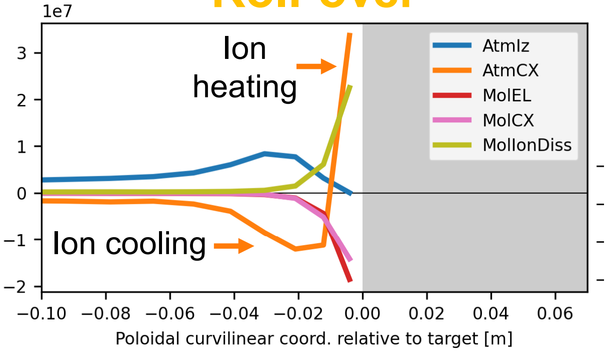
Volume ion energy source [W.m^{-3}]:
(plots include only significant major processes)

Atom CX now source at target (reheating/diffusion)

Attached



Roll-over



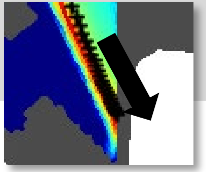
Dominant processes:

AtmCX: $H^+ + H° \rightarrow H° + H^+$

AtmCX: $H^+ + H° \rightarrow H° + H^+$!

MolElastic: $H^+ + H_2 \rightarrow H^+ + H_2$!

Ion energy sources

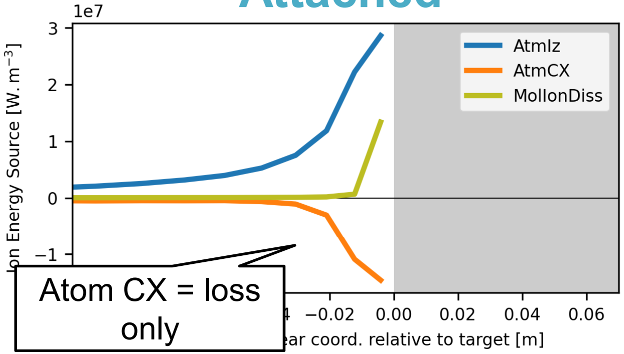


Volume ion energy source [W.m^{-3}]:

(plots include only significant major processes)

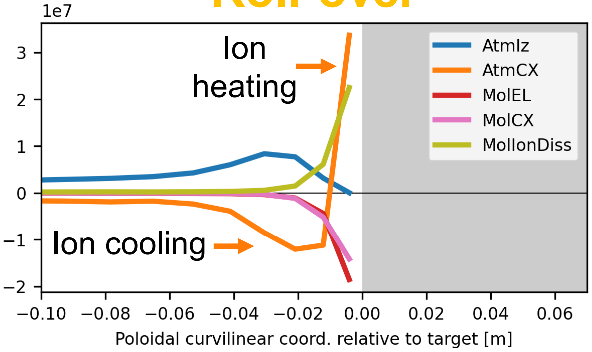
Atom CX now source at target (reheating/diffusion)

Attached

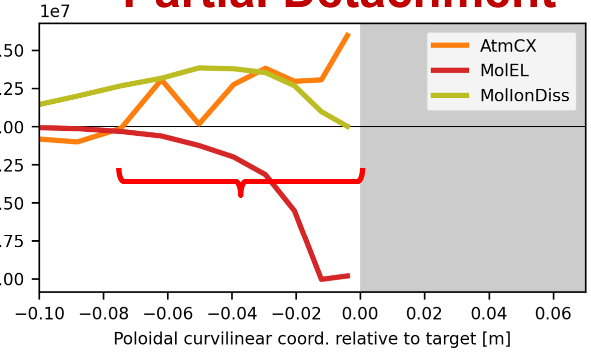


Atom CX = loss only

Roll-over



Partial Detachment



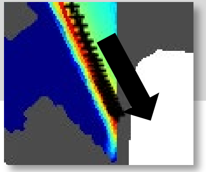
Dominant processes:

Attached:
- AtmCX: $H^+ + H° \rightarrow H° + H^+$

Roll-over:
- AtmCX: $H^+ + H° \rightarrow H° + H^+$!
- MolElastic: $H^+ + H_2 \rightarrow H^+ + H_2$!

Partial Detachment:
- AtmCX: $H^+ + H° \rightarrow H° + H^+$
- MolElastic: $H^+ + H_2 \rightarrow H^+ + H_2$

Ion energy sources

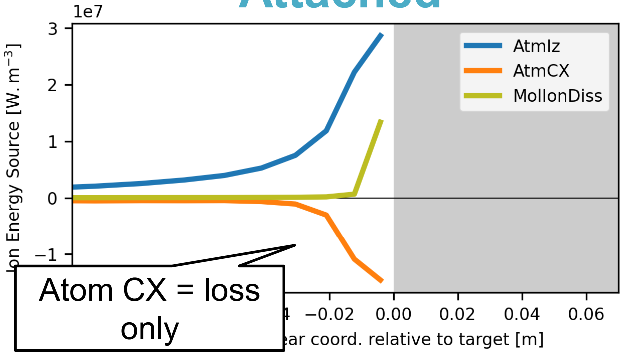


Volume ion energy source [W.m^{-3}]:

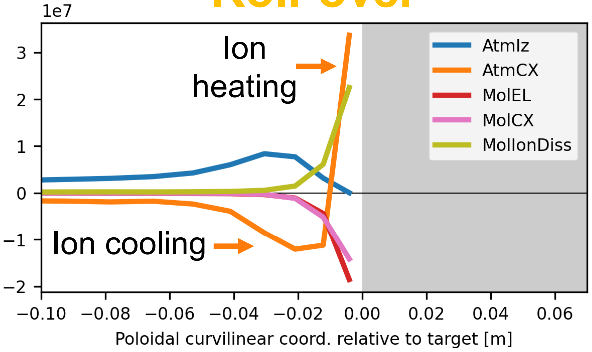
(plots include only significant major processes)

Atom CX now source at target (reheating/diffusion)

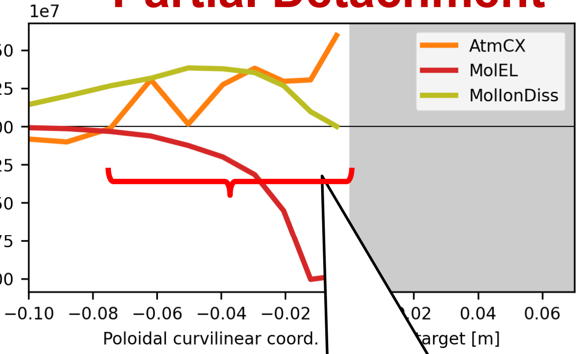
Attached



Roll-over



Partial Detachment

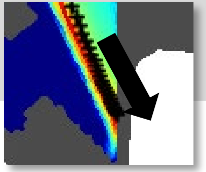


Wide Atom CX positive source in whole region near target

Dominant processes:

Attached	Roll-over	Partial Detachment
AtmCX: $H^+ + H° \rightarrow H° + H^+$	AtmCX: $H^+ + H° \rightarrow H° + H^+$!	AtmCX: $H^+ + H° \rightarrow H° + H^+$
	MolElastic: $H^+ + H_2 \rightarrow H^+ + H_2$!	MolElastic: $H^+ + H_2 \rightarrow H^+ + H_2$

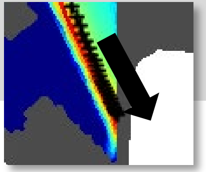
2. Impact of throughput : **Electron energy sources**



Volume electron energy source [W.m^{-3}]:

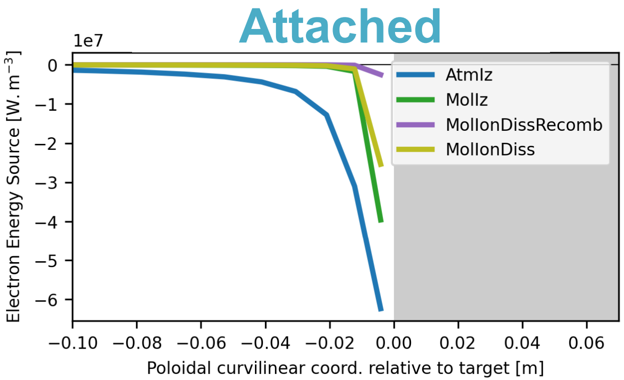
(plots include only significant major processes)

Electron energy sources



Volume electron energy source [W.m^{-3}]:

(plots include only significant major processes)



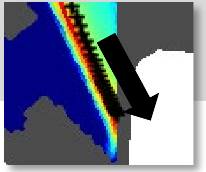
Dominant processes:

AtmIz: $e^- + H° \rightarrow H^+ + 2e^-$

MolIz: $e^- + H_2 \rightarrow H_2^+ + 2e^-$

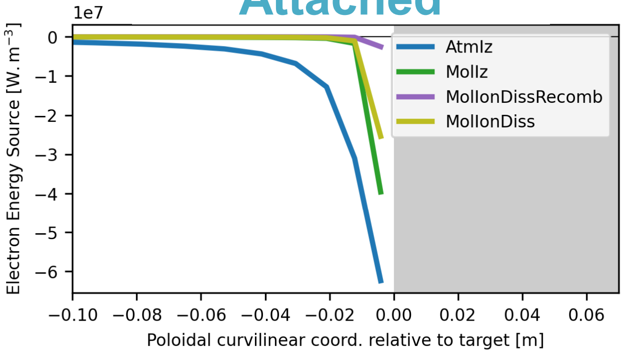
MolIonDiss: $e^- + H_2^+ \rightarrow H^+ + H° + e^-$

2. Impact of throughput :
Electron energy sources

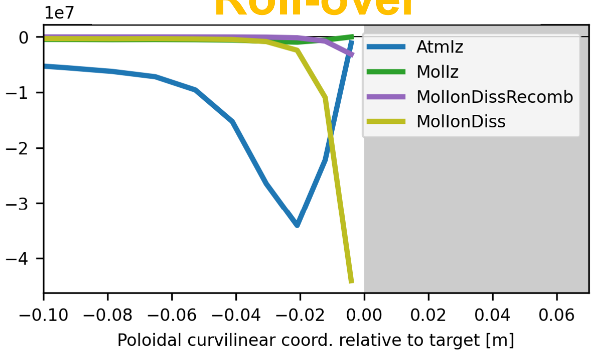


Volume electron energy source [W.m^{-3}]:
(plots include only significant major processes)

Attached



Roll-over



Dominant processes:

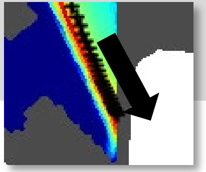
Attached:

- **AtmIz: $e^- + H° \rightarrow H^+ + 2e^-$**
- **MolIz: $e^- + H_2 \rightarrow H_2^+ + 2e^-$**
- **MolIonDiss: $e^- + H_2^+ \rightarrow H^+ + H° + e^-$**

Roll-over:

- **AtmIz: $e^- + H° \rightarrow H^+ + 2e^-$**
- *MolCX: energy taken from the ions*
- **MolIonDiss: $e^- + H_2^+ \rightarrow H^+ + H° + e^-$**

Electron energy sources



Volume electron energy source [W.m^{-3}]:

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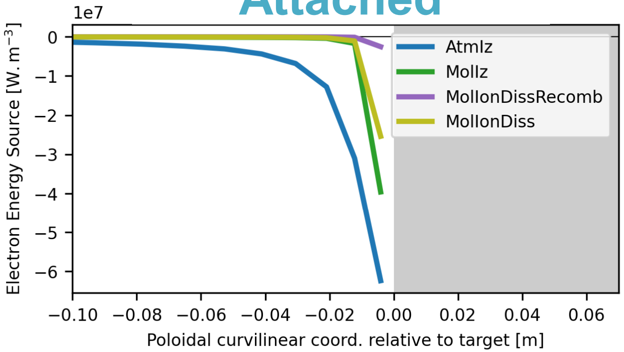
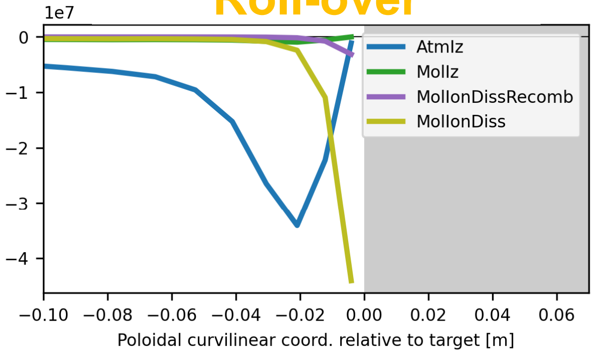
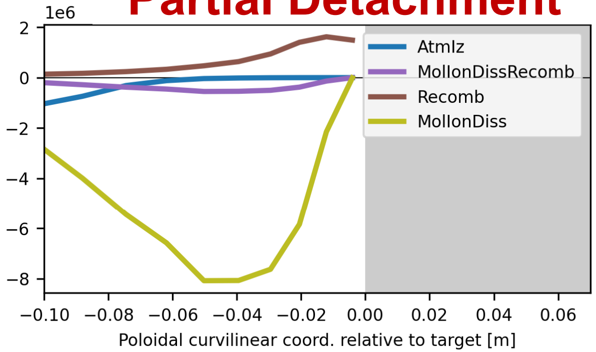
Attached



Roll-over



Partial Detachment



Dominant processes:

Attached:

- AtmIz: $e^- + H° \rightarrow H^+ + 2e^-$
- MolIz: $e^- + H_2 \rightarrow H_2^+ + 2e^-$
- MolIonDiss: $e^- + H_2^+ \rightarrow H^+ + H° + e^-$

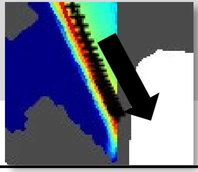
Roll-over:

- AtmIz: $e^- + H° \rightarrow H^+ + 2e^-$
- *MolCX: energy taken from the ions*
- MolIonDiss: $e^- + H_2^+ \rightarrow H^+ + H° + e^-$

Partial Detachment:

- AtmIz: $e^- + H° \rightarrow H^+ + 2e^-$
- MolIonDiss: $e^- + H_2^+ \rightarrow H^+ + H° + e^-$
- MolIonDissRc: $H_2^+ + e^- \rightarrow 2\ H°$!
- Recomb: $e^- + H^+ \rightarrow H°$!

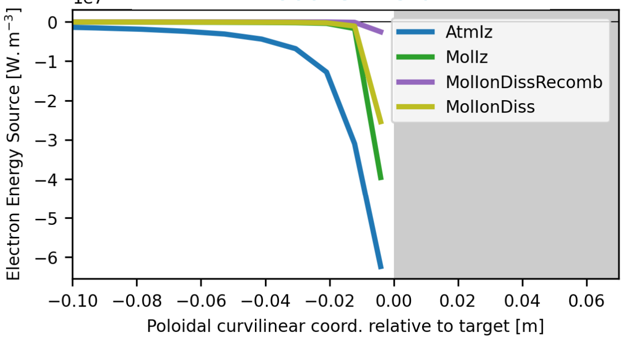
2. Impact of throughput :
Electron energy sources



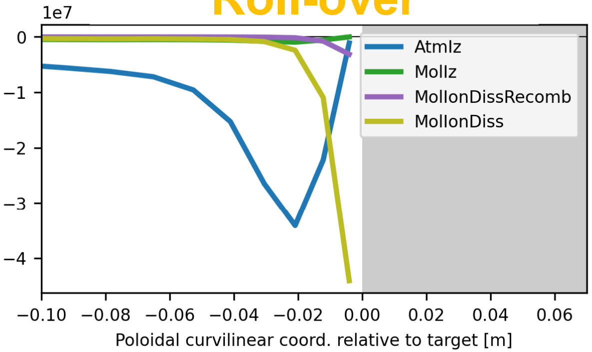
Volume electron energy source [W.m^{-3}]:
(plots include only significant major processes)

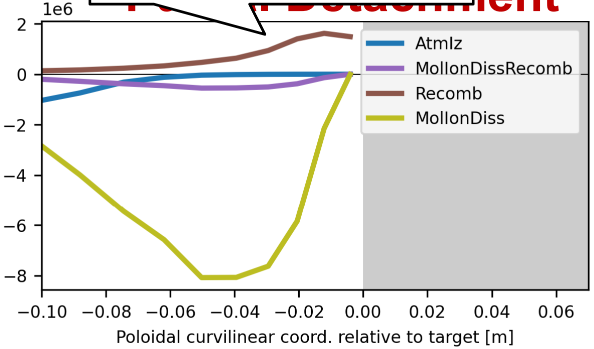
3-body recombination = electron heating at low T

Attached



Roll-over





Dominant processes:

AtmIz: $e^- + H° \rightarrow H^+ + 2e^-$

MolIz: $e^- + H_2 \rightarrow H_2^+ + 2e^-$

MolIonDiss: $e^- + H_2^+ \rightarrow H^+ + H° + e^-$

AtmIz: $e^- + H° \rightarrow H^+ + 2e^-$

MolCX: energy taken from the ions

MolIonDiss: $e^- + H_2^+ \rightarrow H^+ + H° + e^-$

AtmIz: $e^- + H° \rightarrow H^+ + 2e^-$

MolIonDiss: $e^- + H_2^+ \rightarrow H^+ + H° + e^-$

MolIonDissRc: $H_2^+ + e^- \rightarrow 2 H°$!

Recomb: $e^- + H^+ \rightarrow H°$!

Qualitative picture of processes evolution during detachment

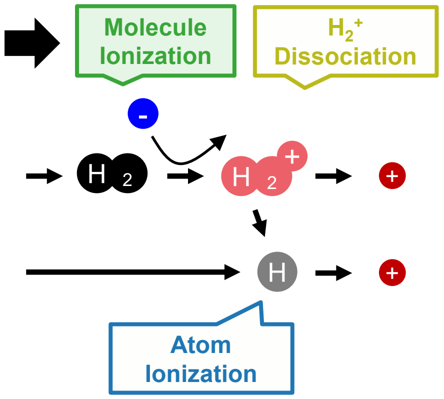
Particle source

Mom. & Energy sources

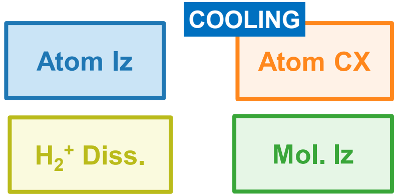
2. Impact of throughput : Qualitative picture of processes evolution during detachment

Attached

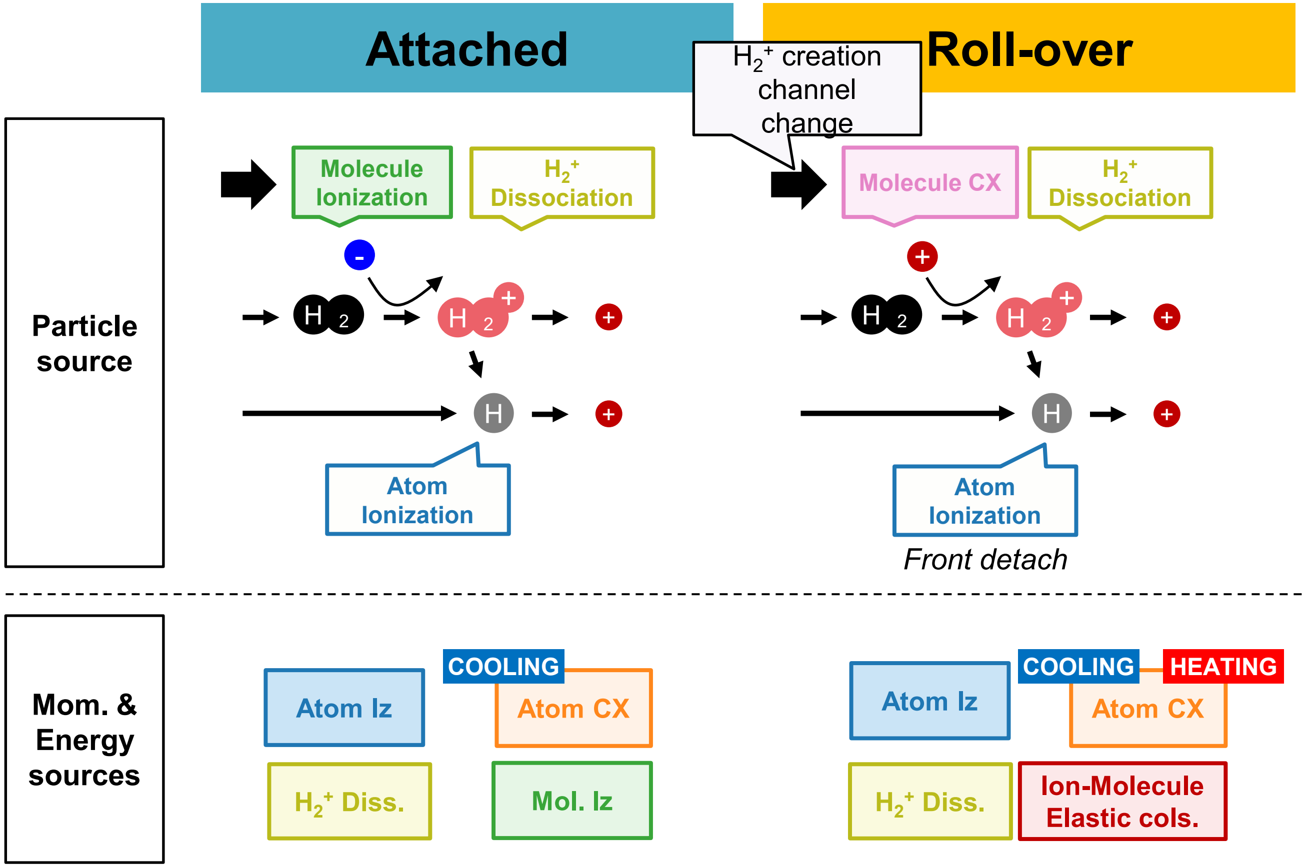
Particle source



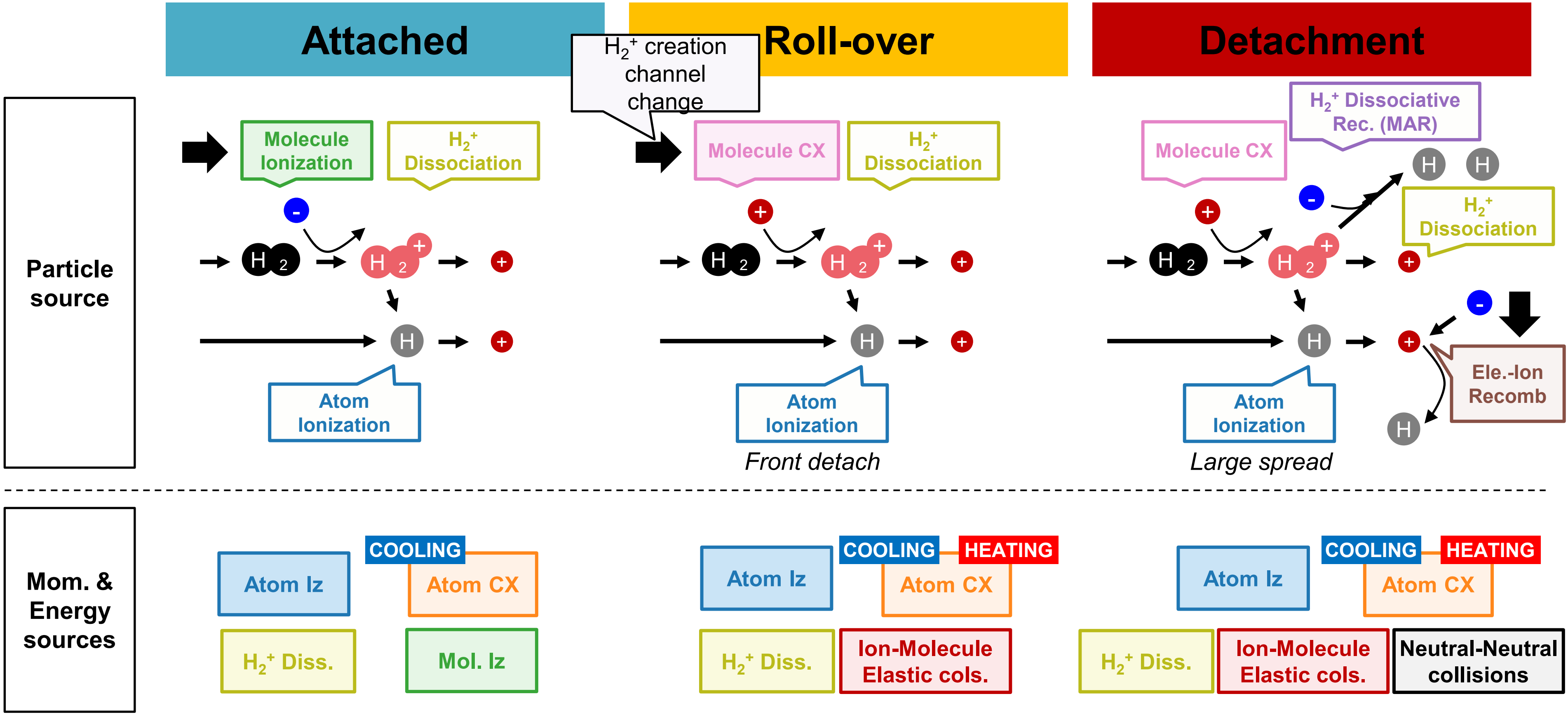
Mom. & Energy sources



Qualitative picture of processes evolution during detachment



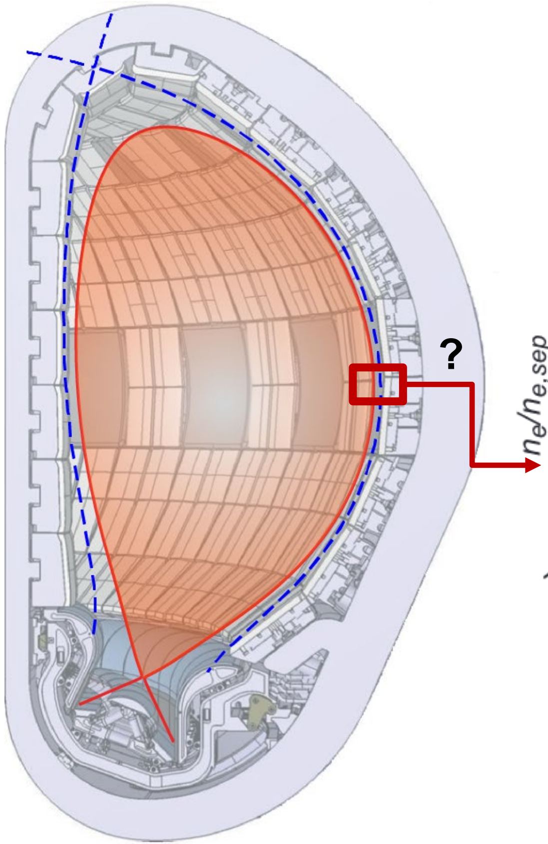
2. Impact of throughput :
Qualitative picture of processes evolution during detachment



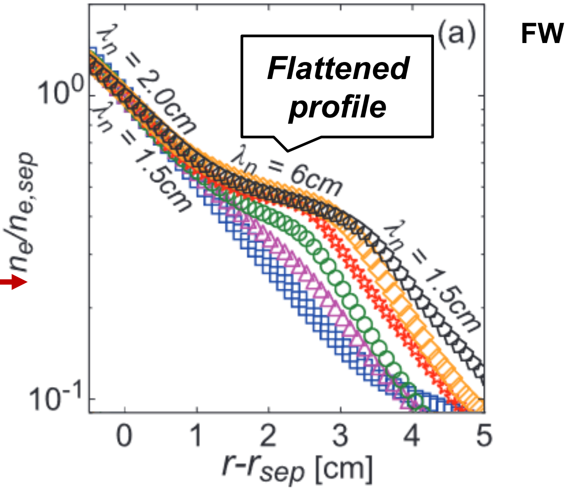
Outline

- 1. Context and motivation
- 2. Impact of throughput
- **3. Impact of enhanced far-SOL transport (shoulder formation)**
- 4. Summary

3. Impact of enhanced far-SOL transport (shoulder formation):
Impact on divertor from formation of shoulders?



Possible formation of "shoulders" in OMP profiles: *(JET example)*



[A. Wynn et al 2018 Nucl. Fusion 58 056001]

Precise shape of profiles in ITER? = Unknown

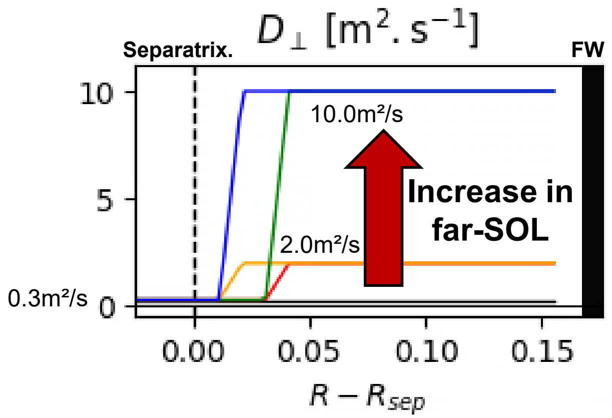
- **Possible formation of shoulders** (turbulence) – not modelled in mean-field codes
- SOLEDGE3X simulation database includes **far-SOL enhanced transport cases** for **FW fluxes studies**

➔ **Question: does this inclusion of shoulders have an impact on what happens in the divertor?**

Modelling & Impact on quantities at the FW

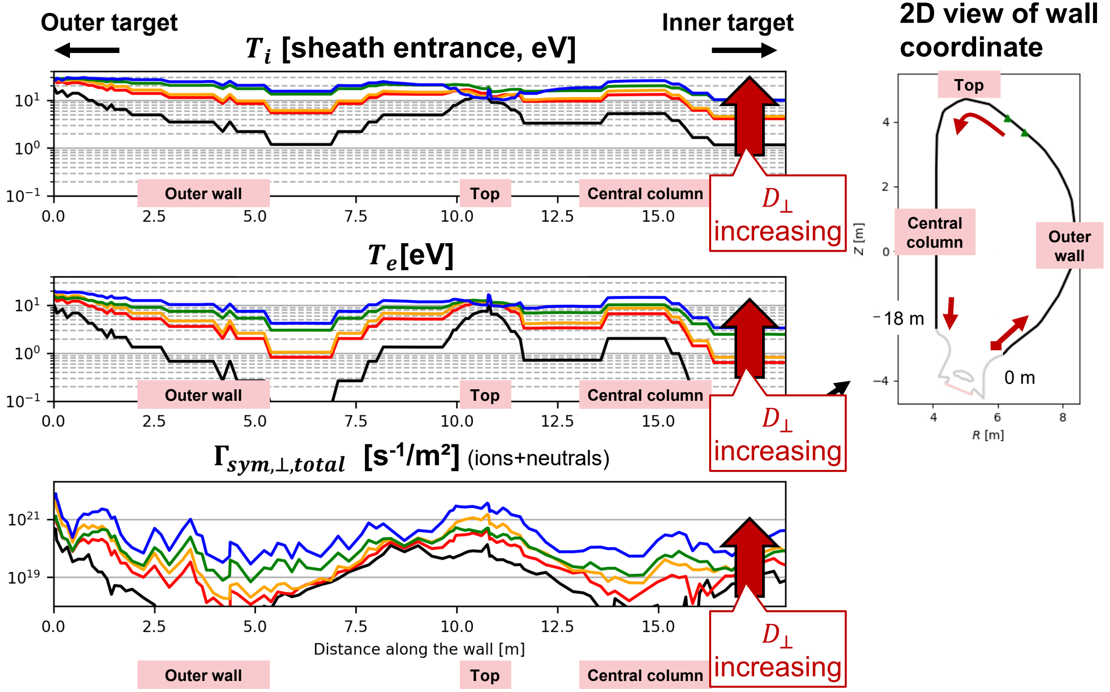
Modelling through $D_\perp, \chi_\perp$

OMP profiles:



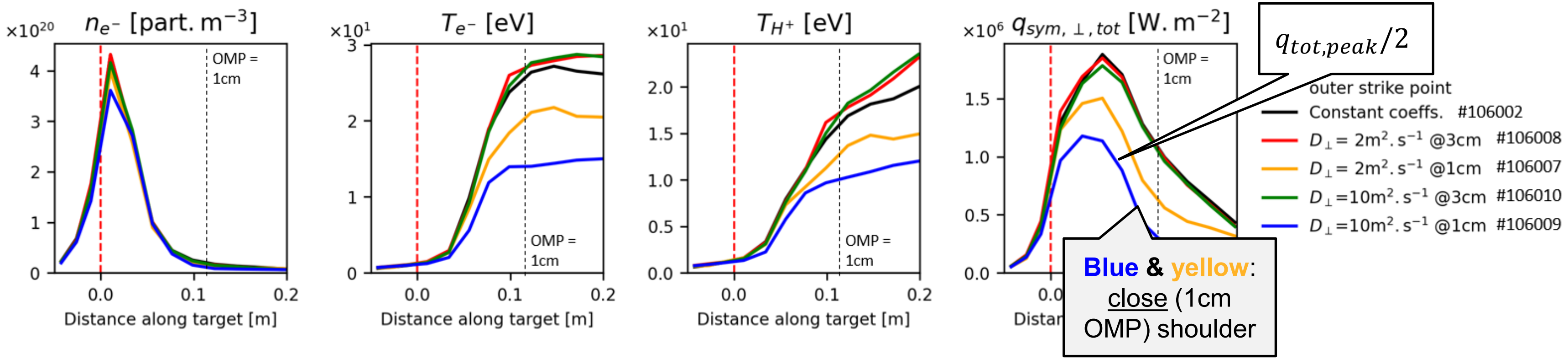
Observed Impact of high far-SOL transport

(low throughput)



Impact on targets: Significant effect only for close shoulders

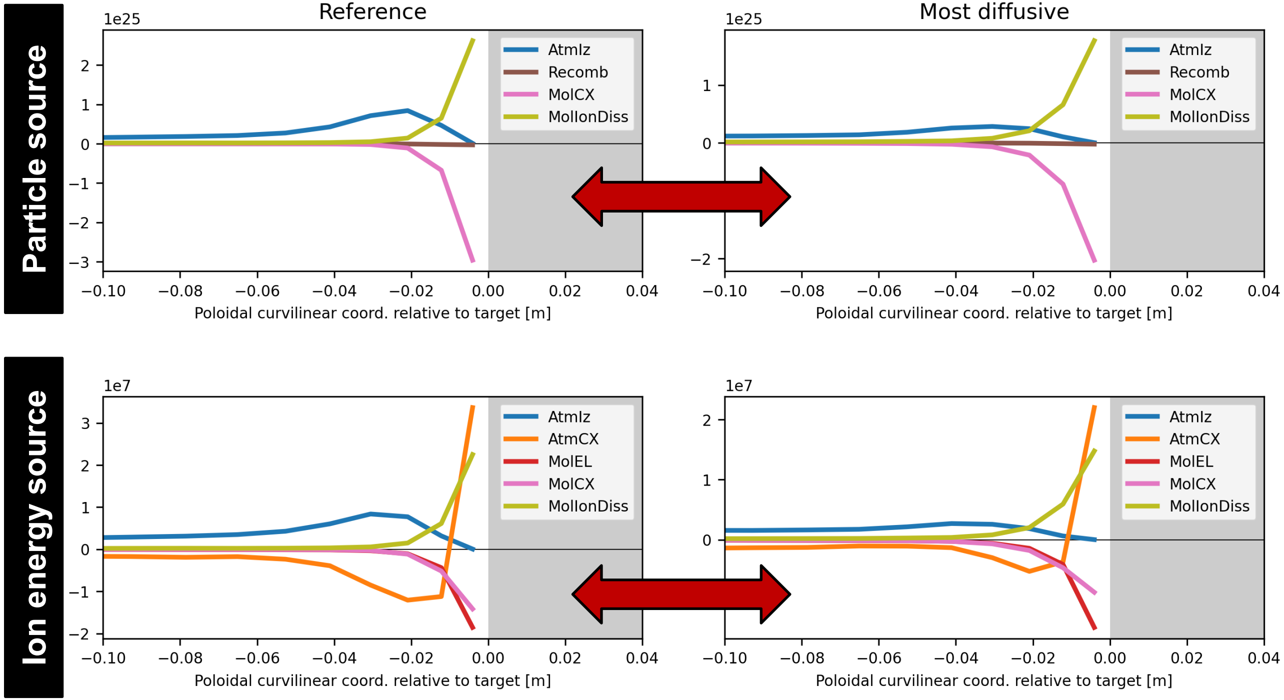
Outer Target



Close and diffusive shoulders have an impact on the divertor

Reaction structures are identical for close shoulders

No shoulder (Roll-over) | **Large & close shoulder**



With strongly enhanced far-SOL transport:

- Almost **identical reaction profiles**
- Simple **reduction** in **amplitude**

Presence of shoulder does not seem to change divertor regime in these simulations

Outline

- 1. Context and motivation
- 2. Impact of throughput
- 3. Impact of enhanced far-SOL transport (shoulder formation)
- 4. Summary

5. Summary

- First **self-consistent full vessel simulations for ITER with SOLEDGE3X** applied to ITER low power phase (20MW), analysed with new detailed **per-reaction source contributions diagnostics**
- Enables **analysis of mechanisms of plasma recycling** and their changes from **attached**, **rollover**, and **partially detached** conditions in ITER simulations
- Macro **picture of plasma-neutral interaction structure in detachment onset**:
  - **Molecule interactions** present **even in attached** cases (H_2^+ dissociation is a major contributor, net source if mol. EI)
  - **Switch mechanism** of **H_2^+ formation**: **molecule electron impacts** at low regime (high T_e), the fully replaced by **molecule CX** at roll-over
  - First **detachment** of **atom ionization** front at **roll-over**, then further spread out with increased detachment
  - Roll-over and after: **momentum** loss dominated by **ion molecule elastic collisions**, **CX** turns into a **heating source** for the plasma at target
  - Electron-ion **recombination** (**EIR**) & molecule assisted recombination (**MAR**) appear **only in (partially) detached cases**, not before, and **neutral-neutral collisions** start taking importance (cloud compression)
- **Enhanced far-SOL transport (shoulders) effect in the divertor**: only with close shoulders, and does not induce change of regime. **No change of PNI structure**, simple amplitude decrease of sources
- **Next steps:**
  - Run to full-power **100MW FPO neon-seeded** cases (WIP)
  - Assess **effect of impurities** on PNI **processes** in simulations

Thank you

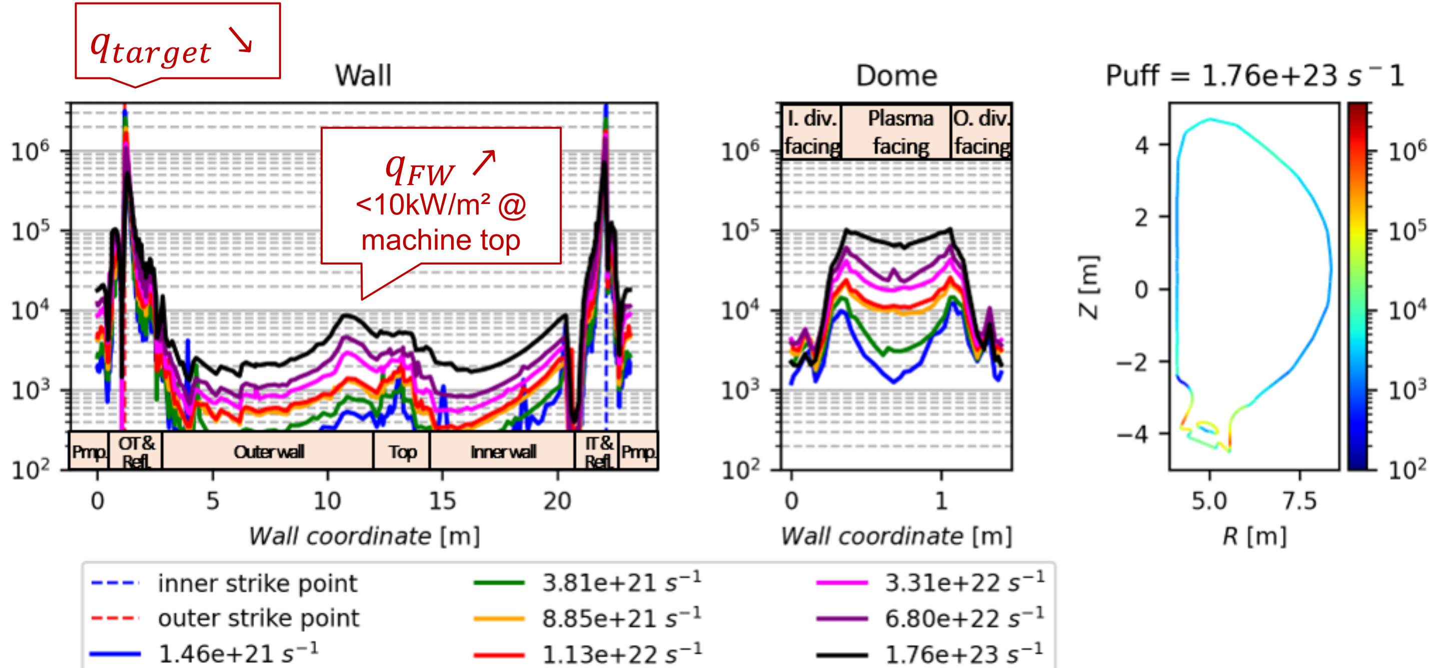
Acknowledgement:
This work was performed under the auspices of the ITER Scientist Fellow Network. The views and opinions expressed herein do not necessarily reflect those of the ITER organization.
This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 — EUROfusion). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them.

Backup slides

FW heat load: well within design limits

Heat flux density deposition on the FW $q_{sym,\perp,total}$ [W/m²]:

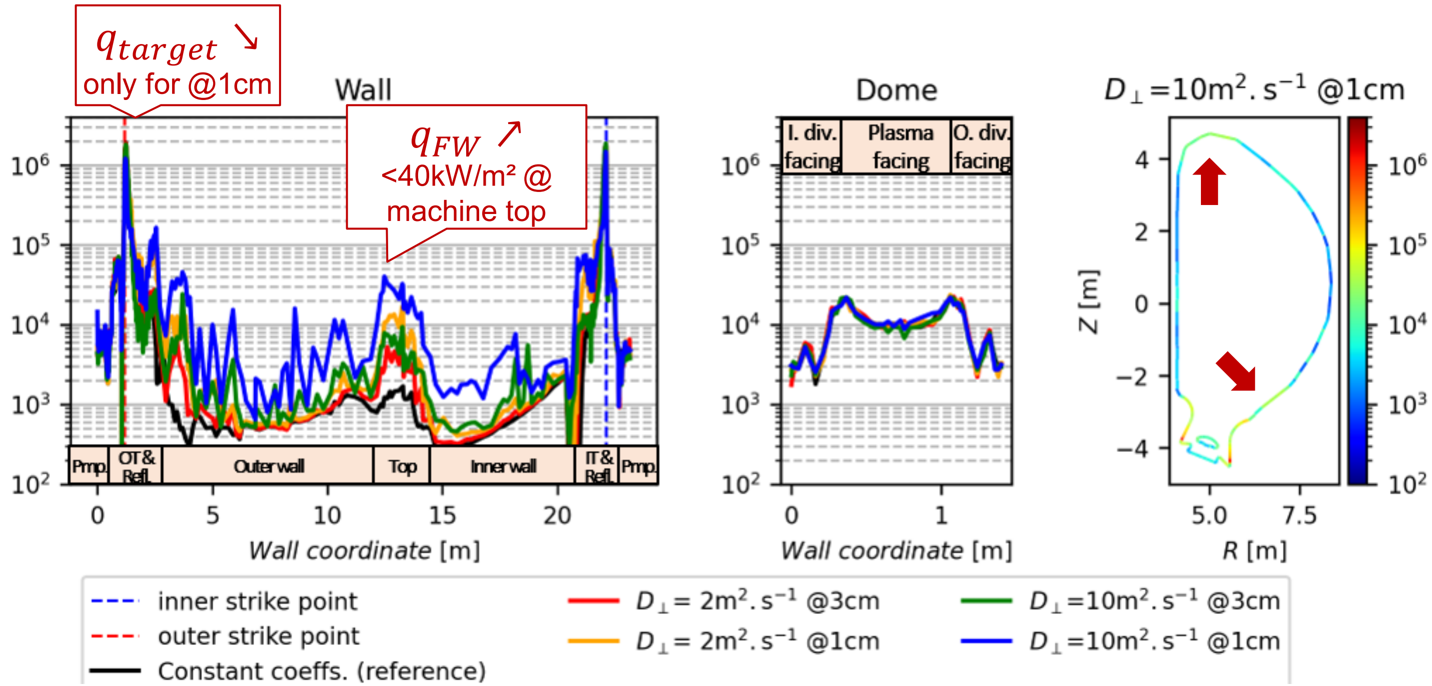
(2D-axisym., perp. no shaping, pl+neut.+rad)



- FW material limits:
  - Inner: 5MW/m²
  - Outer: 3MW/m²,
  - Top: 2MW/m²
    [ITER Research Plan, 2018]
- Max FW load: **up to 20 % of input power** at highest throughput

Heat flux density deposition on the FW $q_{sym,\perp,total}$ [W/m²]:

(2D-axisym., perp. no shaping, pl+neut.+rad)



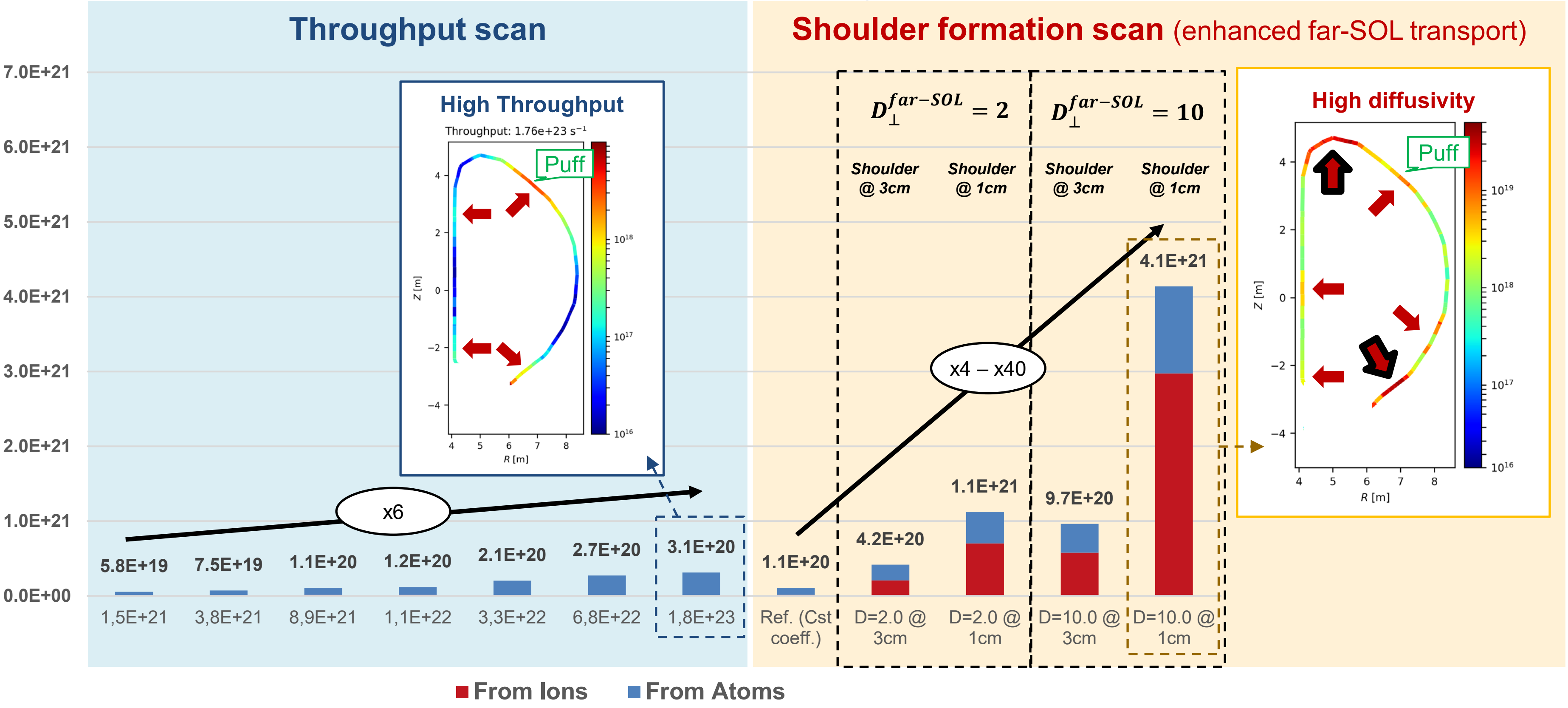
- FW material limits:
  - Inner: 5MW/m²
  - Outer: 3MW/m²,
  - Top: 2MW/m²

  [ITER Research Plan, 2018]
- Max FW load: **up to 30 % of input power** at highest throughput

Summary of throughput and shoulder formation on FW gross erosion rate

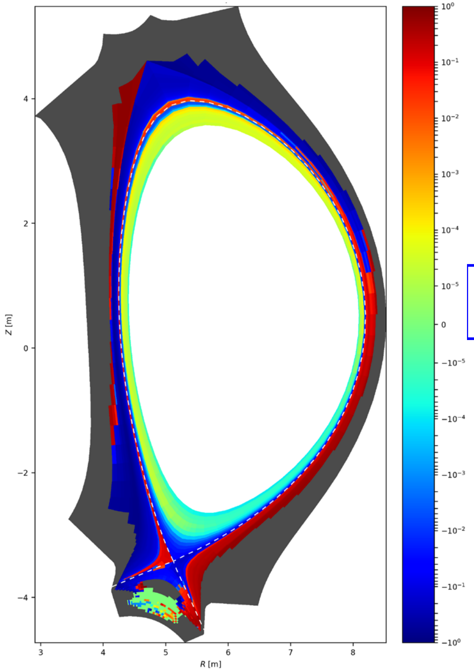
First Wall total gross sputtering rate [s^{-1}]:

Caveat: Trends analysis only (sputtering from H⁺ & H° only), rough estimation, better calculations done with specialized codes ERO, WALLDYN

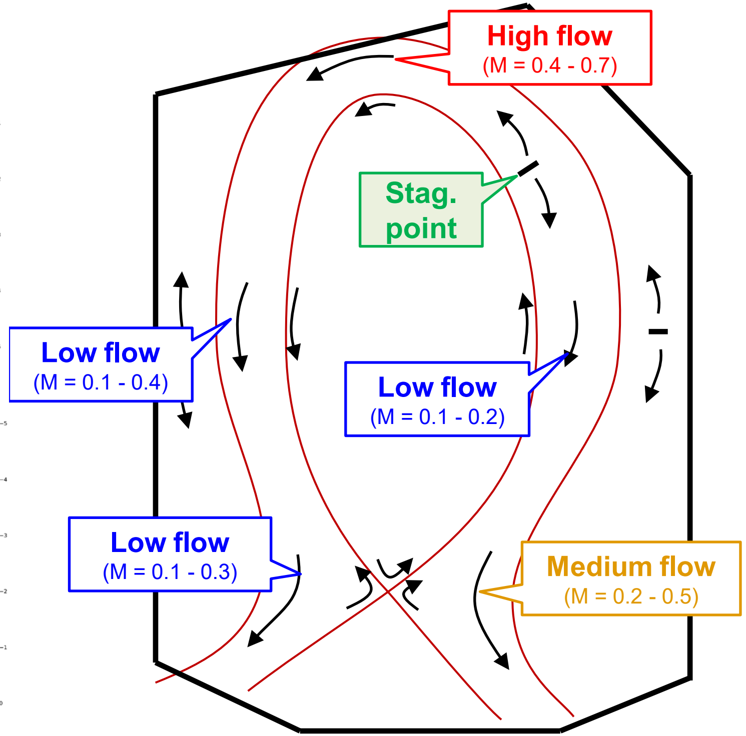


Plasma conditions in far-SOL: SOL flows

Mach Number



Low throughput



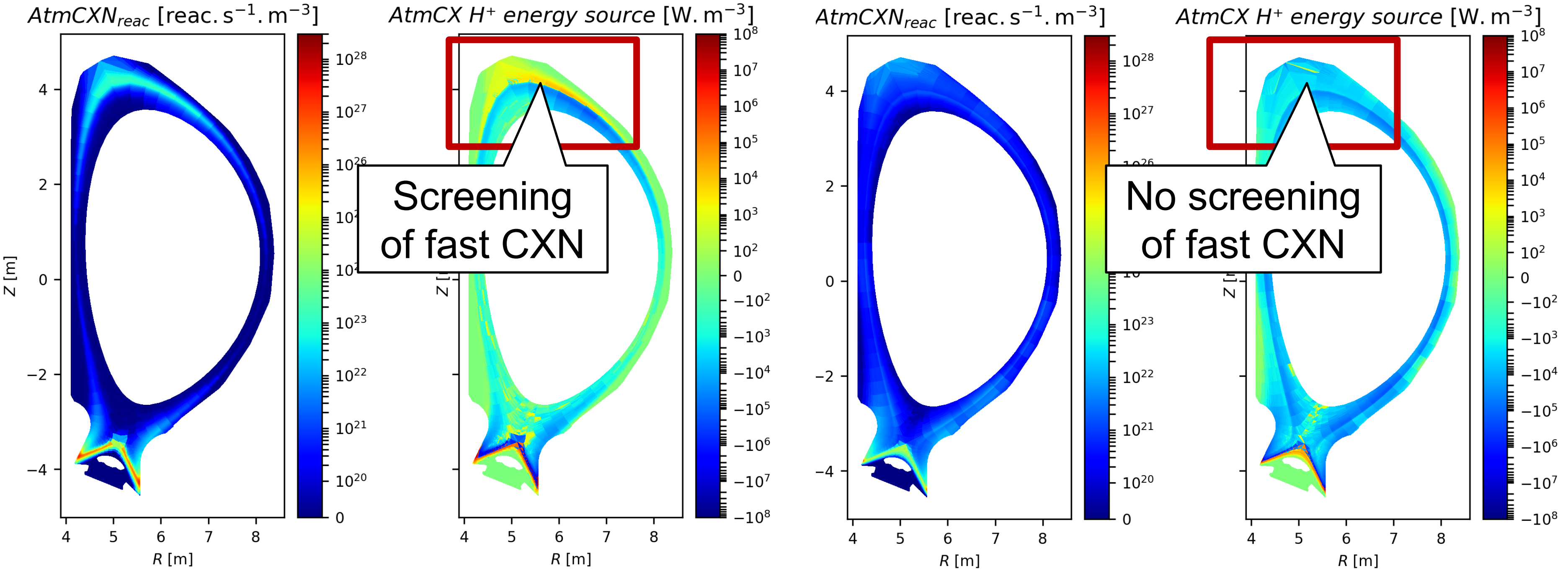
SOL flows:

- Key input for erosion codes and impurity transport
- **Mach ↗** with **increasing throughput**
- **Mach ↘** in presence of **shoulder**
- Stagnation point around the upper outer section

CX atoms are screened at high TP, not with enhanced transport

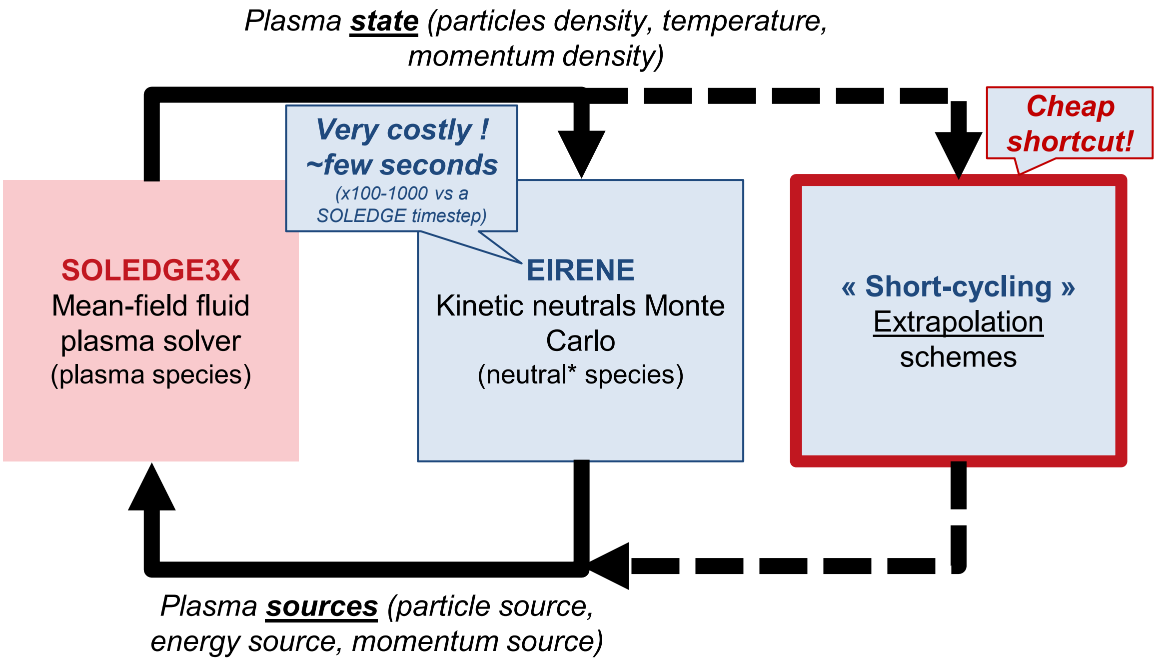
High Throughput

Large shoulder



Computation time: neutral sources extrapolation schemes

SOLEDGE3X-EIRENE coupling workflow:



- Time step ~10^{-7}s (CFL)
- ITER solution equilibrium time: ~ 1s
- **Requires "shortcuts" i.e. extrapolations**

Sources extrapolation:

- $S_n = n_{atom} \, n_e < \sigma_{iz} v >$

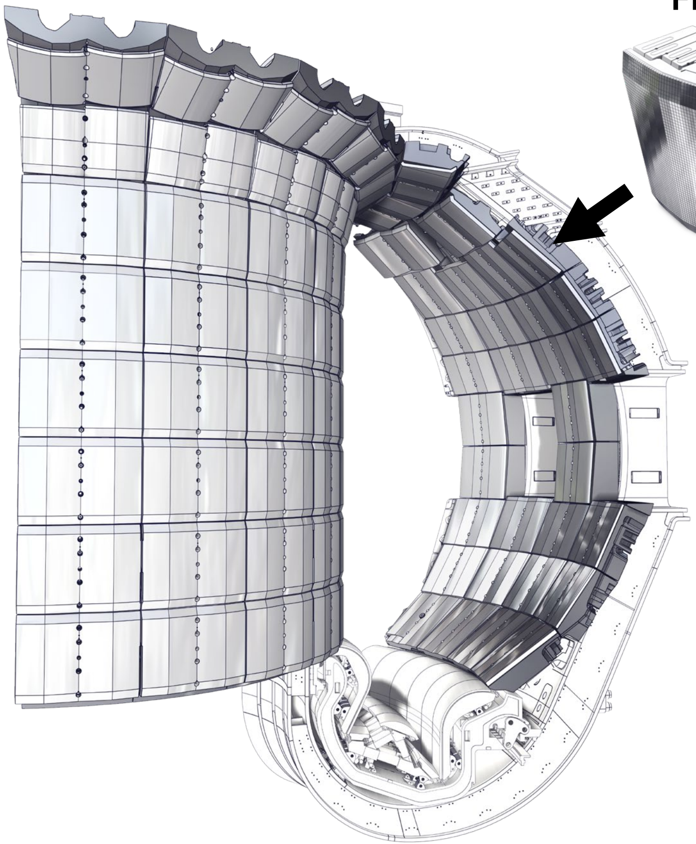
S_n: Extrapolated source from neutrals

n_{atom}: Keep spatial distrib.

n_e, $< \sigma_{iz} v >$: Updated from plasma background

[Details to be published]

ITER simulations: addressing the First Wall (FW) challenge



Impacts of plasma-FW Panels interaction

- **Panel erosion:**
  - FW lifetime (incl. # of spares)
  - Dust generation (Be)
  - Fuel retention
- **Plasma performance:**
  - Contamination (sputtering)
  - Impurity transport & redeposition

Requires a tool for estimating **FW fluxes** and **full vessel plasma backgrounds** of key plasma scenarios
➔ ***SOLEDGE3X***

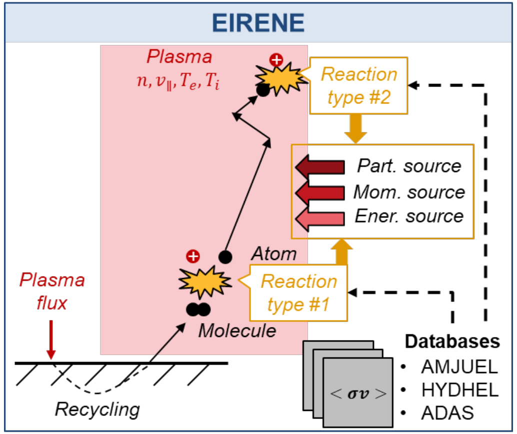
Feed input for other codes:

→ **ERO2.0**
WALLDYN
…

This talk focus: Contributions analysis from simulations

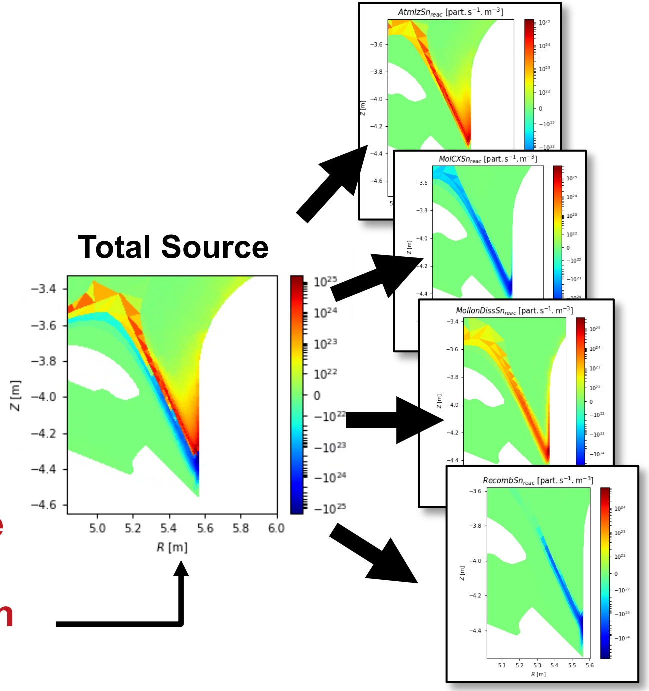
Plasma-Neutral Interactions

- Highly **non-linear**
- **Large number of processes** involved
- State of the art simulation is kinetic Monte Carlo: **difficult to analyse** a priori



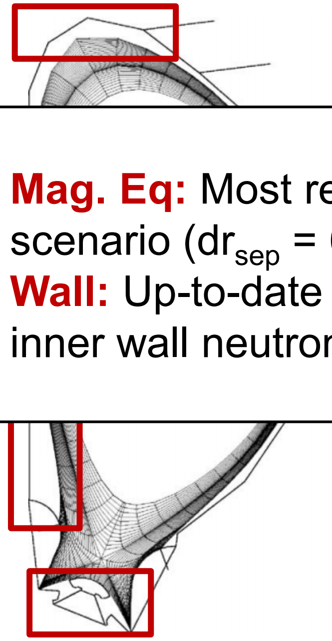
Goal of this talk:

- **From full domain ITER simulations** with **SOLEDGE3X**…
  - Divertor
  - Main chamber & FW
- …**impact analyses of 2 parameters**…
  1. Throughput
  2. Density shoulder formation
- … and description of **structure of plasma-neutral processes** involved with **new contribution code diagnostics**



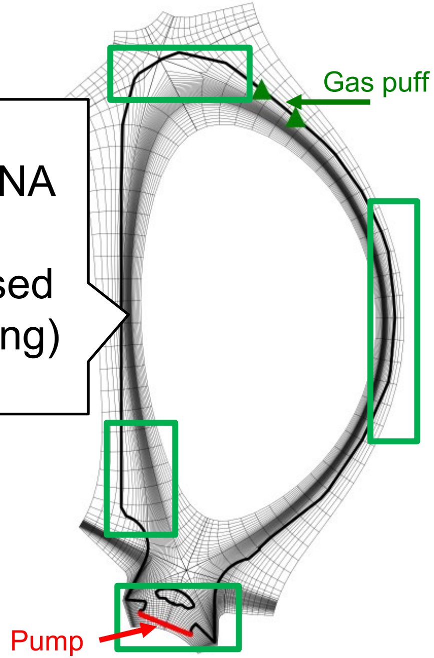
Full vessel plasma numerical domain with SOLEDGE3X

SOLPS-ITER domain



- **Mag. Eq:** Most recent DINA scenario (dr_{sep} = 6.5cm)
- **Wall:** Up-to-date (increased inner wall neutron shielding)

SOLEDGE3X domain



"Self-consistent" plasma simulations :

- Grid **extends up to all PFCs** (no distinction main SOL vs far SOL)

\+

- **"Up-to-date" divertor solution** (SOLPS-ITER like plasma-neutral interaction model with EIRENE)

Output → Erosion/Imp. transport codes:

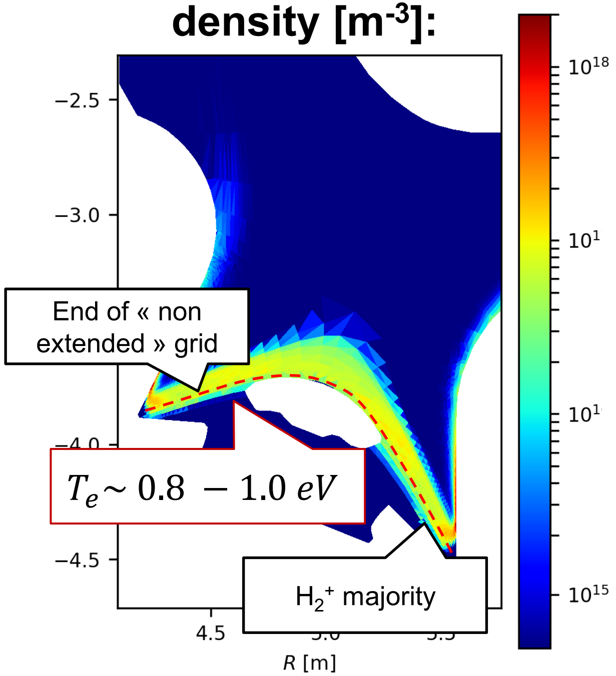
- FW fluxes
- Plasma backgrounds up to the FW

Outline

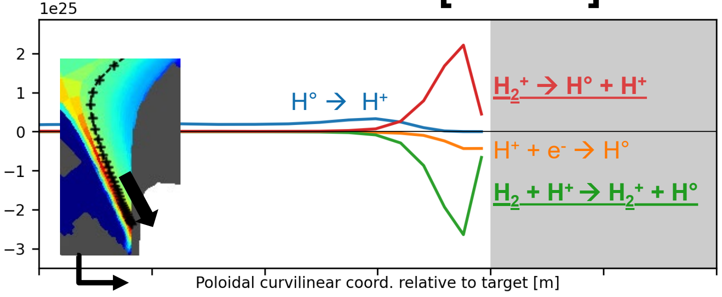
- 1. Context and motivation
- **2. Up-to-the-wall domain challenge for ITER cases**
- 2. Impact of throughput
- 3. Impact of enhanced far-SOL transport (shoulder formation)
- 5. Summary

Key role of H_2^+ molecular ion near divertor legs

Molecular ion H_2^+ density [m^{-3}]:



H^+ particle source main contributors [$s^{-1}.m^{-3}$]:



➔ Many still open/unresolved questions in divertor A&M modelling and simulations

H_2^+ ion role:

- **H2+ : intermediate product** in "molecule-assisted" processes (MAR, MAI)
- Significant $n_{H_2^+}$ just below the end of "common SOL" domain, even majority species there
- $\lambda^{pol}_{mfp\ H_2^+} \sim 5cm > d_{cell}$

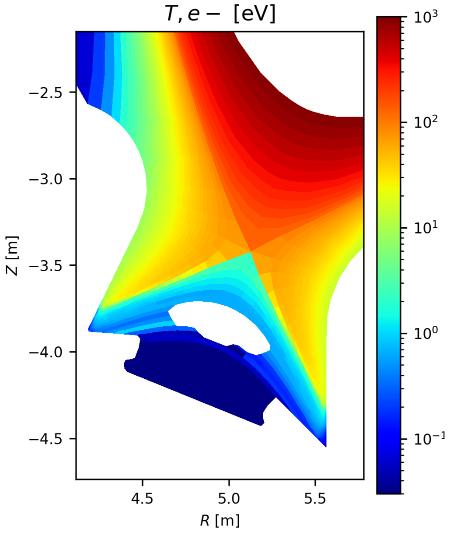
➔ **requires transport** tracking (esp. in transients)

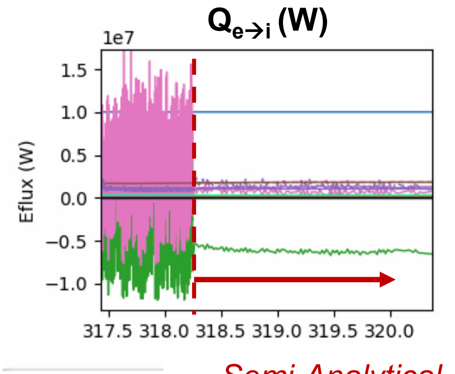
Stiffness of physics in cold divertor conditions

Example: Electron-ion energy equipartition:

$$Q_{e\to i} = \frac{m_e Z^2 e^4 \Lambda}{m_i (2\pi)^{\frac{3}{2}} \varepsilon_0^2 \sqrt{m_e}} n_e n_i \frac{1}{T_e^{\frac{3}{2}}} (T_i - T_e)$$

Strong at low temperature !



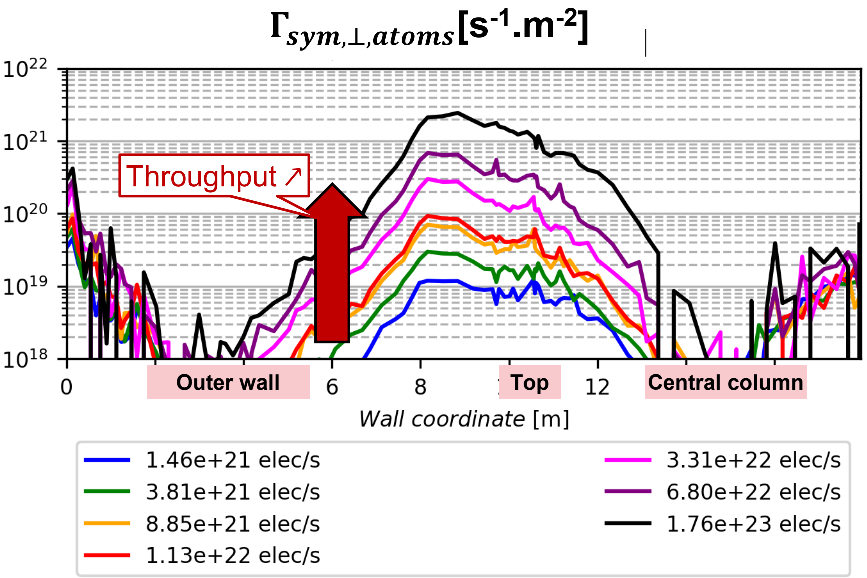


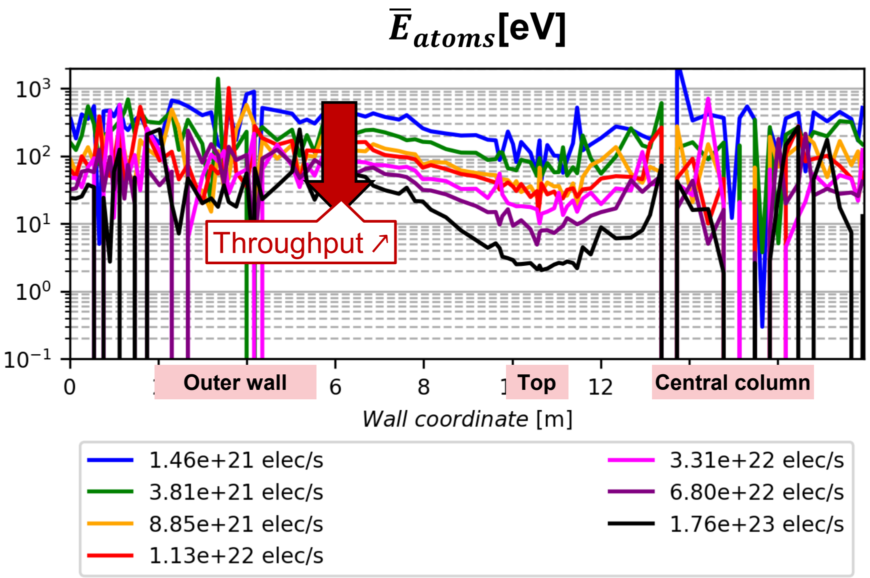
Semi-Analytical solution

- Collisional **energy exchange & friction force** terms become very large at **low T**, especially during transients
- **Coulomb Log Λ** produces unphysical values in Braginskii/Zhdanov formulation at T→0 : Quantum effects correction [Hong-sup Hahn and E. A. Mason, The Physics of Fluids 14, 278 (1971)]
- **Revisited numerical scheme** for collisional terms for increased stability

[Details to be published]

CX atoms: FW incident flux & average energy, counter action





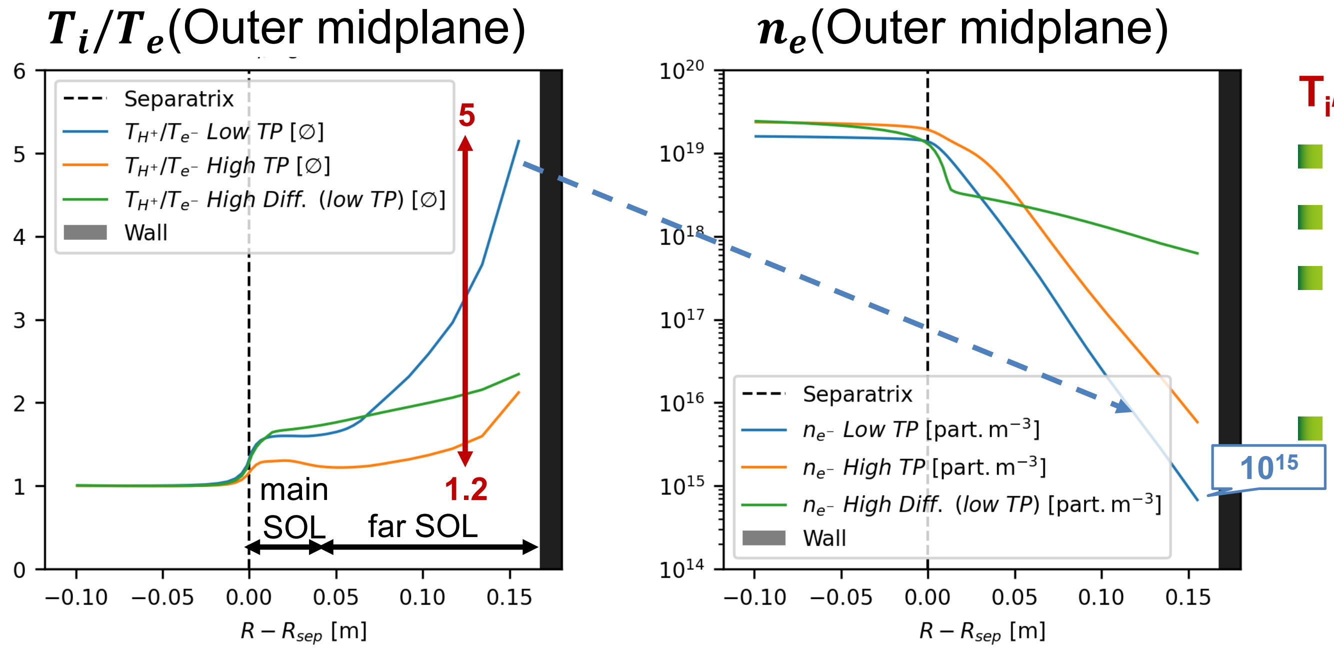
Impact on incident atom flux density:

- **Large increase** at machine **top and outer top: x100**

Impact on average atom energy:

- **Large decrease** ÷10 – 100
- 100 eV → 3 eV at machine top

Comparing current assumptions in far-SOL: T_i/T_e ratio



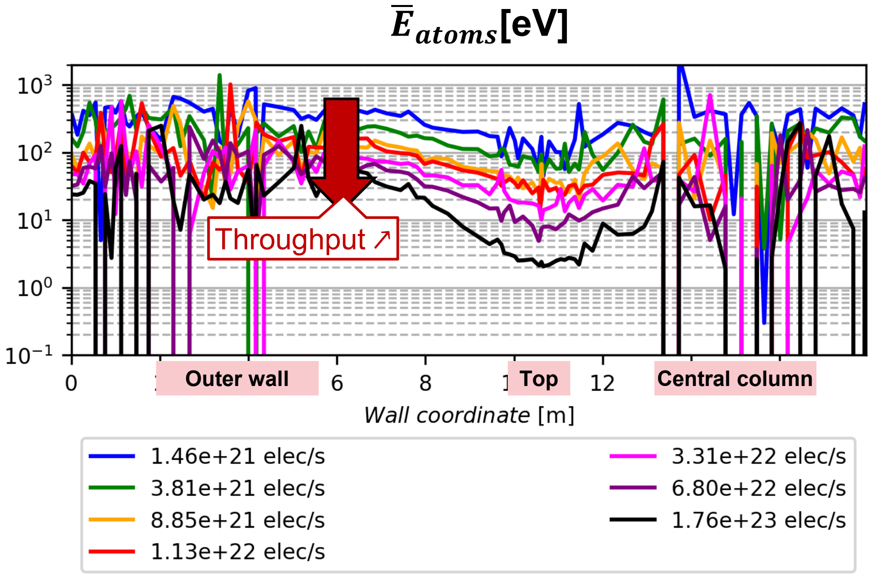
T_i/T_e ratio in far-SOL:

- **Main SOL: T_i/T_e ~ 1.2 – 2**
- **Far SOL: T_i/T_e ~ 1.2 – 5**
- Ratio ↘ **with throughput and diffusivity** (**low: 5, high: 2)**
- ~Correlation with n_e, but not only (collisionality)

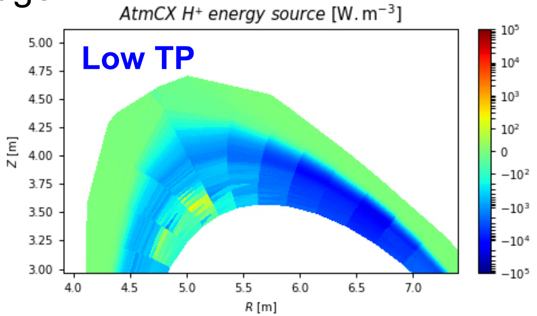
5. Summary

- First **self-consistent full vessel simulations for ITER with SOLEDGE3X** applied to ITER low power phase (20MW): **grid up to the FW in main chamber critical** for **FW impact studies**
- Overall **good agreement with SOLPS** on throughput scan **on common parts of the domain**
- In both scans, increase in $q_{\perp,sym}$ on FW, but still very low values (for 20MW cases)
- Impact of **throughput**:
  - **Counter action Γ ↗ while T ↘ at the FW**
  - Overall throughput **impact moderate on FW gross erosion rate** (x6 between scan extremes, only **from CX atoms**)
- Impact of **enhanced far-SOL transport (shoulders)**:
  - **Combined increase of Γ ↗ and T ↗ at the FW**
  - Much **greater impact than throughput on FW gross erosion rate** (x40 between scan extremes, **mainly from ions**)
- **Higher impact of shoulders ➔ Importance of refinement on $D_\perp, \chi_\perp$ assumptions !**

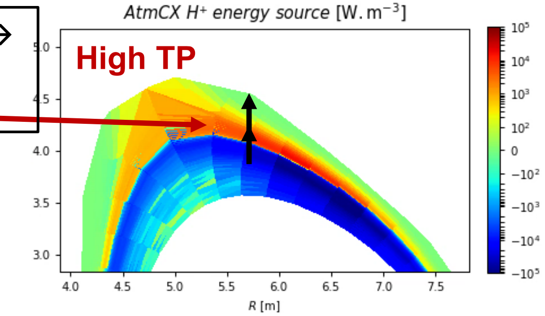
2. Impact of throughput :
CX atoms: FW incident flux & average energy, counter action



- Energy decrease from T decrease from Ionisation
- Further TP increase cold ions screen CXN from core edge



Energy atom → ion (atom cooling)

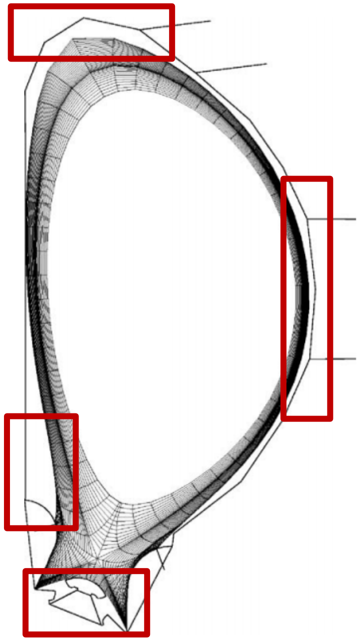


Impact on average atom energy:

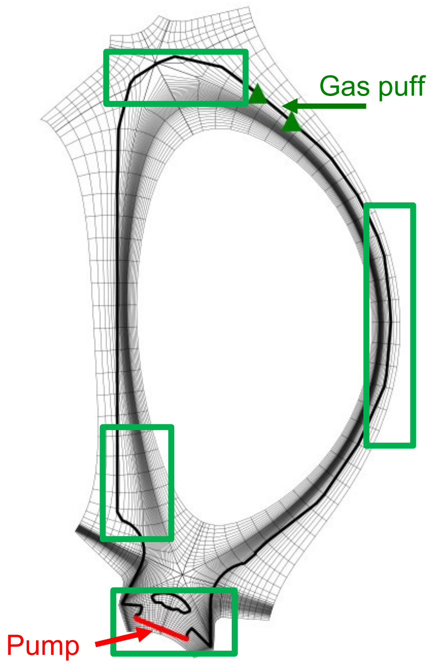
- **Large decrease** ÷10 – 100
- 100 eV → 3 eV at machine top

Full vessel plasma numerical domain with SOLEDGE3X

SOLPS-ITER domain



SOLEDGE3X domain



"Self-consistent" plasma simulations :

- Grid **extends up to all PFCs** (no distinction main SOL vs far SOL)

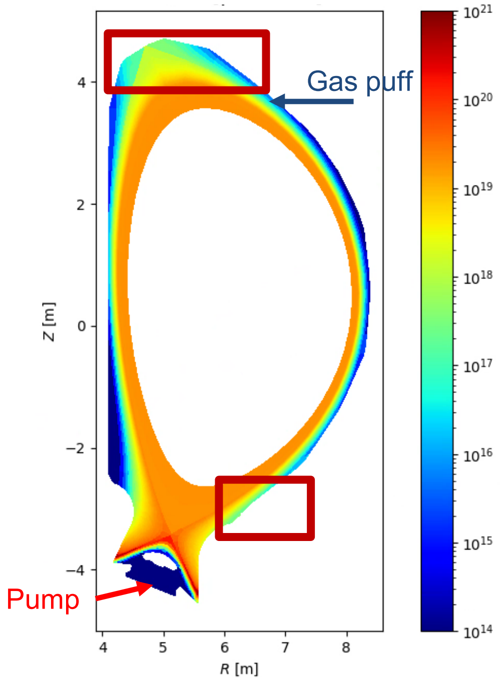
+

- **"Up-to-date" divertor solution** (SOLPS-ITER like plasma-neutral interaction model with EIRENE)

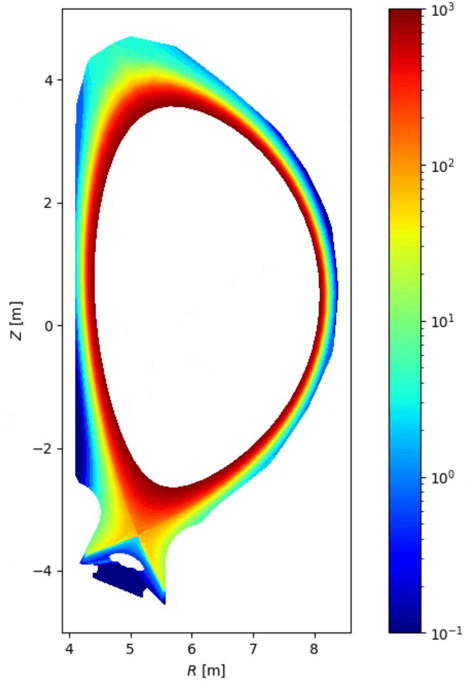
Significant plasma at machine top, broadening of λ_q

Illustration case at medium throughput (3.31 x 10[22] e-.s-1):

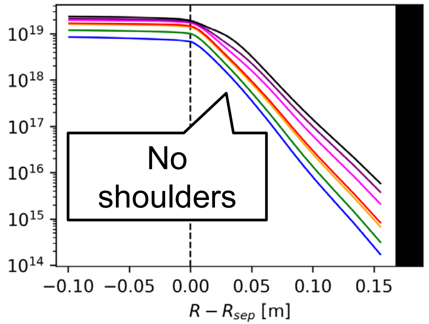
n_e[m-3]



T_e[eV]



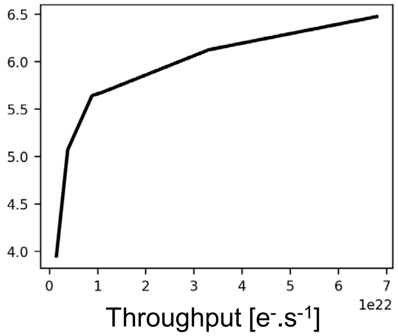
n_e[m-3] OMP



Throughput [e-.s-1]:

- 1.46e+21 s^{-1}
- 3.81e+21 s^{-1}
- 8.85e+21 s^{-1}
- 1.13e+22 s^{-1}
- 3.31e+22 s^{-1}
- 6.80e+22 s^{-1}
- 1.76e+23 s^{-1}

λ_q[mm]



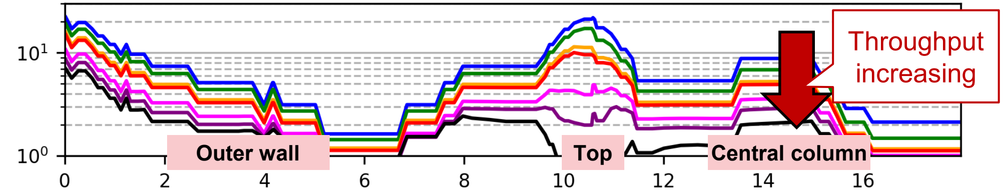
- **Probable plasma-wall interactions**:
  - Top
  - Outer lower wall
- λ_q increase with throughput

Quantities at the FW: counter action of Γ vs *T*

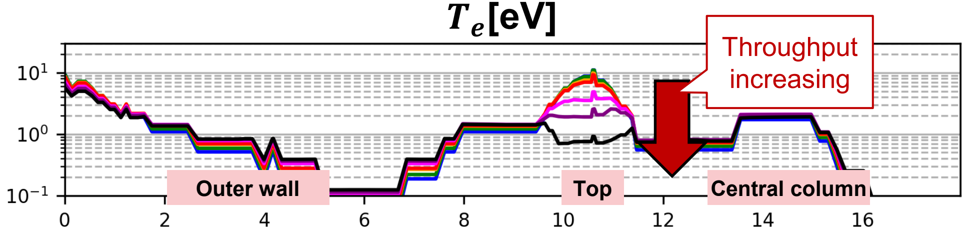
Impact of throughput on FW T and total particle flux:

Outer target ← → Inner target

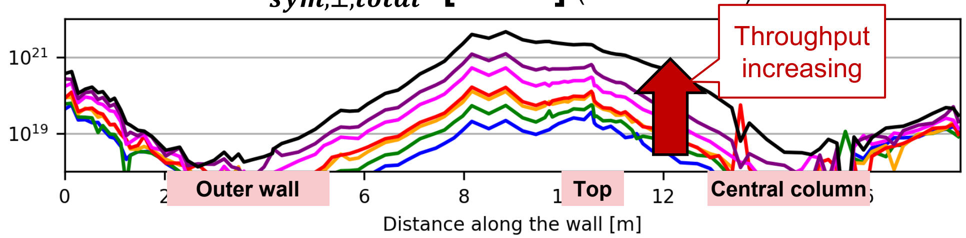
T_i [sheath entrance, eV]



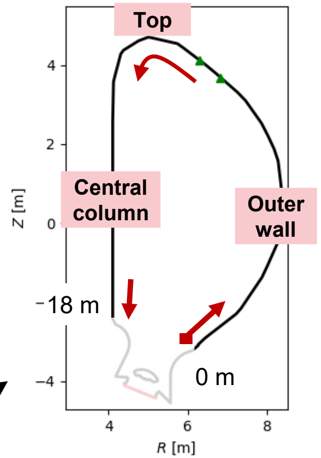
T_e[eV]



$\Gamma_{sym,\perp,total}$ [s⁻¹/m²] (ions+neutrals)



2D view of wall coordinate



Throughput: [e⁻.s⁻¹]

- 1.46e+21 s^{-1}
- 3.81e+21 s^{-1}
- 8.85e+21 s^{-1}
- 1.13e+22 s^{-1}
- 3.31e+22 s^{-1}
- 6.80e+22 s^{-1}
- 1.76e+23 s^{-1}

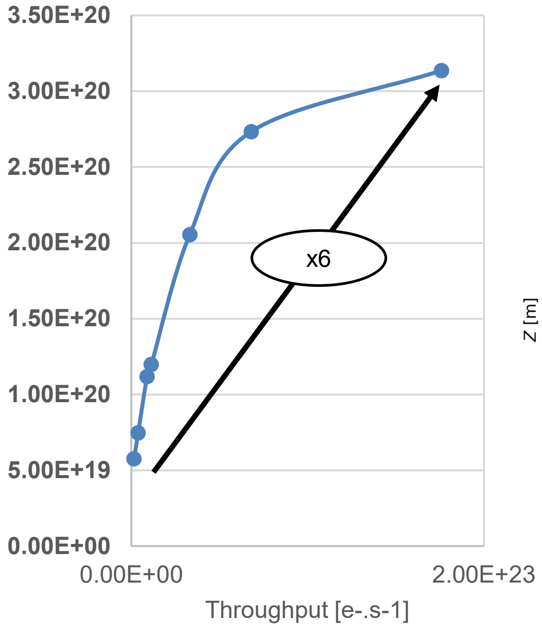
When increasing throughput:

- $T_{i,wall}$ ↘ : 20 → 7 eV
- $T_{e,wall}$ → : No effect (except machine top: 10 ↘ 1 eV)
- FW part. fluxes x 100
- **Counter action *Γ* ↗ while *T* ↘**

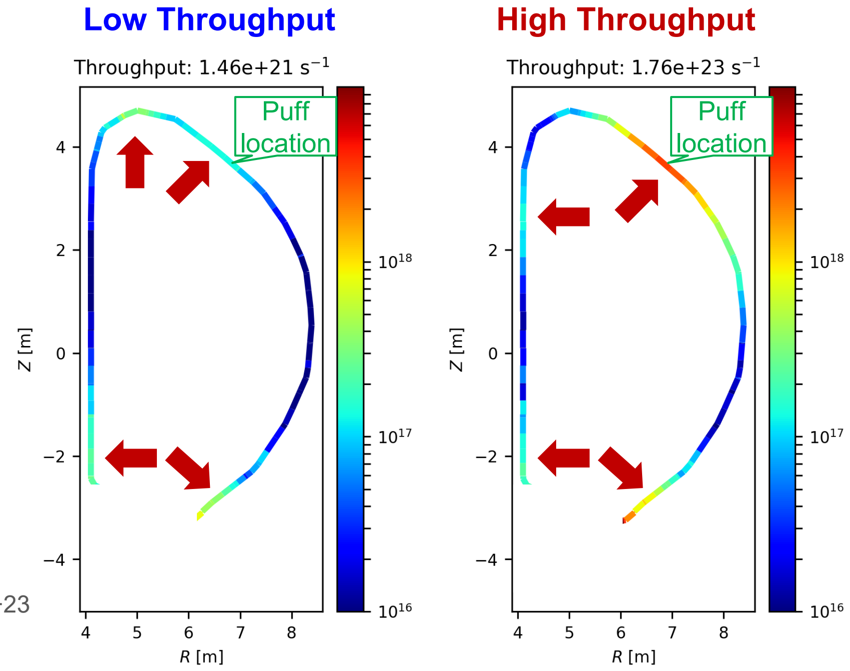
Gross Be erosion figures: x6 between scan extremes

Caveat: Trends analysis only (rough estimation, H^+ & H° only, no 3D), better calculations done with specialized codes (ERO, WALLDYN)

First Wall total gross sputtering rate [s^{-1}]



Gross sputtering rate density [$s^{-1}.m^{-2}$]

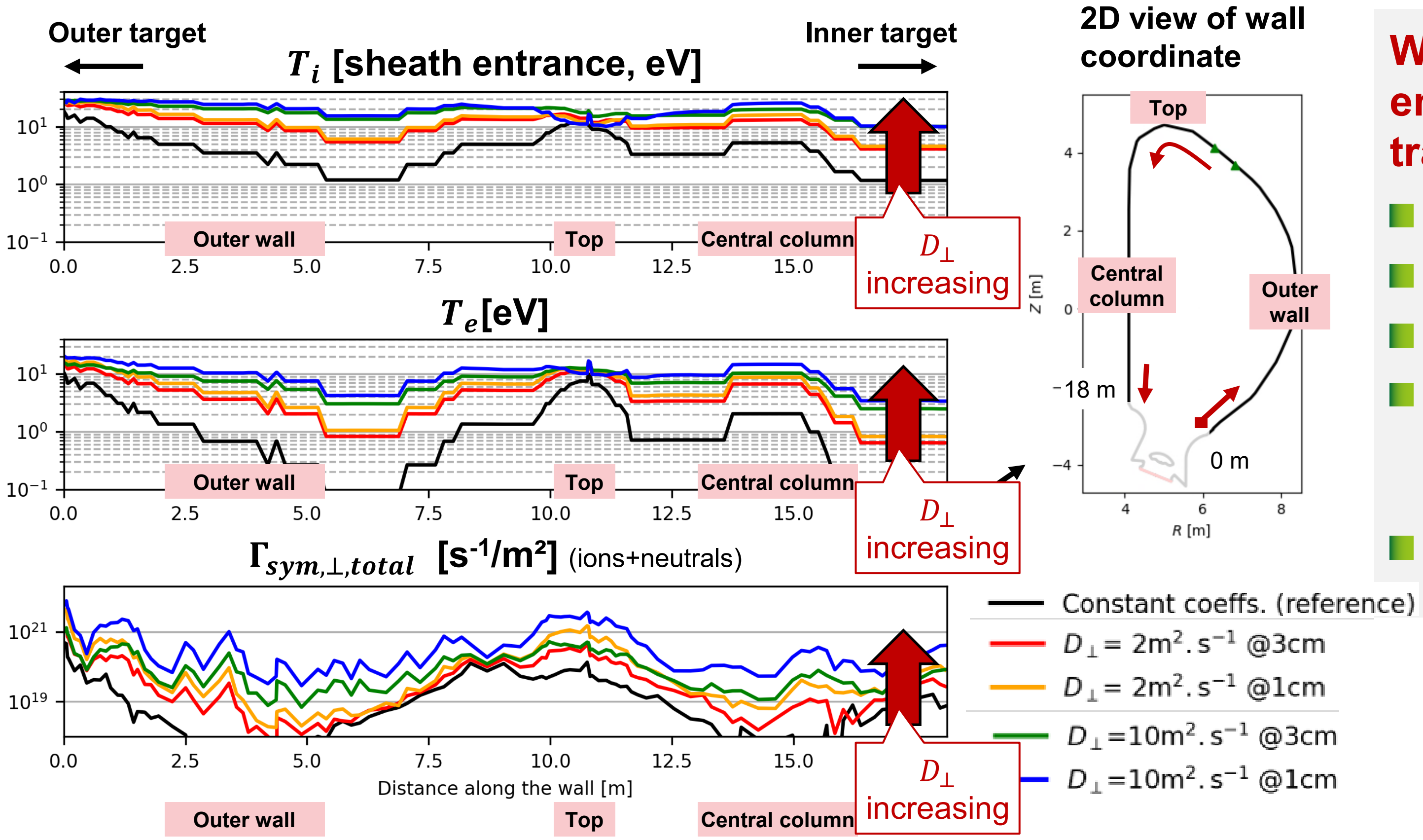


Trends:

- ~90% from **CX atoms**, **increasing** with throughput
- From **ions**: ~**independent** of throughput
- Factor 4 underestimation vs more complete ERO2.0 (not same bg, 3D effects?) [J. Romazanov et al 2022 Nucl. Fusion 62 036011]

Impact on quantities at the FW: combined action of Γ & T

Impact of high far-SOL transport (low throughput):



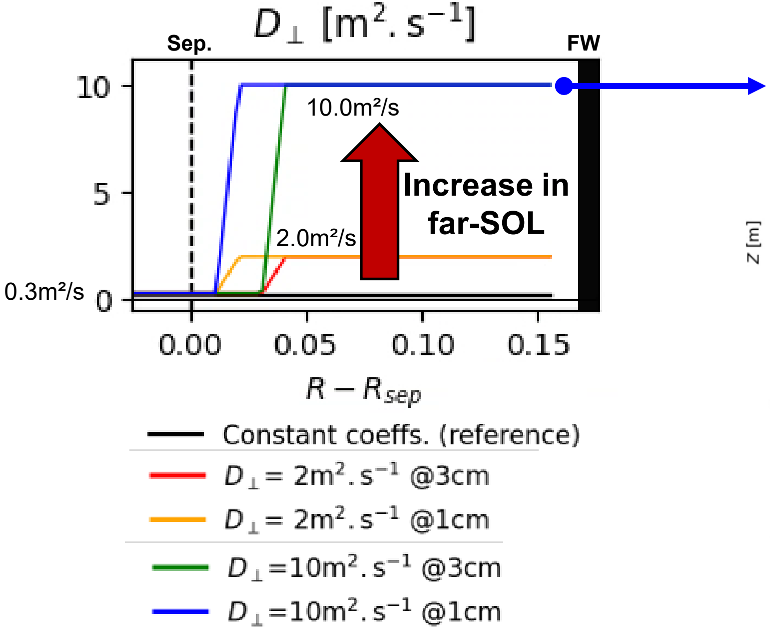
With strongly enhanced far-SOL transport:

- FW fluxes x 10-20
- $T_{i,wall}$ ↗ : 20 - 30 eV
- $T_{e,wall}$ ↗ : 10 - 20 eV
- $q_{sym,\perp,total}$ = 40kW/m² @ machine top
- **Combined increase Γ ↗ and T ↗**

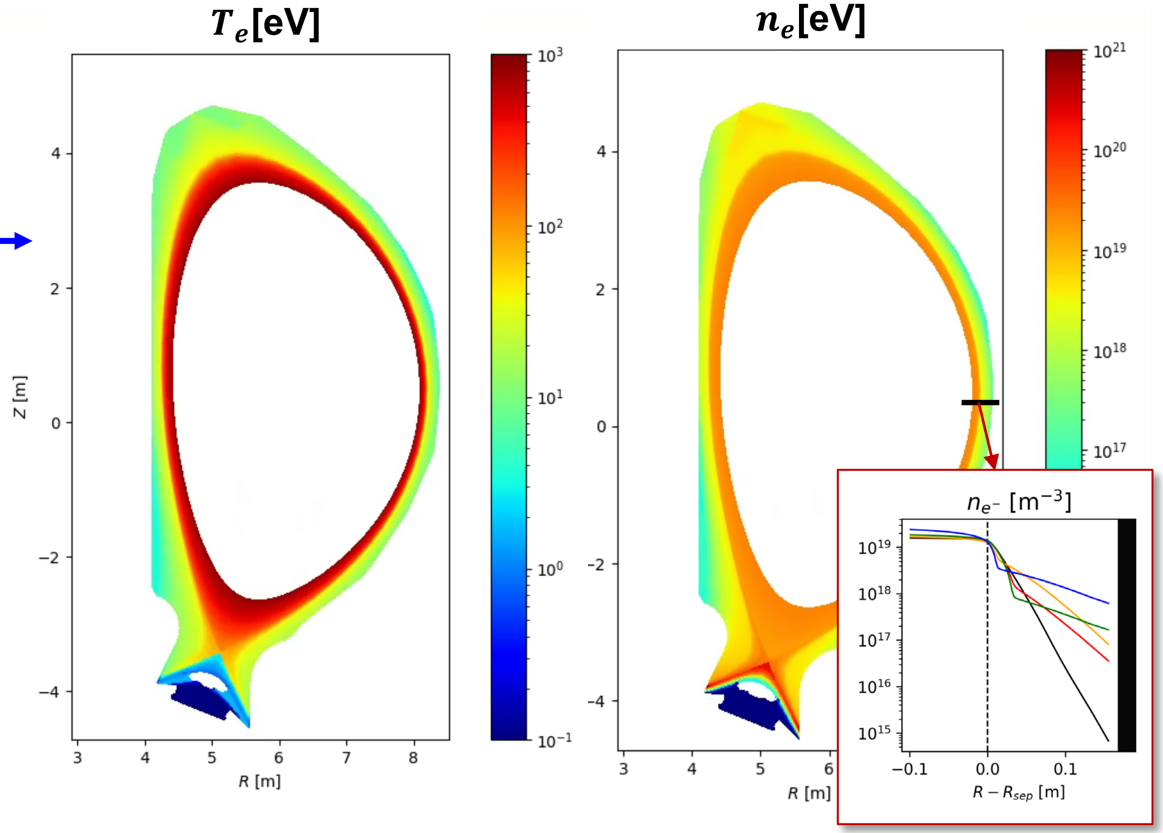
Modelling through increased coeff. in far-SOL

Modelling:

Prescribed perpendicular diffusivity coefficients $D_\perp, \chi_{\perp e}, \chi_{\perp i}, \nu_\perp$ profile at the outer midplane:



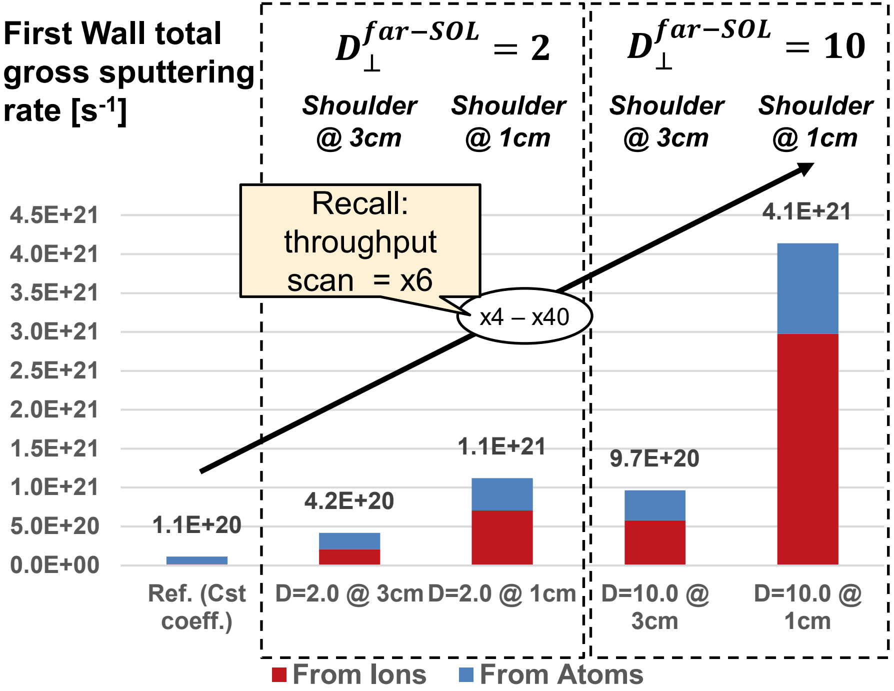
Example: Strongest & closest shoulder (in blue):



3. Impact of enhanced far-SOL transport (shoulder formation): **Gross Be erosion figures: x40 between scan extremes**

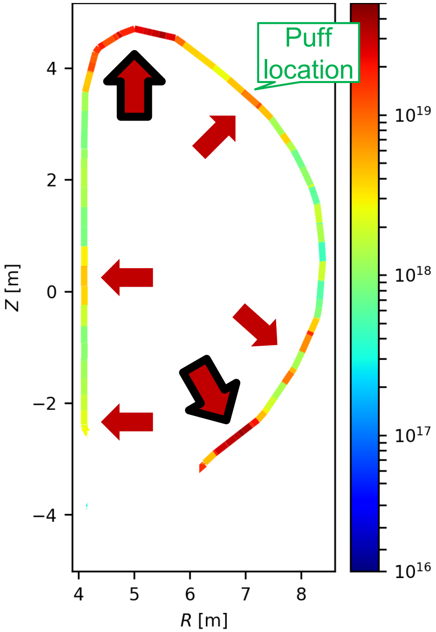
Caveat: Trends analysis only (sputtering from H+ & H° only), rough estimation, better calculations done with specialized codes ERO, WALLDYN

First Wall total gross sputtering rate [s^{-1}]



Gross sputtering rate density [$s^{-1}.m^{-2}$]

Highest diffusivity



Trends:

- Shoulders ➔ **ions now dominant** (50-70%)
- **Large increase**
- Top & outer lower tiles (#8,#9 & #18)
- Factor 10 underestimation vs ERO2.0 (not same bg, 3D effects)

[J. Romazanov et al 2022 Nucl. Fusion 62 036011]

2. Impact of throughput
Overall good agreement with SOLPS-ITER runs

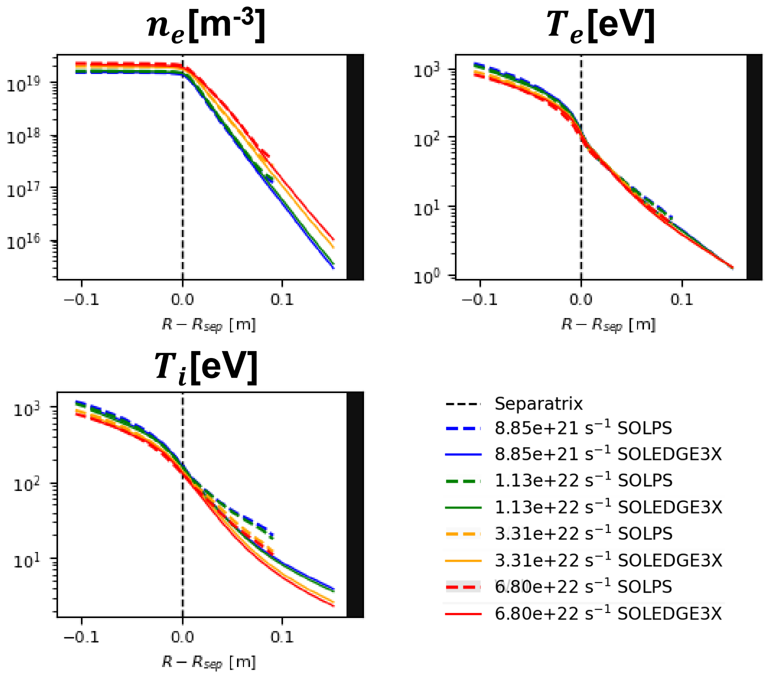
Throughput scan, from attached to partially detached

(colors are different throughputs – blue: low → red: high)

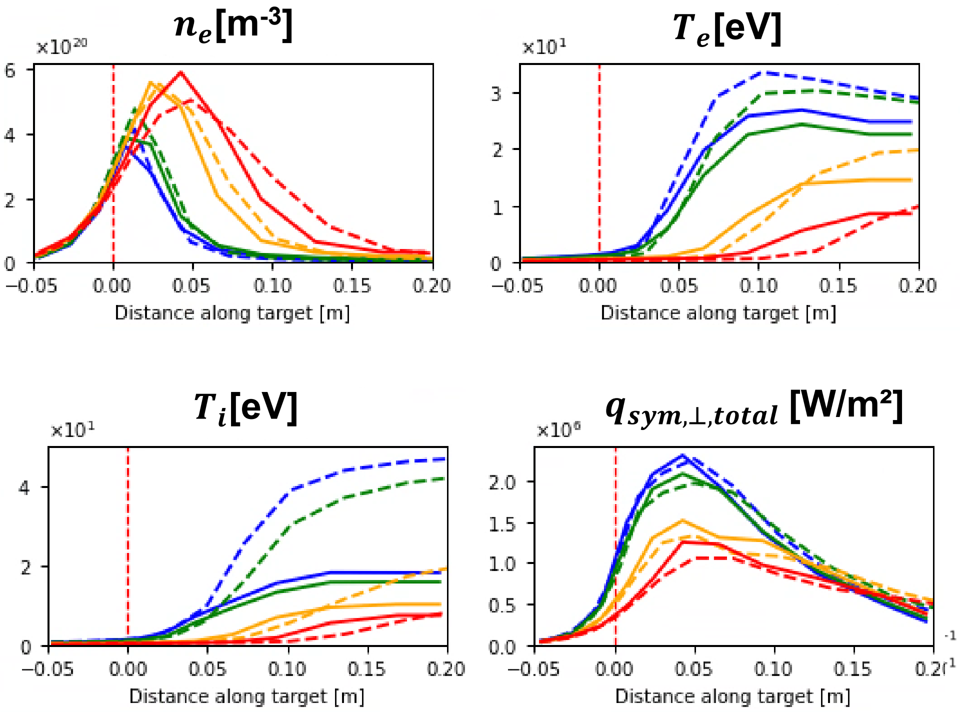
Solid lines: SOLEDGE3X

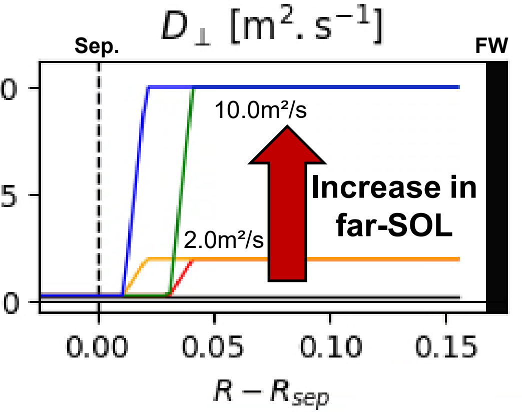
Dashed lines: SOLPS-ITER

Upstream (Outer midplane)

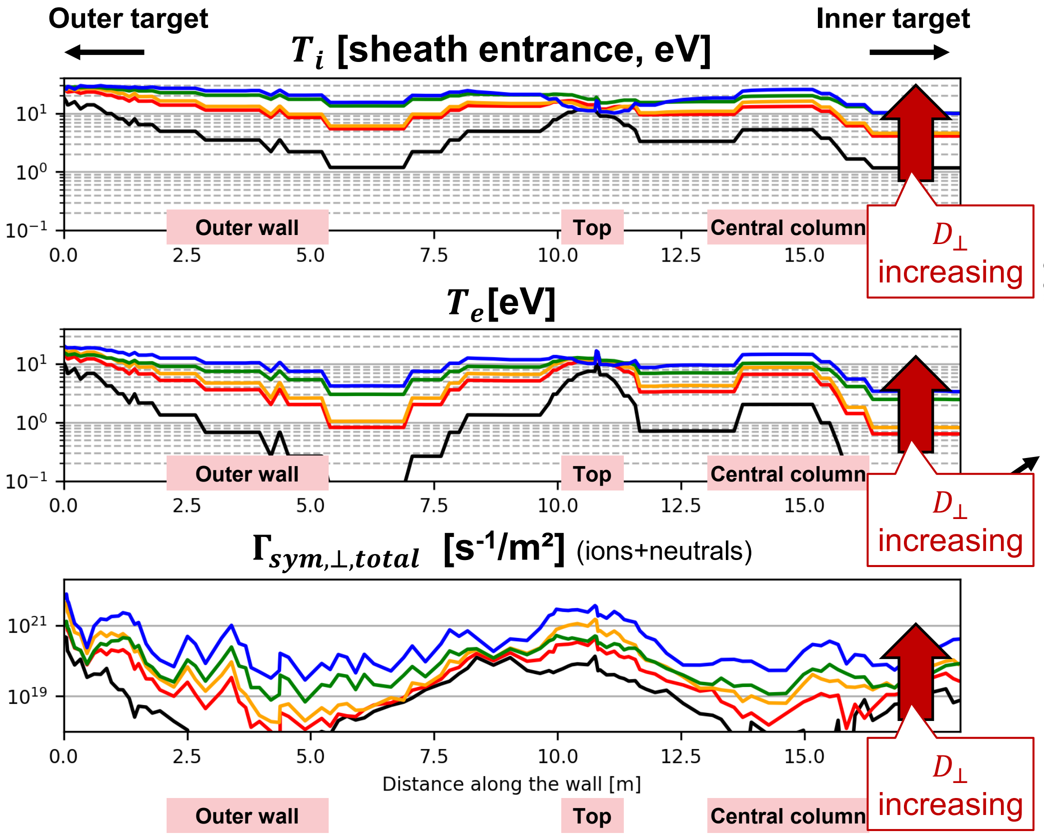


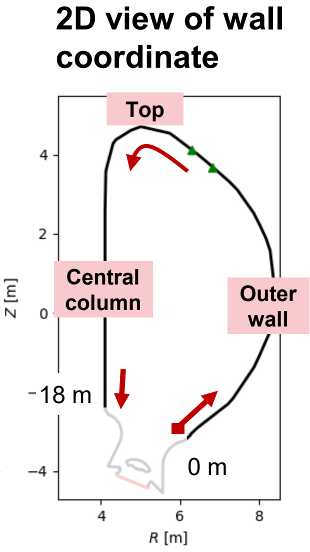
Outer Target



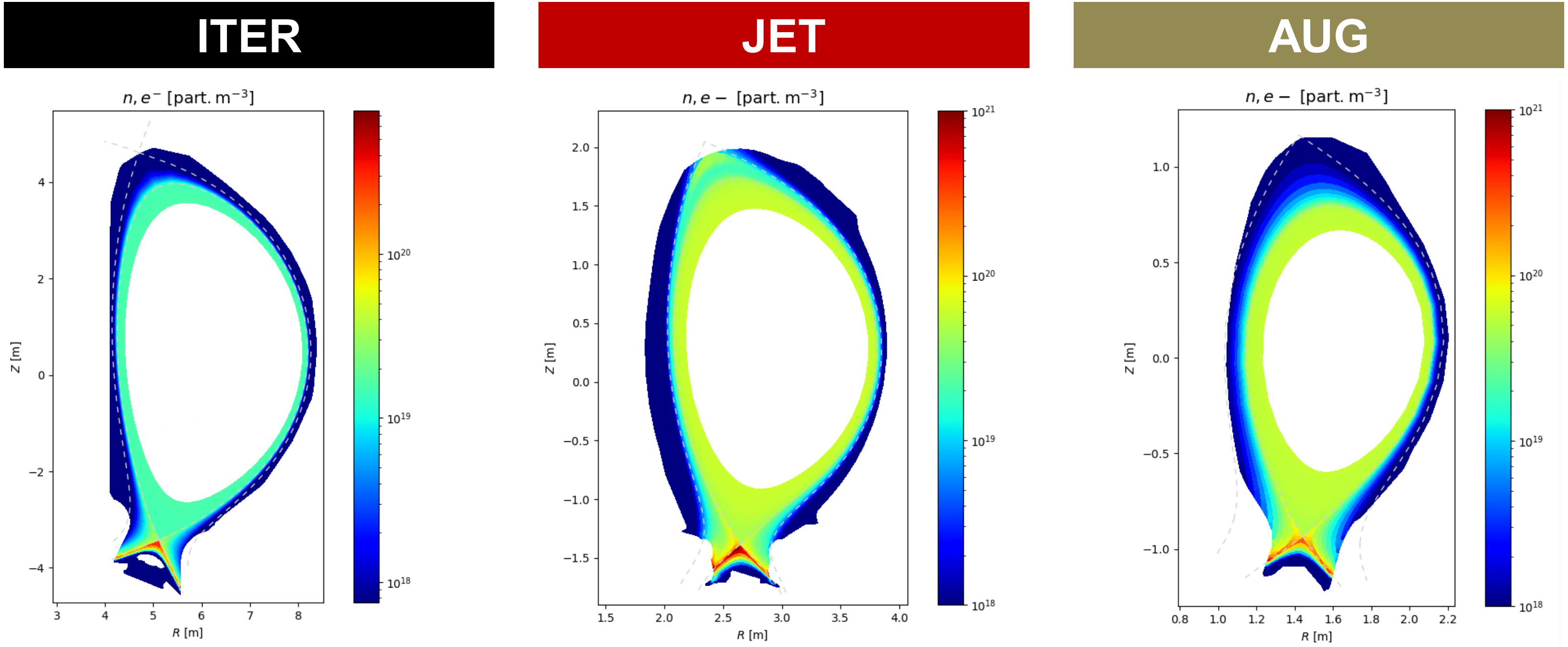


Impact of high far-SOL transport (low throughput):





3x throughput scans, unseeded



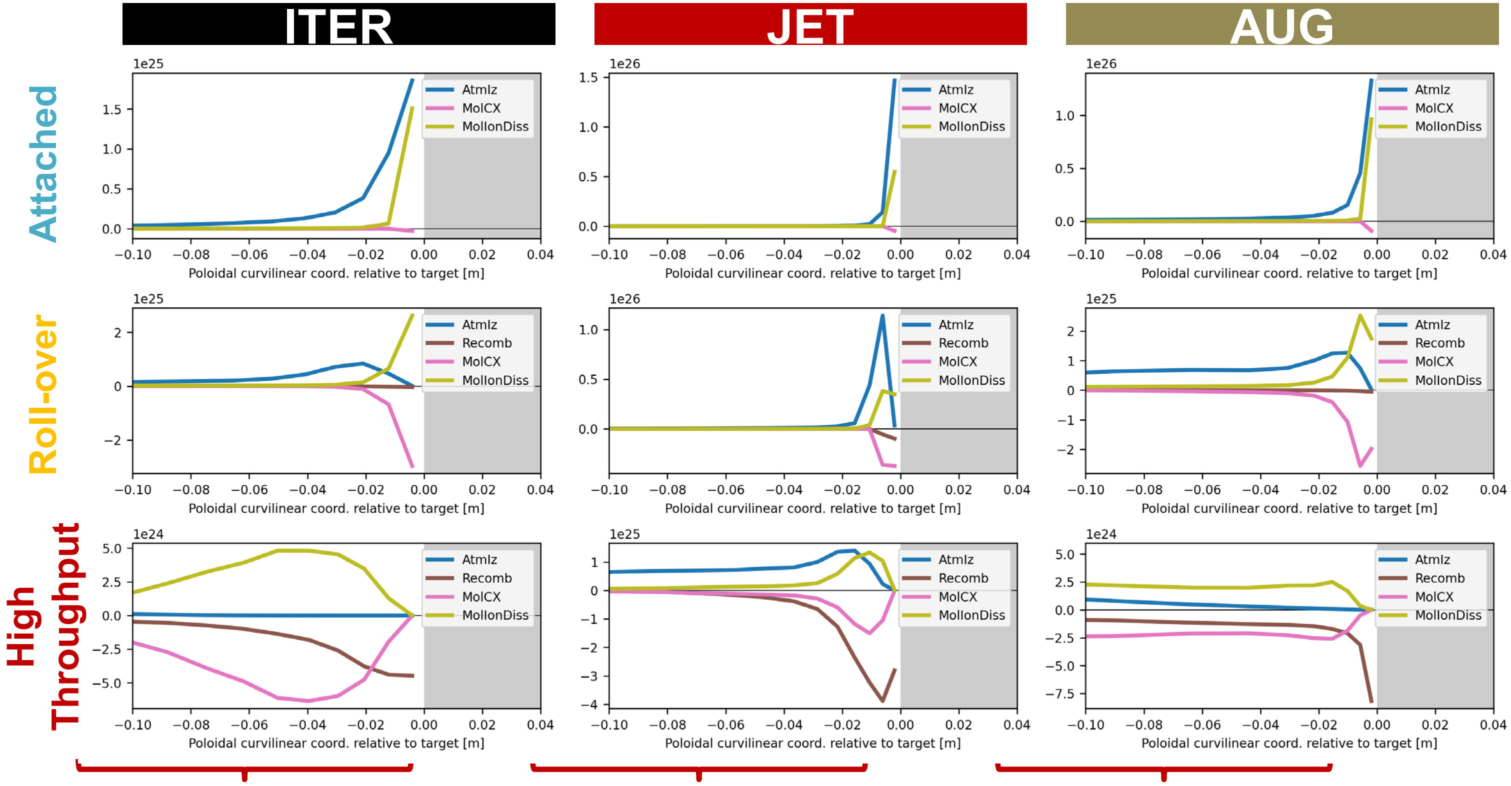
First attempt at simple look on obtained plasma-neutral processes:

- Do contributions importance vary widely ?
- Do we observe the same trends as in ITER cases ?

CAVEAT: Preliminary work, exploration

4. First comparison attempt with other MST cases
Same overarching trends recovered across machines

Volume ion particle source [$s^{-1}.m^{-3}$]:



Observations:

- Many differences but…
- **Same overall patterns**
- **Similar trends**
- **Same spatial scales** (cf. mfp)
- Requires further analysis and additional cases

Same scale size in meters along divertor leg (large divertors → better PNI confinement)