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EUROfusion

The role of plasma-atom/molecule interactions on power, particle and momentum balance during detachment

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[*] See author list of: S. Coda et al. 2019 Nucl. Fusion 59 112023

[**] See author list of: B. Labit et al. 2019 Nucl. Fusion 59 086020

Material is featured in:

- K Verhaegh *et al* 2021 *Plasma Phys. Control. Fusion* **63** 035018
- K Verhaegh *et al* 2021 *Nucl. Mater. Energy* 1000922
- IAEA FEC conference proceedings pre-print & Nucl. Fusion article (in preparation)

Detachment physics

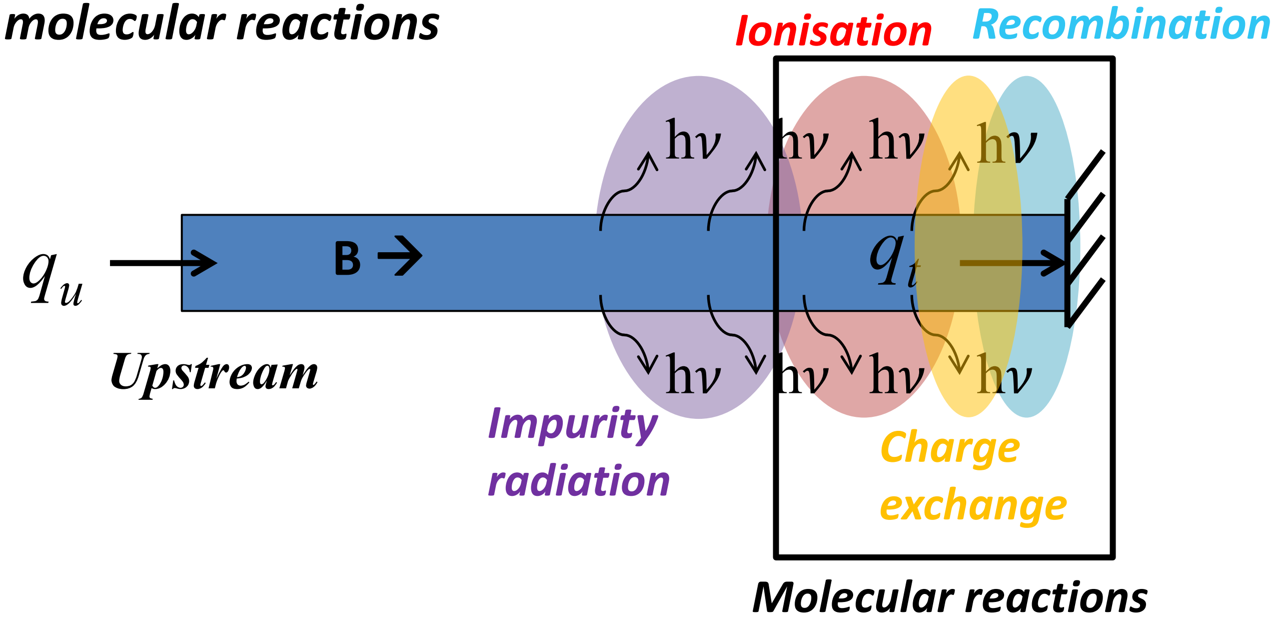
Detachment is necessary to mitigate power exhaust for ITER/DEMO:
<u>reduces target particle and heat load</u>

Detachment is driven by atomic/molecular reactions through dependencies between power, particle and momentum balances

Detachment requires:

- **Power loss**
- **Momentum loss**
- **Particle loss** (↓ ionisation and/or ↑ ion sink)

Detachment induced by chain of **atomic and *molecular reactions***



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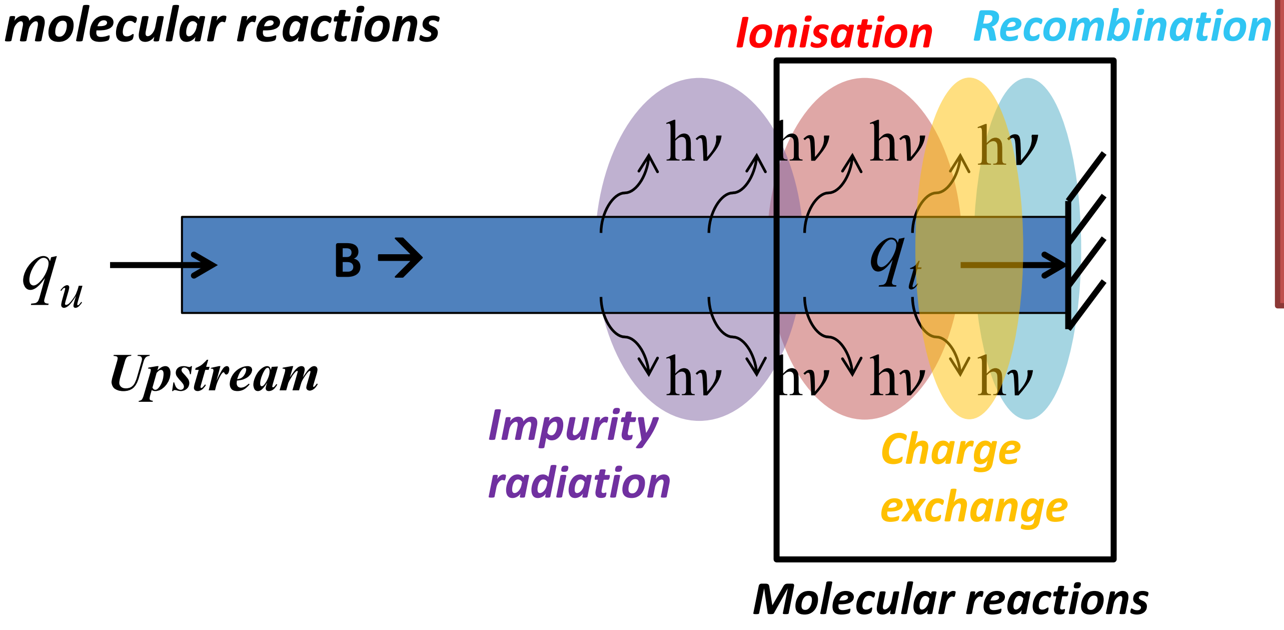


Detachment is driven by atomic/molecular reactions through dependencies between power, particle and momentum balances

***Plasma-molecule* interactions alter all three of these balances. However, this is not well understood.**

Our goal is to investigate these interactions experimentally to estimate:
- **impact on detachment (power/particle balance)**
- **Impact on diagnostic interpretation**

‘Detachment’ and plasma-molecule interactions

Detachment requires:

- **Power loss**
- **Momentum loss**
- **Particle loss**

Two different ‘flavours’ of plasma-molecule interactions

1. ***Collisions*** **between the plasma and H_2**

2. ***Reactions*** **between the plasma and ‘molecular species’**

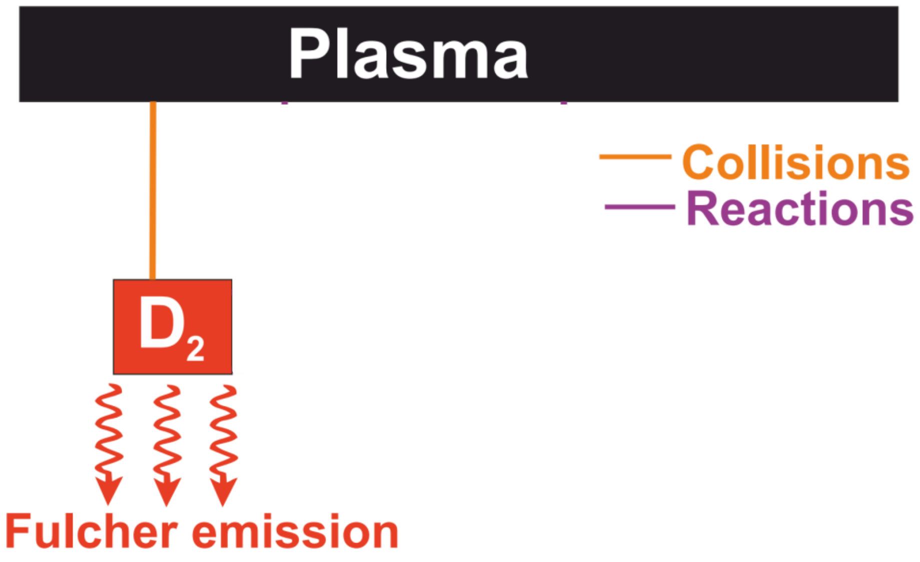
'Detachment' and plasma-molecule interactions

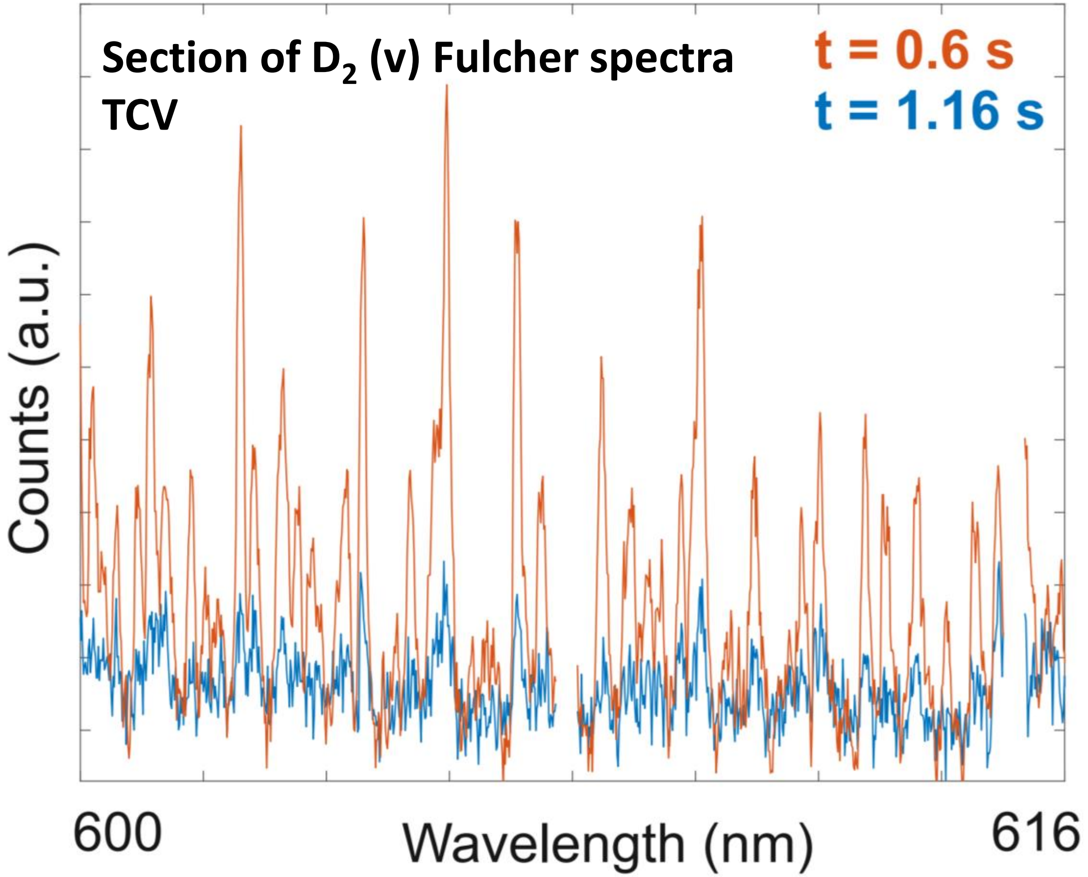
Detachment requires:
- Power loss
- Momentum loss
- Particle loss

1. ***Collisions*** **between the plasma and H_2**
   a) Transfers momentum/power plasma -> molecules,
   b) Excites D_2 (v) **-> Molecular spectra** (negligible radiation)

2. ***Reactions*** **between the plasma and 'molecular species'**

Studied experimentally in tokamaks [Fantz, 2002, et al.; Fantz, 2001, et al.; Groth, 2019, et al. ….]





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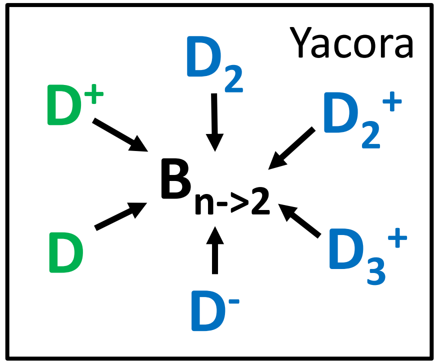
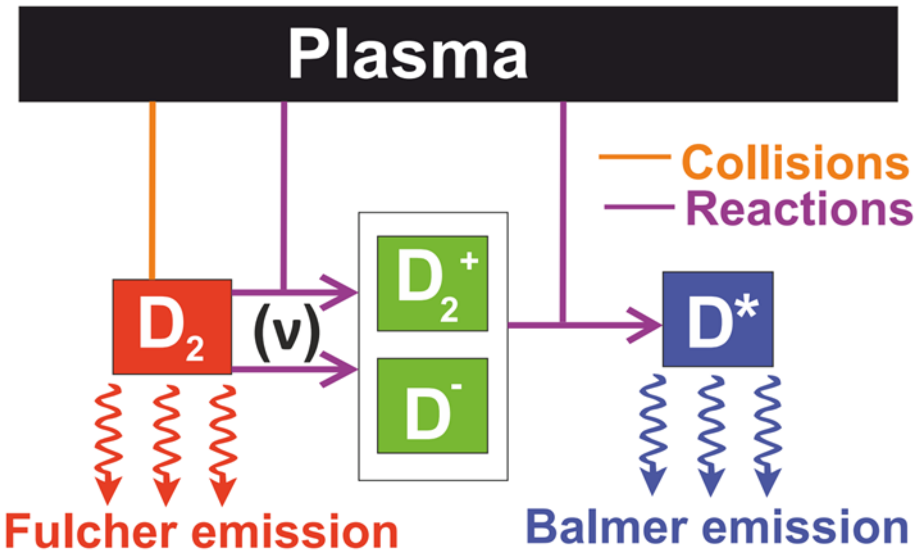
   For instance: $D_2 + D^+ \rightarrow D_2^+ + \mathbf{D}$; $D_2^+ + e^- \rightarrow$ **D*** + **D***
   [Molecular Activated Recombination (**MAR**)]
   a) Impacts particle (MAR & MAI) and momentum balance
   b) Leads to ***excited (*) hydrogen atoms*** -> **atomic line emission & radiation**

[Wünderlich, et al. *JQSRT* 2020]



‘atomic’
‘molecular species’



Hydrogen Balmer spectrum

‘Detachment’ and plasma-molecule interactions

Detachment requires:
- Power loss
- Momentum loss
- Particle loss

Impact plasma-mol. inter. on H emission during detachment relatively unknown

<u>In this work:</u> we investigate this and use it as a diagnostic.

2. <u>*Reactions*</u> between the plasma and ‘molecular species’

For instance: $D_2 + D^+ \rightarrow D_2^+ + \mathbf{D}$; $D_2^+ + e^- \rightarrow$ **D*** + **D***

[Molecular Activated Recombination (**MAR**)]

a) Impacts particle (MAR & MAI) and momentum balance

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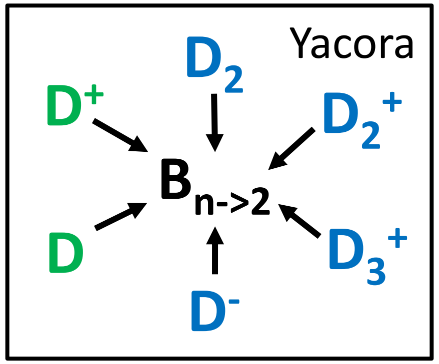

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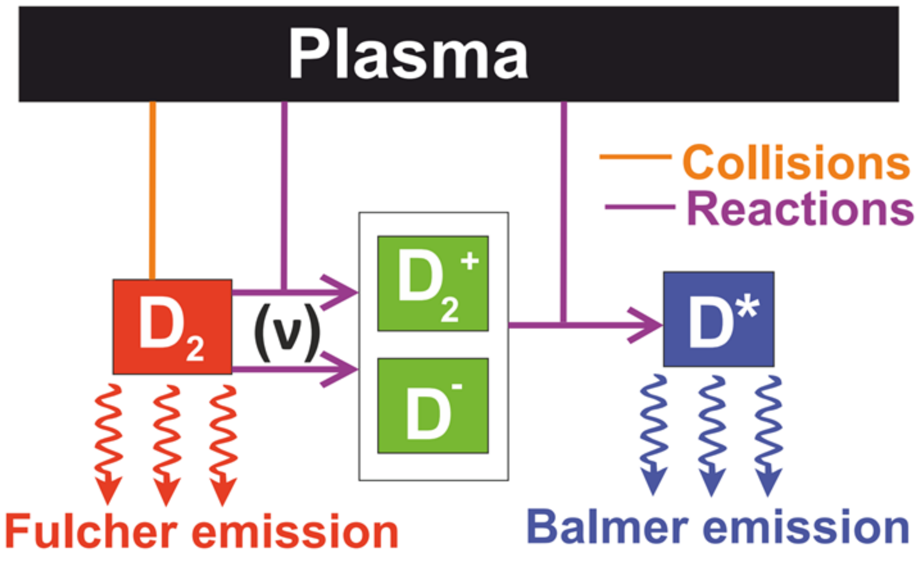
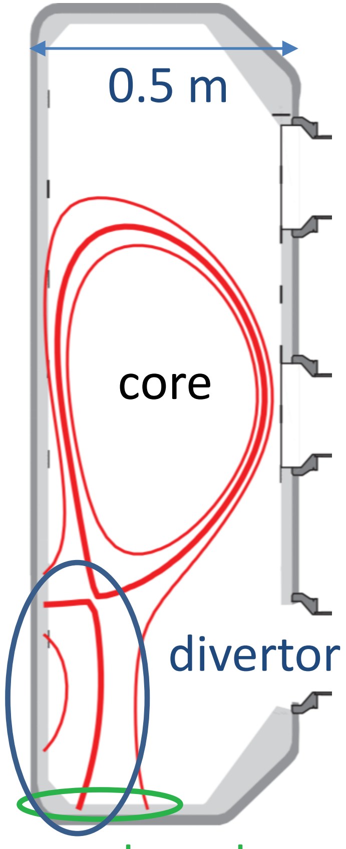


Hydrogen Balmer spectrum

Detachment on TCV



TCV – 'Medium Sized' tokamak:

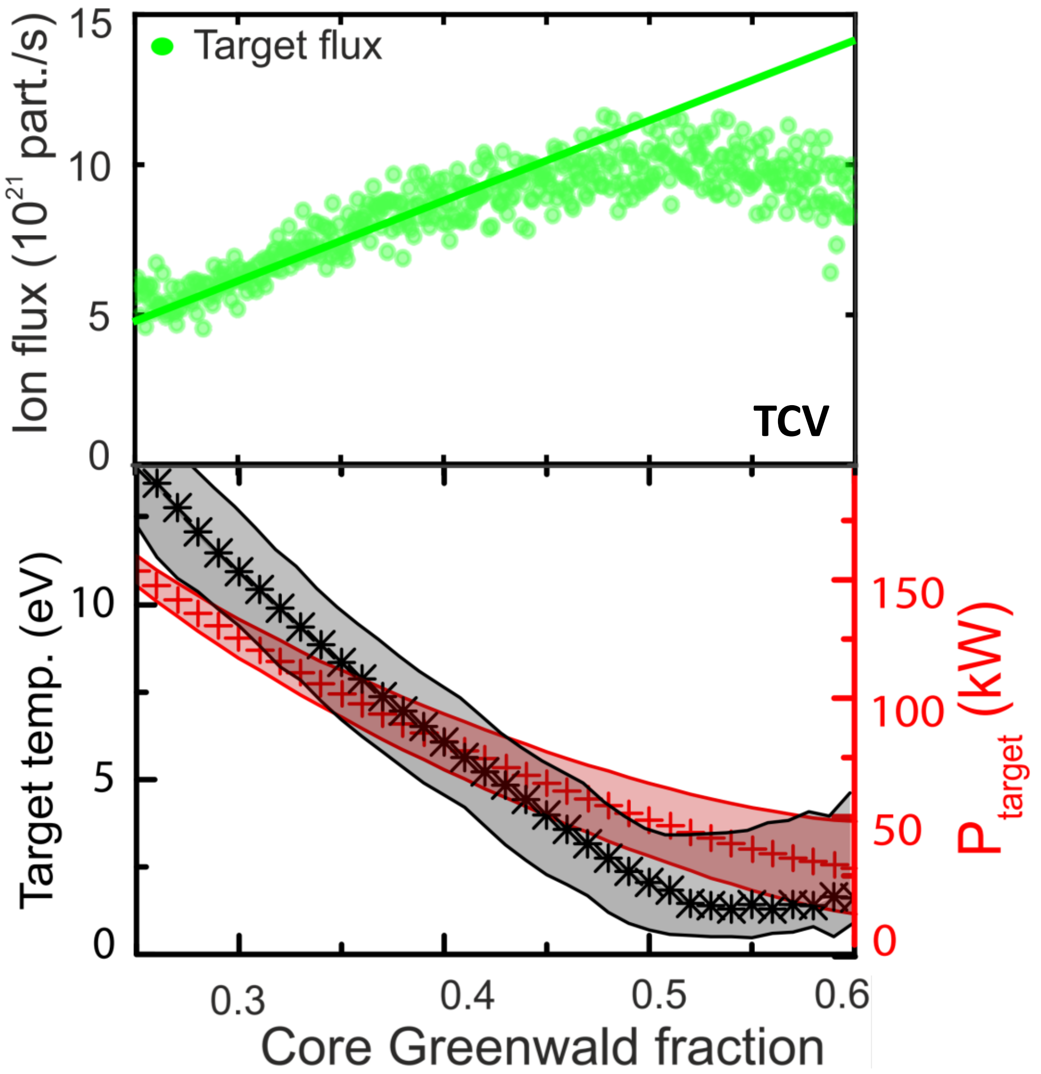
- Carbon wall, open divertor

For the discharges discussed

- Ohmic, L-mode, deuterium , I_p = 340 kA
- Conventional single null

TCV core density ramp:

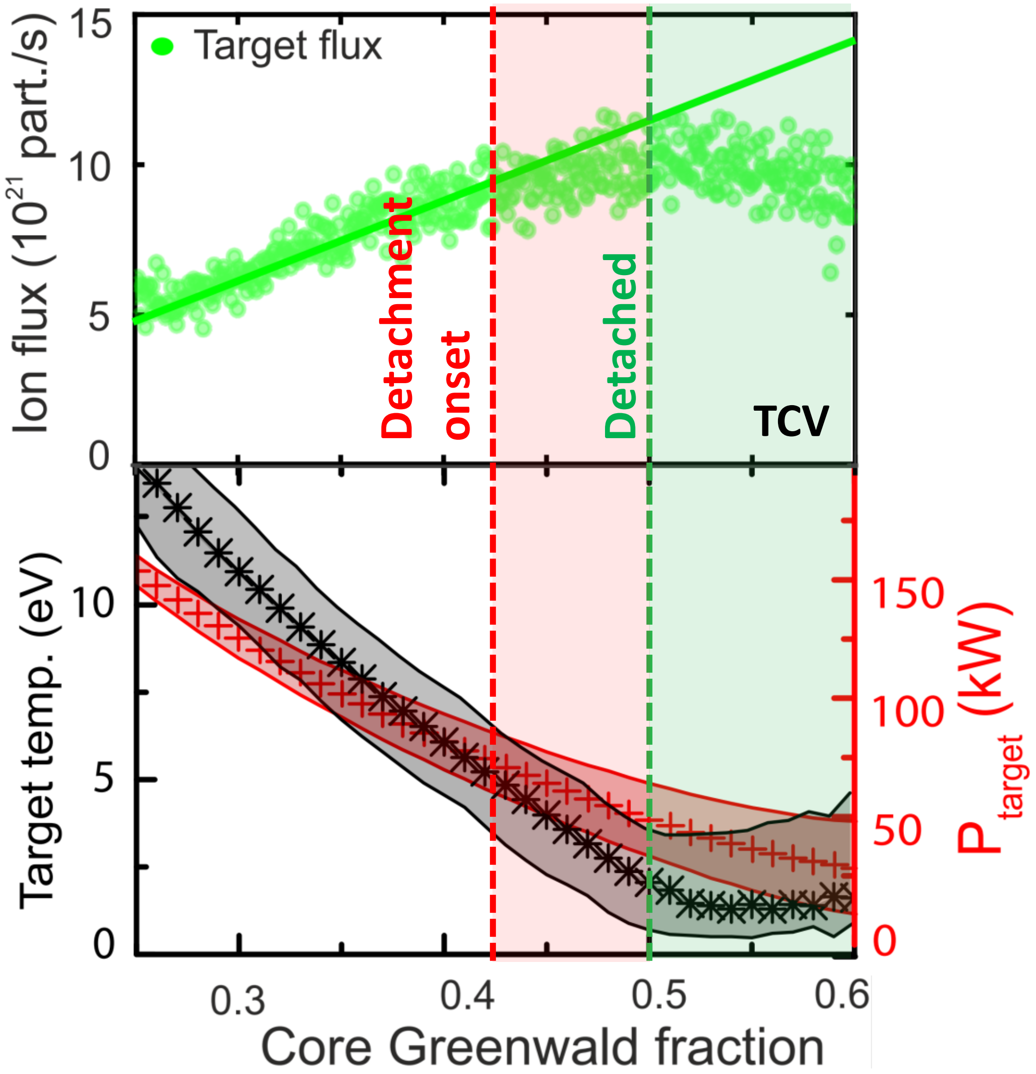
- **Integrated ion target flux (I_t)** rises linearly, flattens and rolls-over
- Target temperature / power load drops



Detachment on TCV

Three phases in the density ramp:

1. **Attached**
2. **Detachment onset (I_t deviates from linear)**
3. **'Roll-over' detached**



We will discuss these three different phases throughout the talk

Goals and outline

- Motivation and introduction

1. **Investigate how plasma-molecule interactions impact hydrogenic line emission, and how Balmer series measurements can be used to study molecular effects**

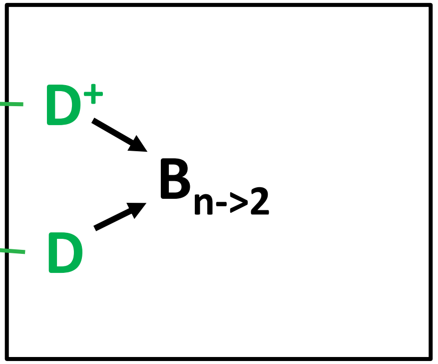
2. Investigate how plasma-atom/molecule interactions can impact detachment through power/particle losses

3. Investigate under which conditions plasma-molecule interactions impact detachment and how this compares to simulations

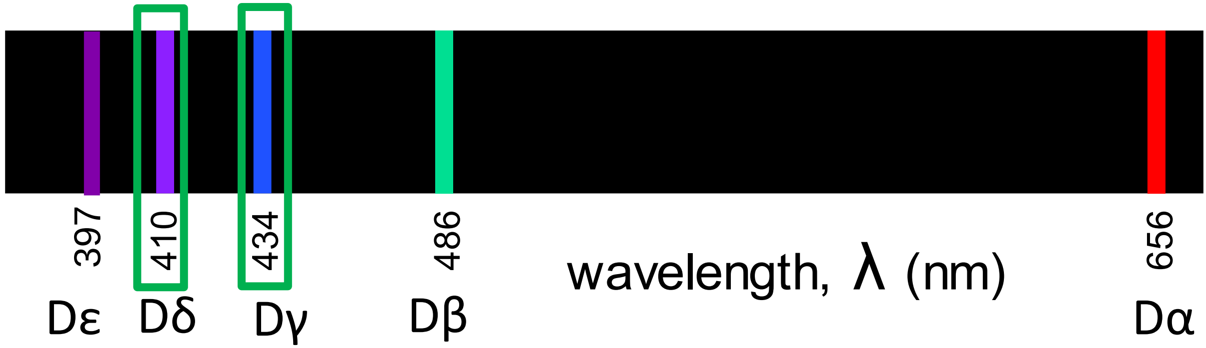
- Conclusions

$H\alpha$ emission and molecules

- Previously, developed tools for analysing excitation and recombination contributions using two Balmer lines [Verhaegh, et al. 2019, PPCF; Verhaegh, et al. 2019, NF]
  - **Electron-ion recombination rates** (EIR)
  - **Ionisation rates** (from excitation)
- Lower-n Balmer lines are less influenced by EIR -> ‘effectively’ more influenced by plasma-molecule interactions (-> avoid using this for the ‘atomic analysis’)



Hydrogen Balmer spectrum



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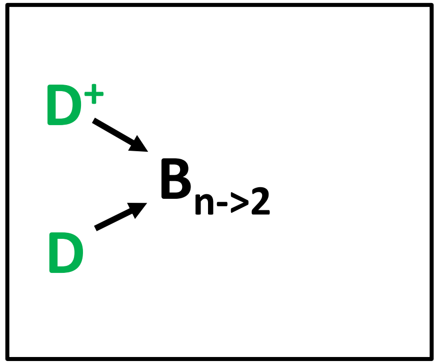
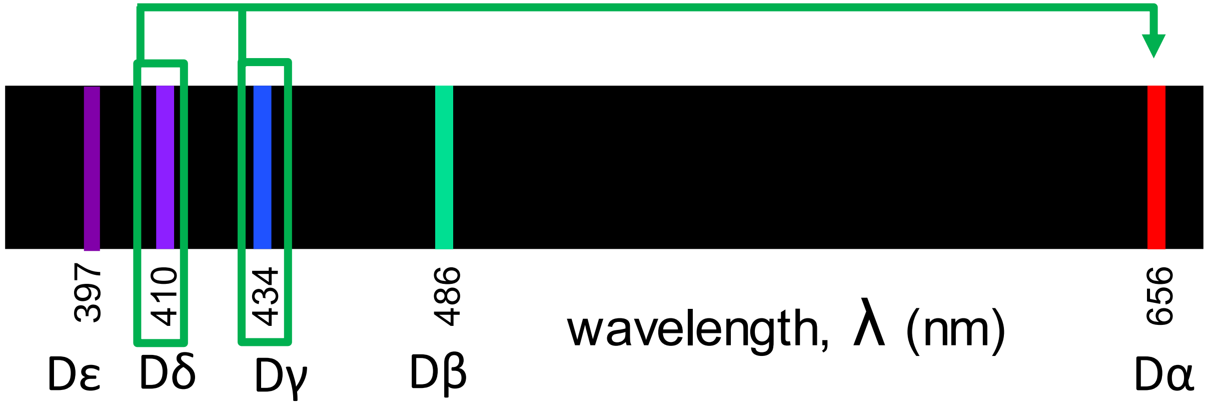


Investigate molecules:

1. Apply **atomic analysis** to **medium-n Balmer line pair**
2. Use result to estimate **atomic contribution Hα,** compare against measurement

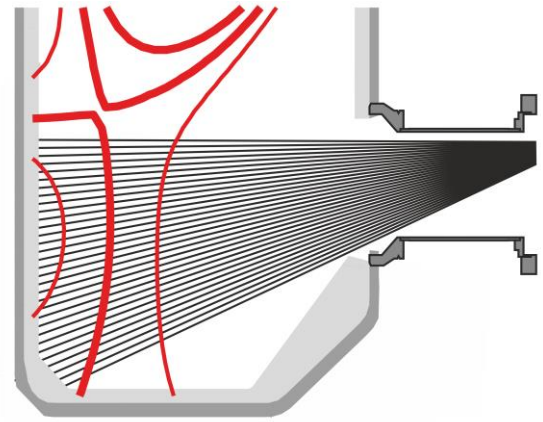
Hydrogen Balmer spectrum

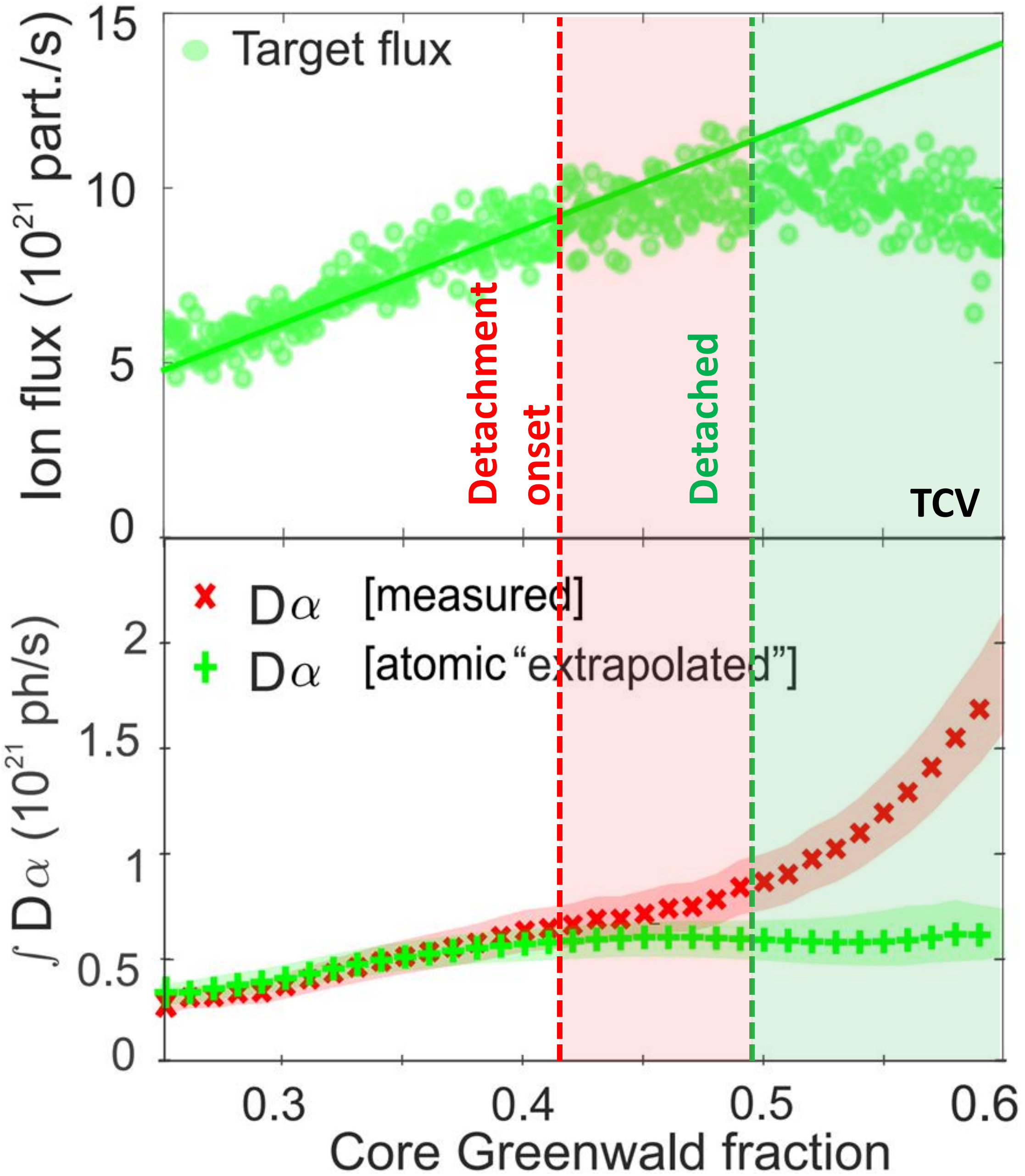


$D\alpha$ emission and molecules - results

[Verhaegh, et al. NME 2021]

- **Measured $D\alpha$ emission** increases during detachment beyond **$D\alpha$ emission expected purely on the basis of atomic reactions**





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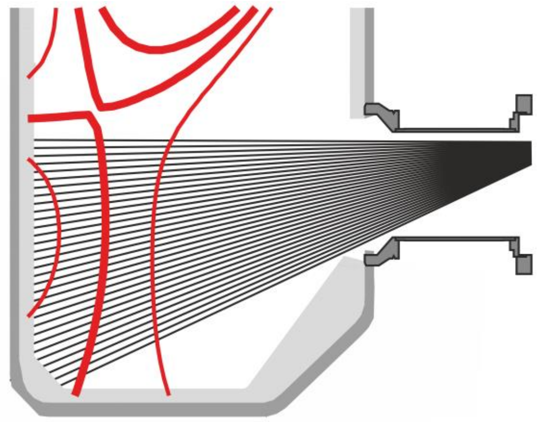
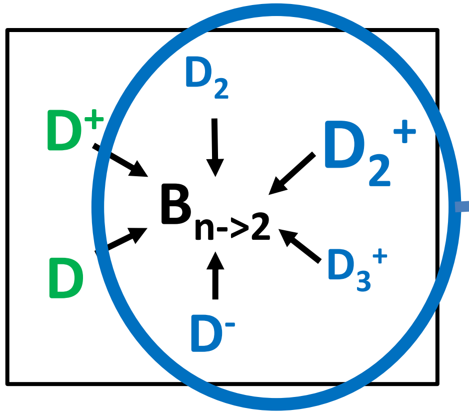
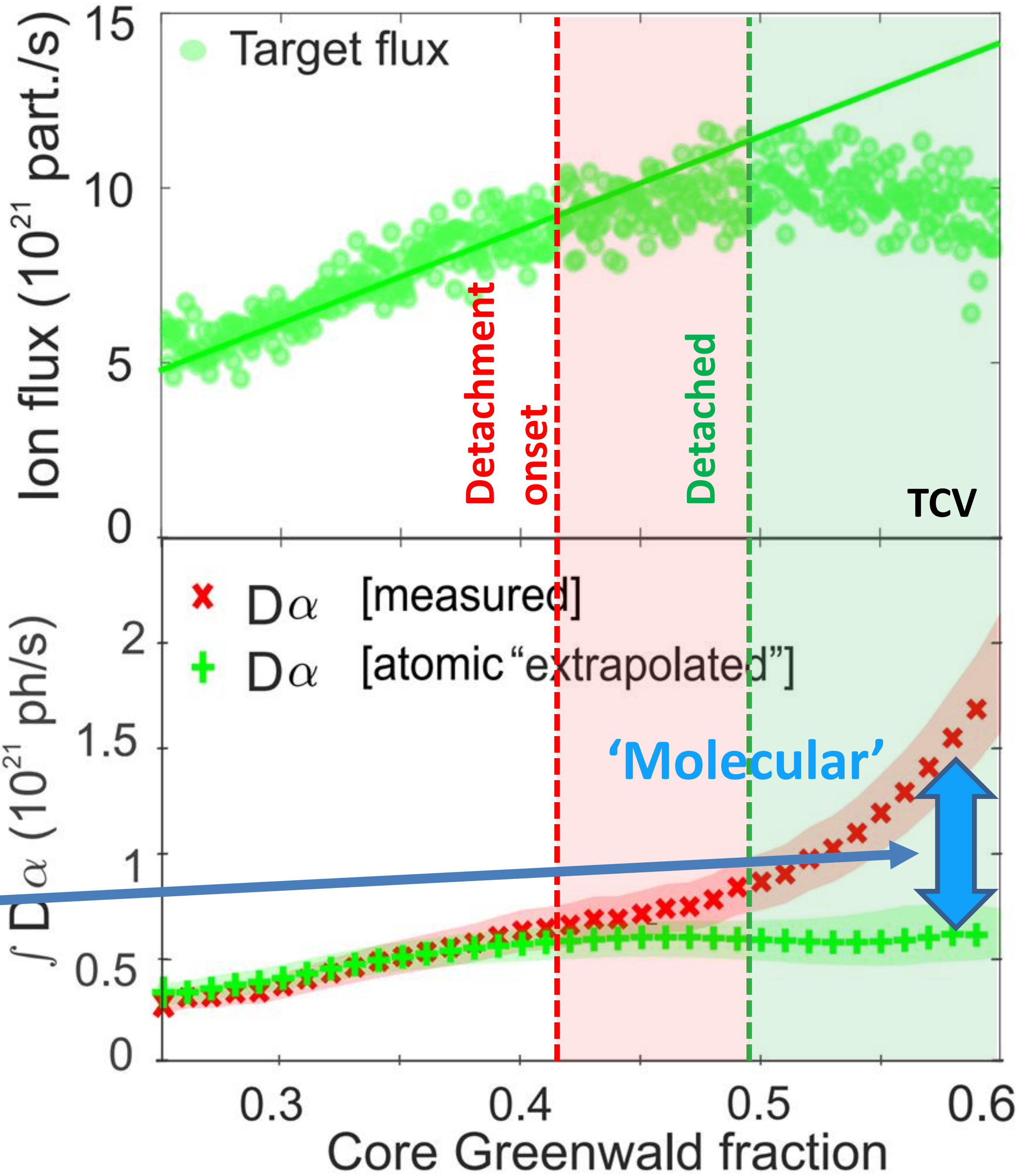






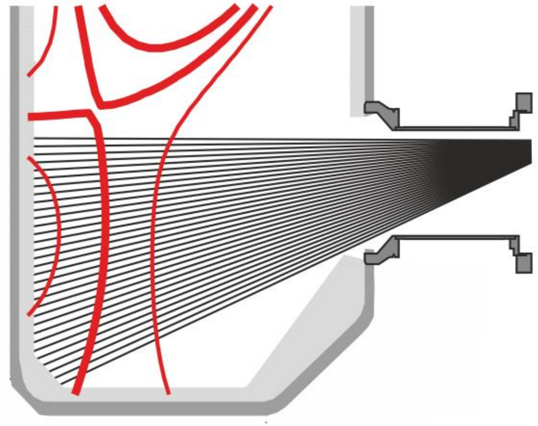
$D\alpha$ emission and molecules - results

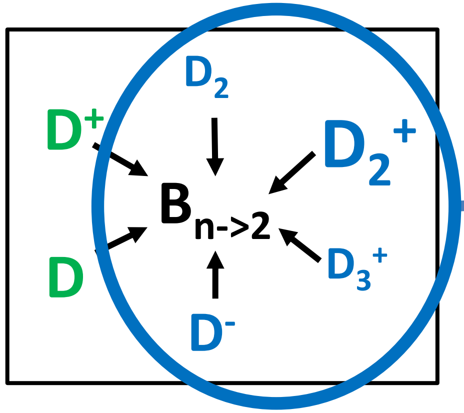
[Verhaegh, et al. NME 2021]

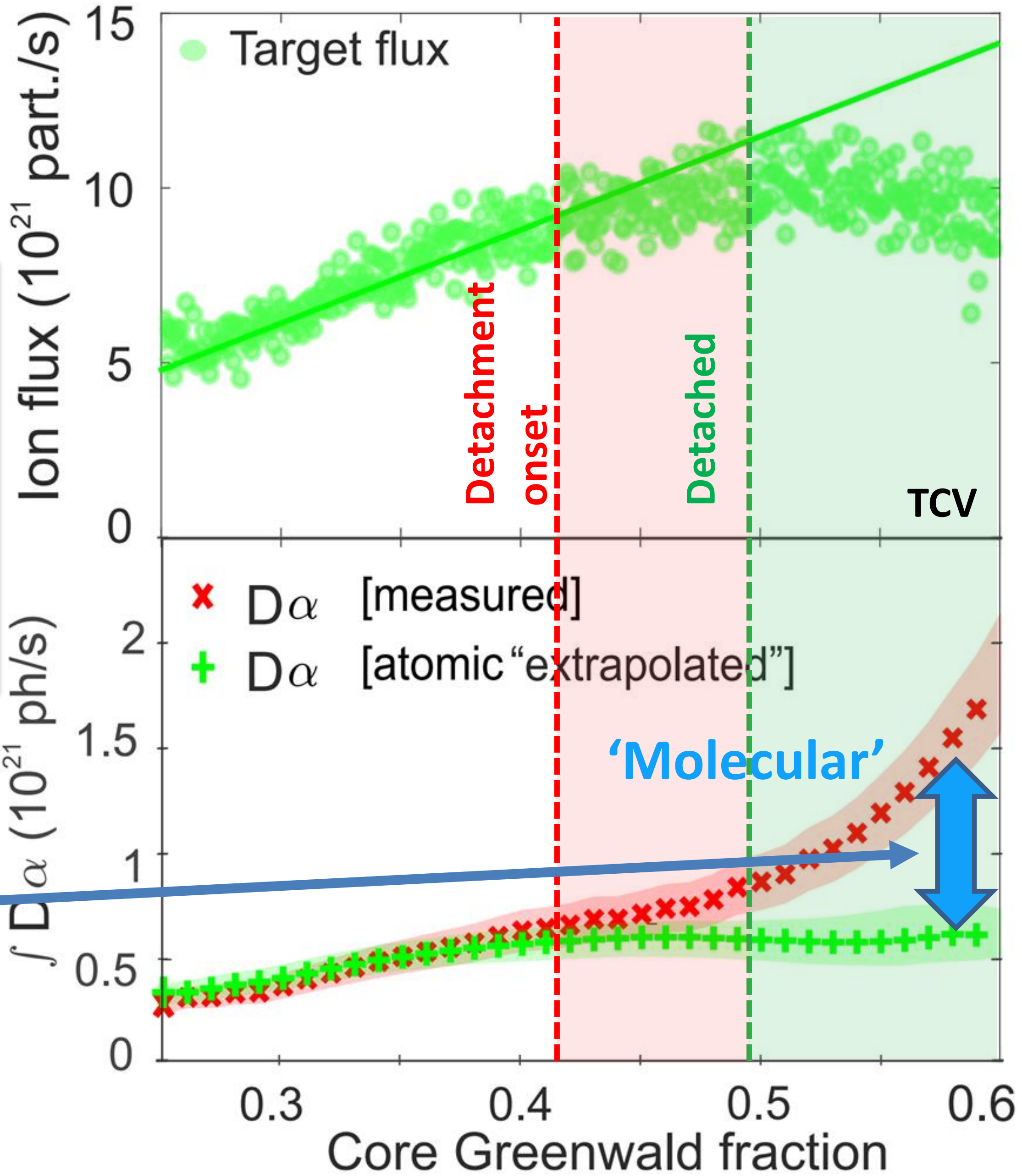
- Measured $D\alpha$ emission increases during detachment beyond $D\alpha$ emission expected purely on the basis of atomic reactions
  -> $D\alpha$ from excited atoms after plasma-molecule interactions

This mismatch of Dα is an indicator for:
1. Particle losses through MAR
2. Strong contribution plasma-mol. inter. Balmer lines
3. Power losses from D* after plasma-mol. interactions

We developed a technique for extracting this quantitatively from Dα, Dβ, Dγ, Dδ BaSPMI - [Verhaegh, et al. 2021, PPCF]





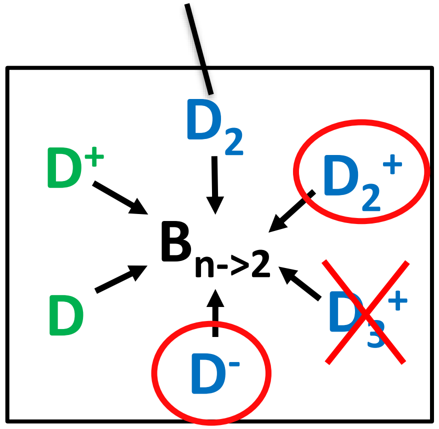


Novel Balmer line spectra analysis - BaSPMI

Spectroscopic analysis: [Verhaegh, et al. 2021, PPCF]

1. Apply this **atomic analysis** to **medium-n Balmer line pair**
2. Use result to estimate **atomic contribution** **Dα, Dβ**
3. **Measured Dα, Dβ = 'Atomic' + 'Molecular' emission**
4. Iterate to **self consistent separation Dα, Dγ, Dδ** (and Dβ for D_2^+, D^- separation)
5. Multiply **separate brightnesses** with **'reaction/radiation per photon' ratios** to obtain:
   1. **Particle sinks/sources** (MAR, MAI, ionisation, electron-ion recombination)
   2. **Radiative power losses**

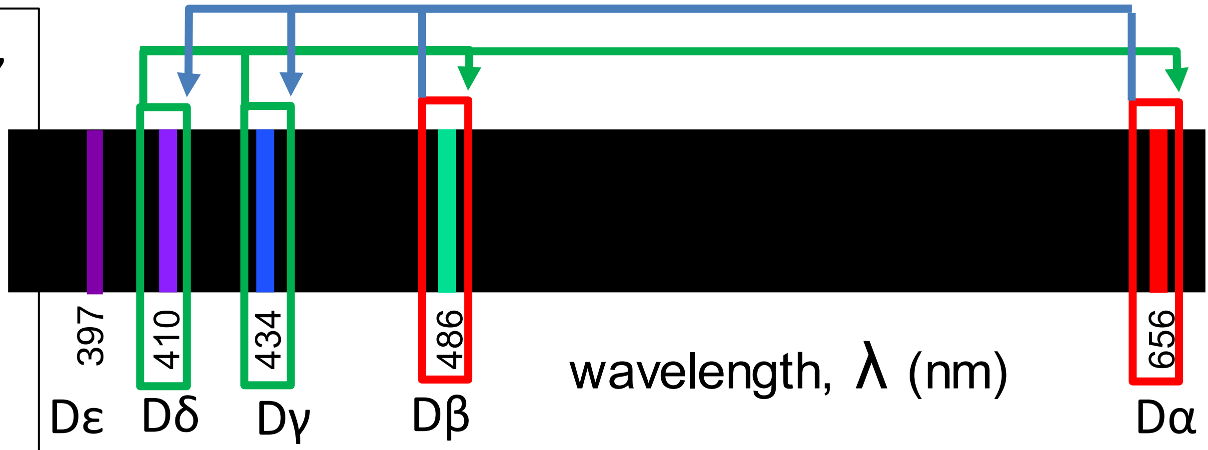
Negligible impact, estimated with SOLPS



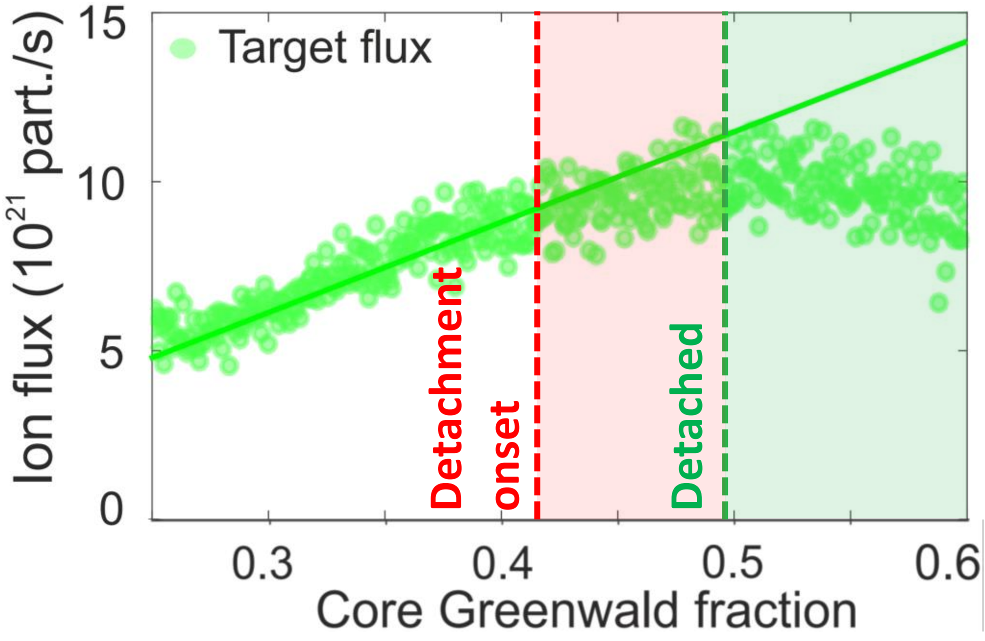
[Wünderlich, et al. Yacora]

- Uses **hydrogen CR** model Yacora on the Web –Wünderlich, et al., results for MAR/MAI and population coefficients (**applied to deuterium plasma**)
- Does not rely on creation cross-sections for D_2^+ and D^-
- Monte Carlo **uncertainty** propagation (line ratios (13%), brightnesses (18%), … 12.5/25% **atomic/molecular coefficients**)

Hydrogen Balmer spectrum



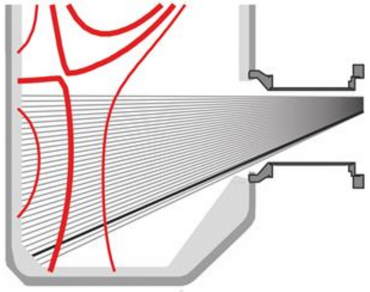
How plasma-mol. interaction impacts hydrogenic line emission

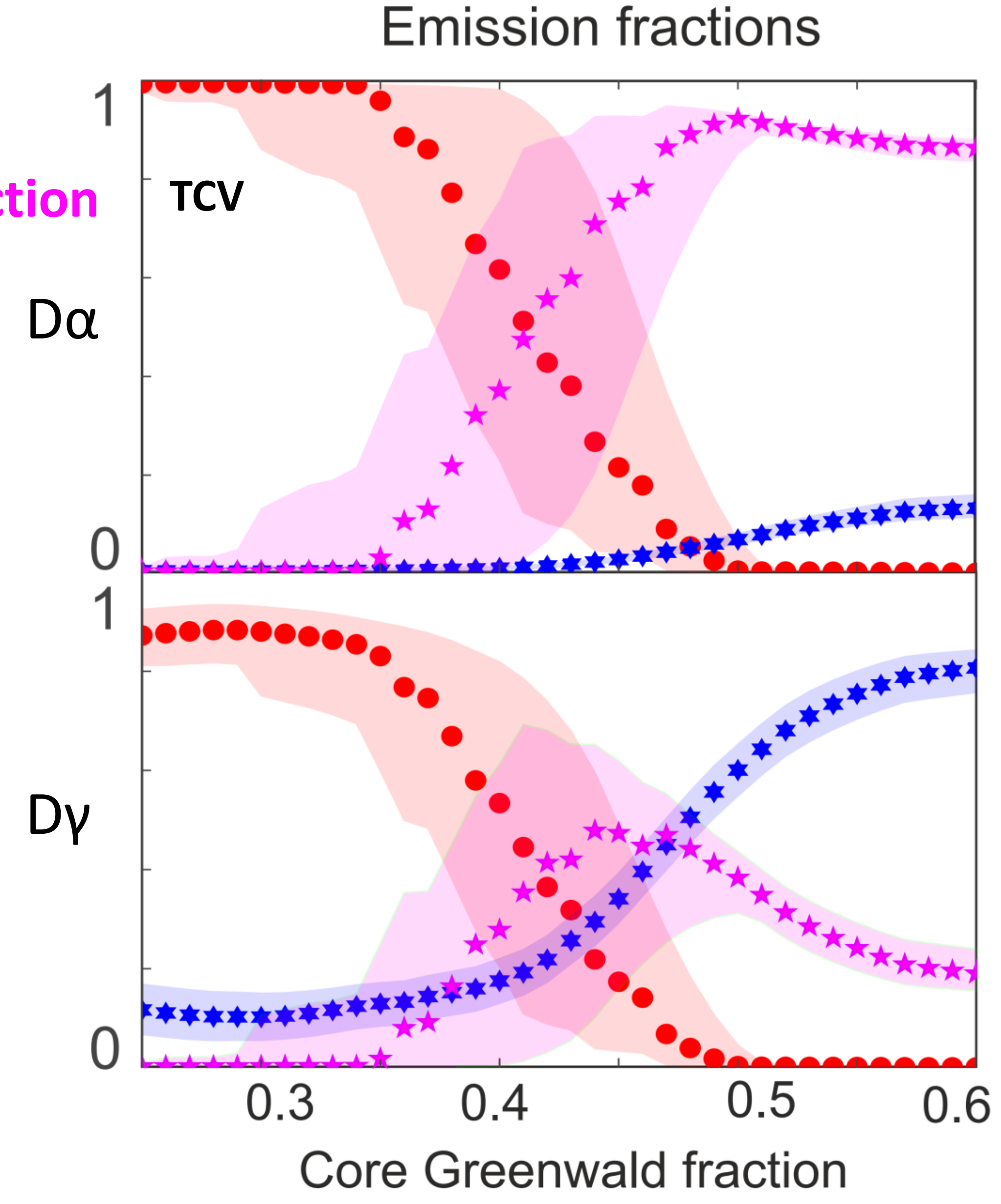


Excitation (D)

EIR – (D^+)

Plasma-mol. interaction





[Verhaegh, et al. NME 2021]

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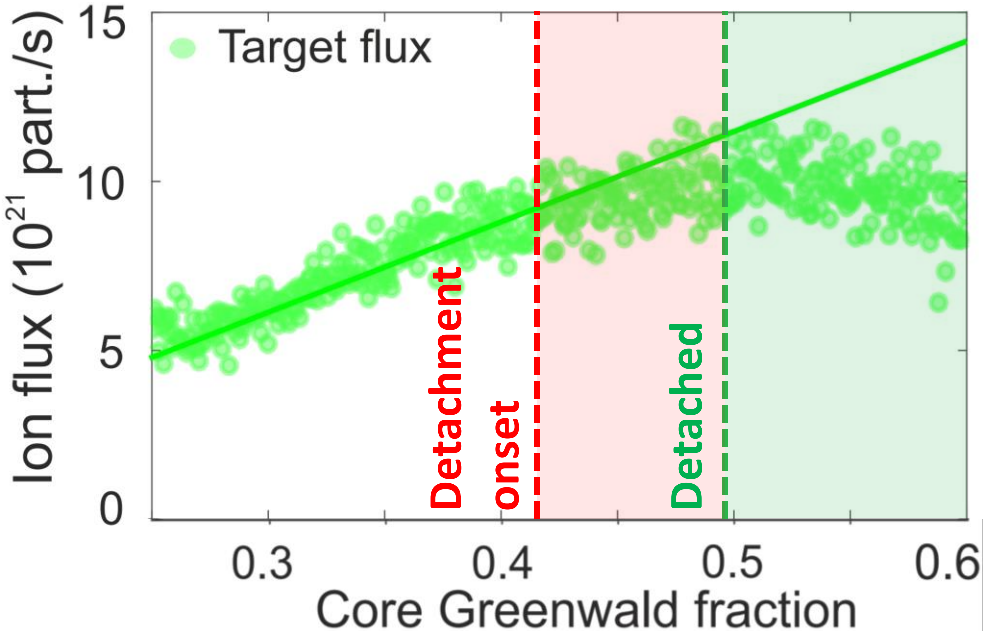

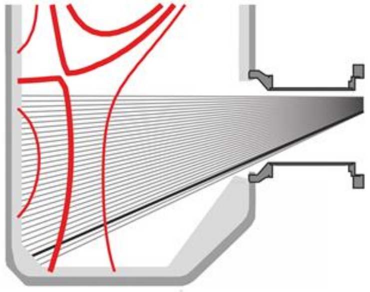

Excitation (D)

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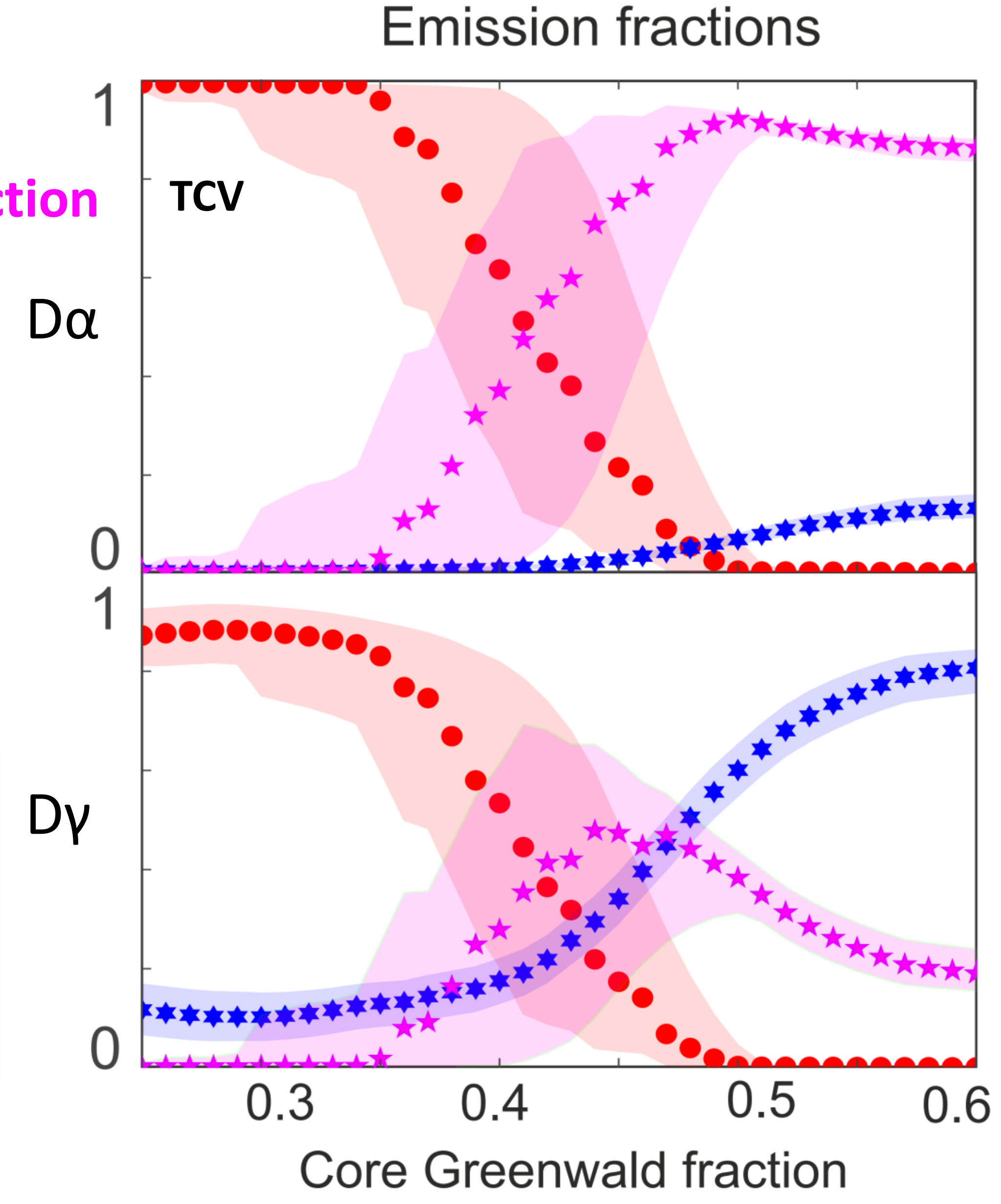
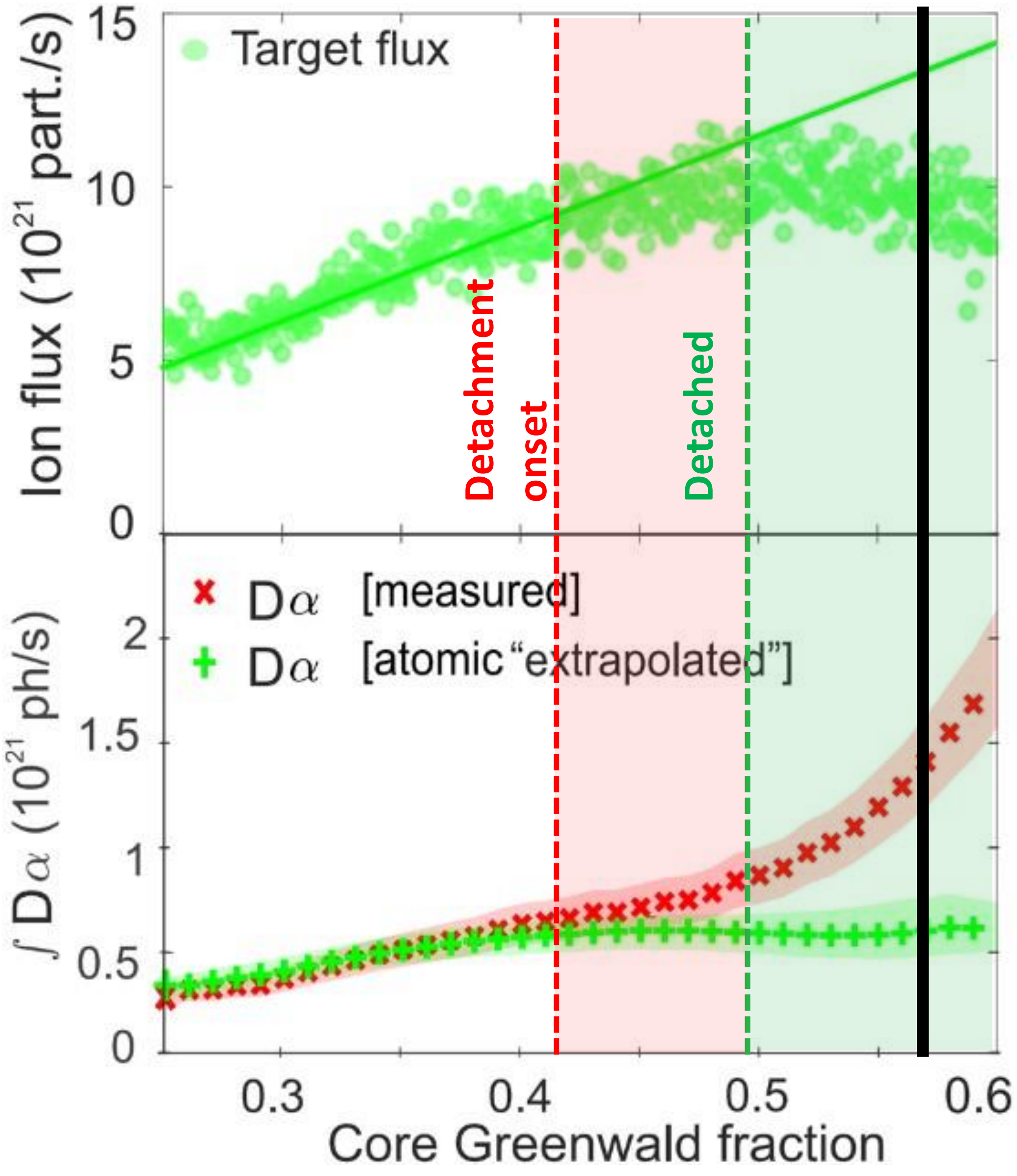
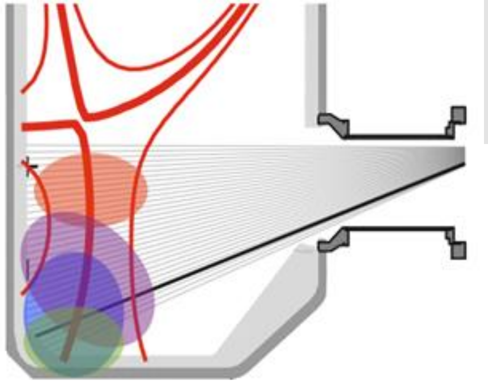


Plasma-molecule interactions:

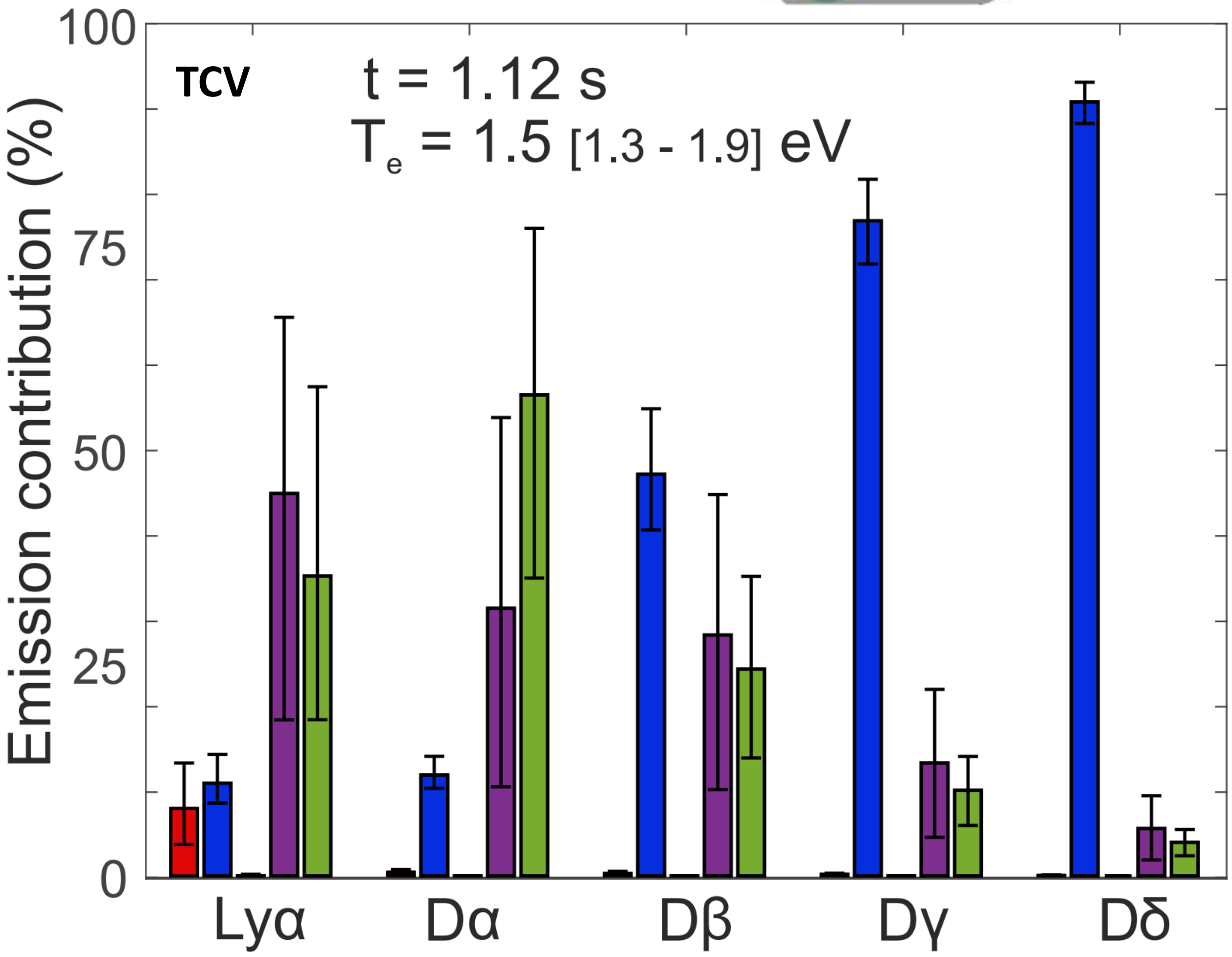
- Start to impact the hydrogenic spectra at **detachment onset**
- Impact Hα particularly (90% near target)
- Have a non-negligible impact on medium-n Balmer lines (<40%, needs to be accounted for ionisation estimates)

How plasma-mol. interaction impacts hydrogenic line emission





Excitation (D)
EIR – (D^+)
Molecules (D_2^+, D_2, D^-)



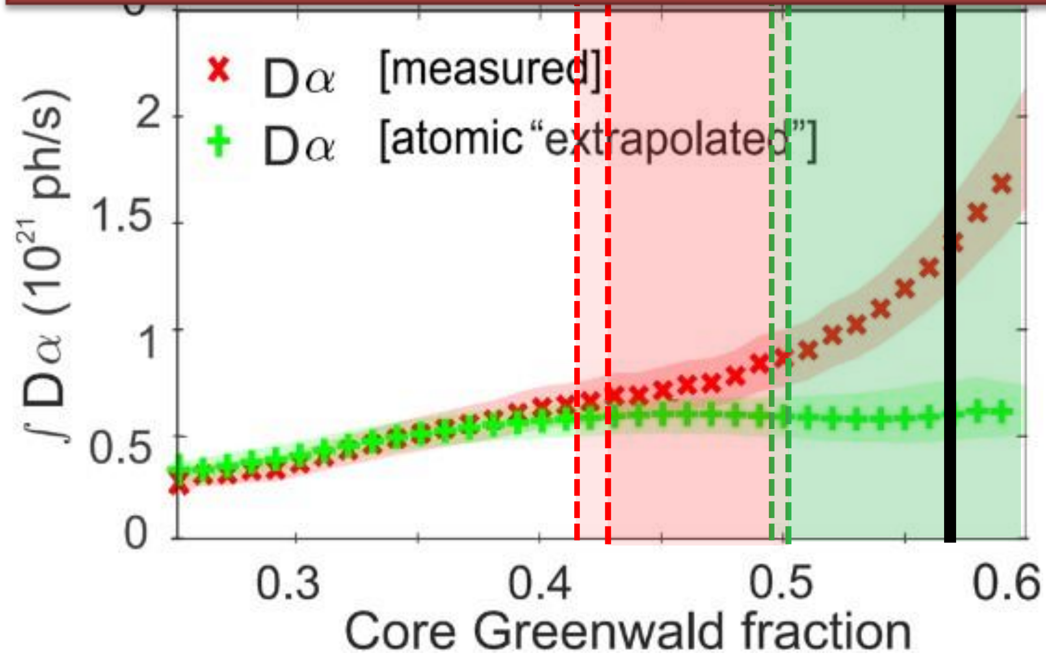
[Verhaegh, et al. 2021, PPCF]

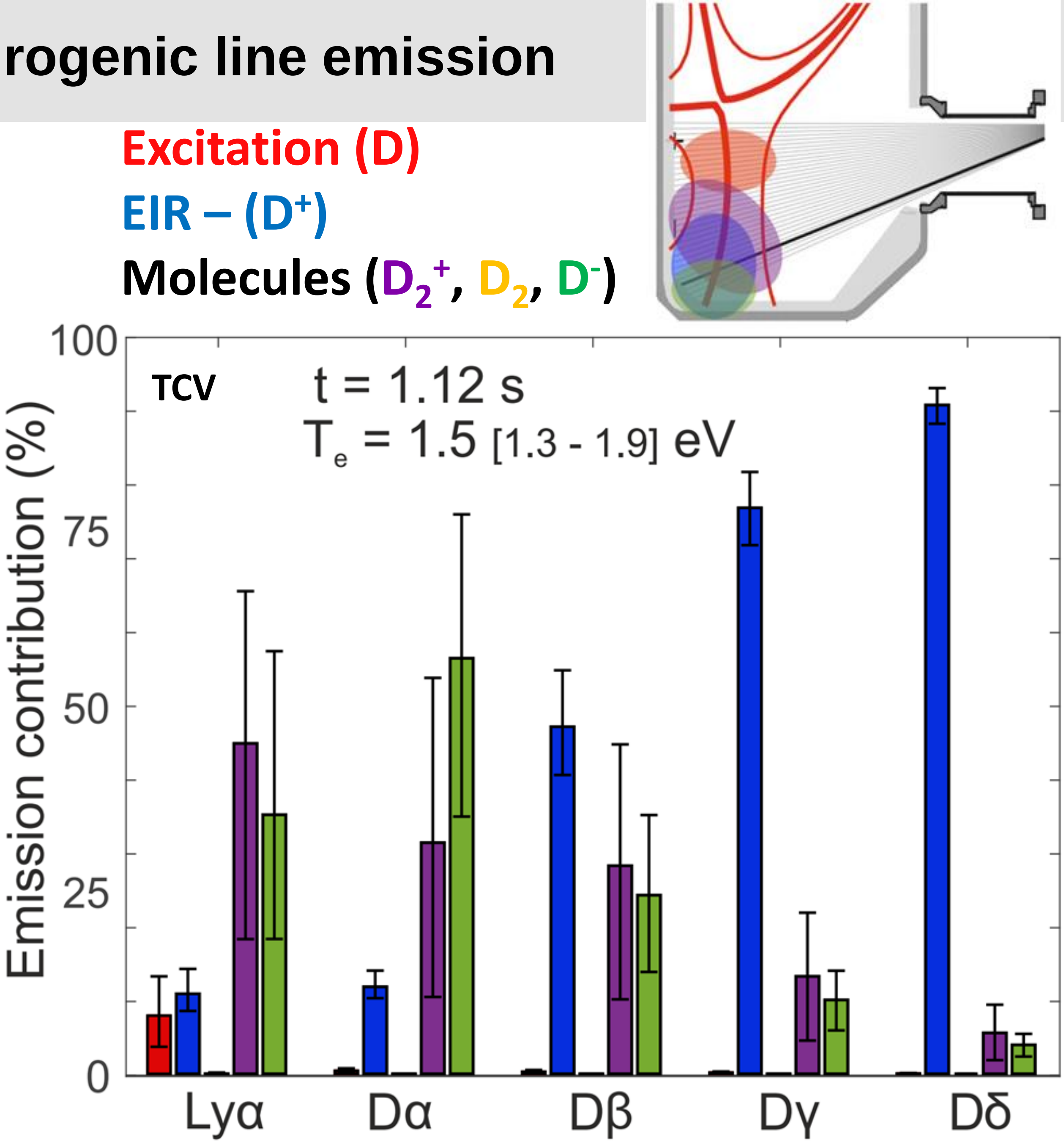
How plasma-mol. interaction impacts hydrogenic line emission

Analysis suggests D^- may be present despite low cross-section for D [Krishnakumar, et al. PRL, 2011]

If D^- is not accounted for, Dβ would be overestimated by 34 [25-44]% near the target

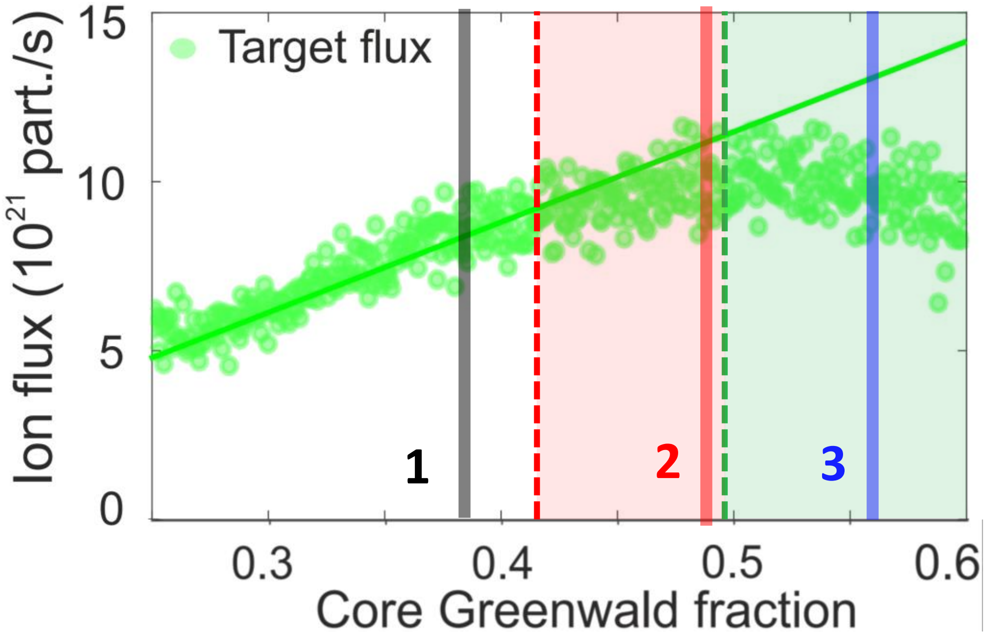
MAR/power losses similar (given the uncertainties) whether D^- is accounted for or not

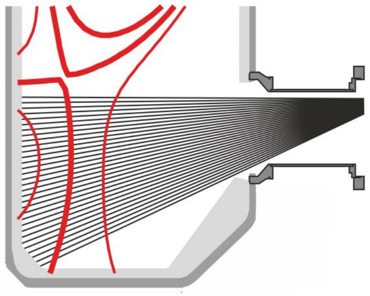


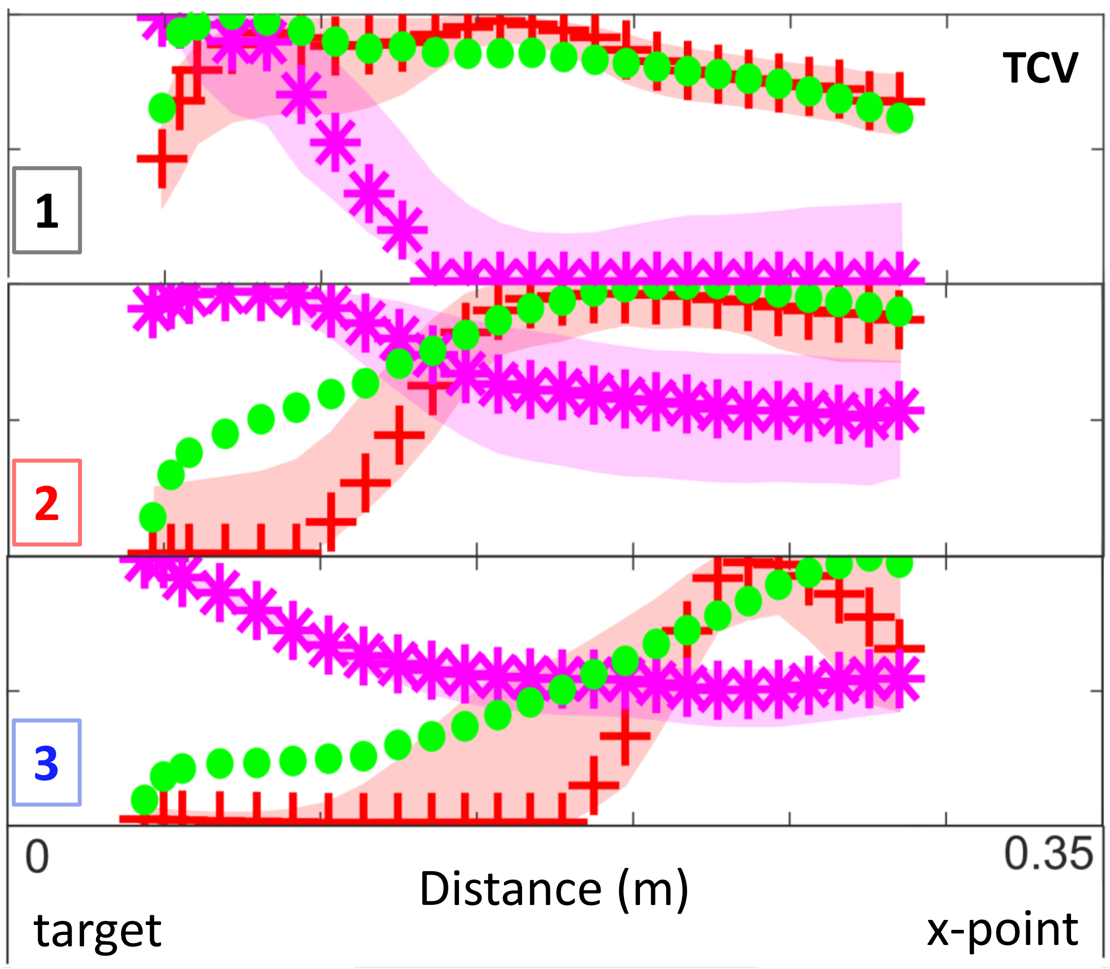


[Verhaegh, et al. 2021, PPCF]

Plasma-molecule interactions along the divertor leg





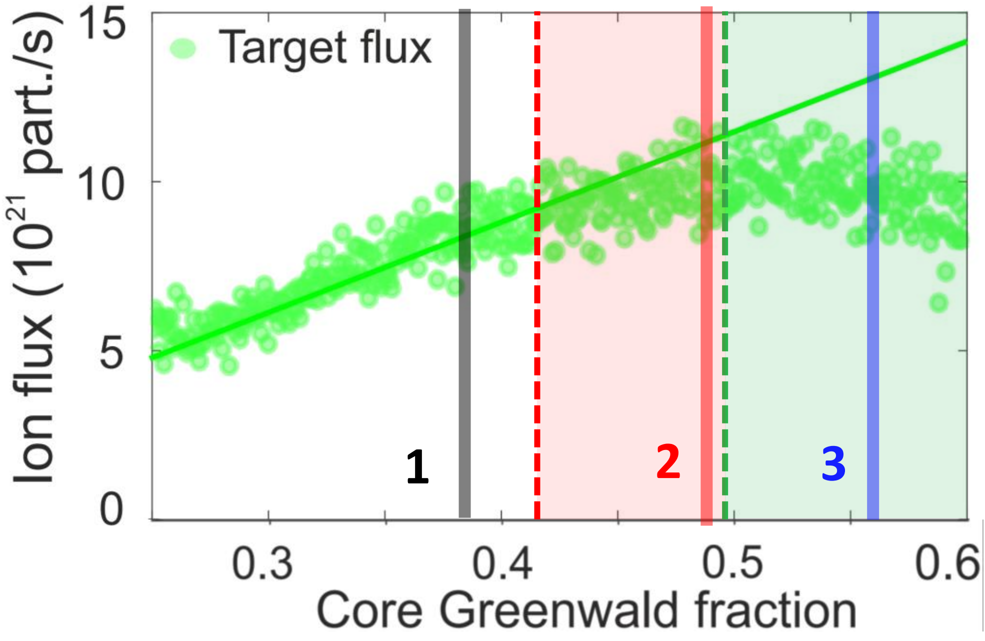


[Verhaegh, et al. NME 2021]

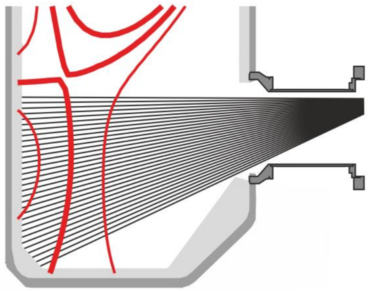
In **Dα (H excitation)** region

D mfp ~ 5-10 cm

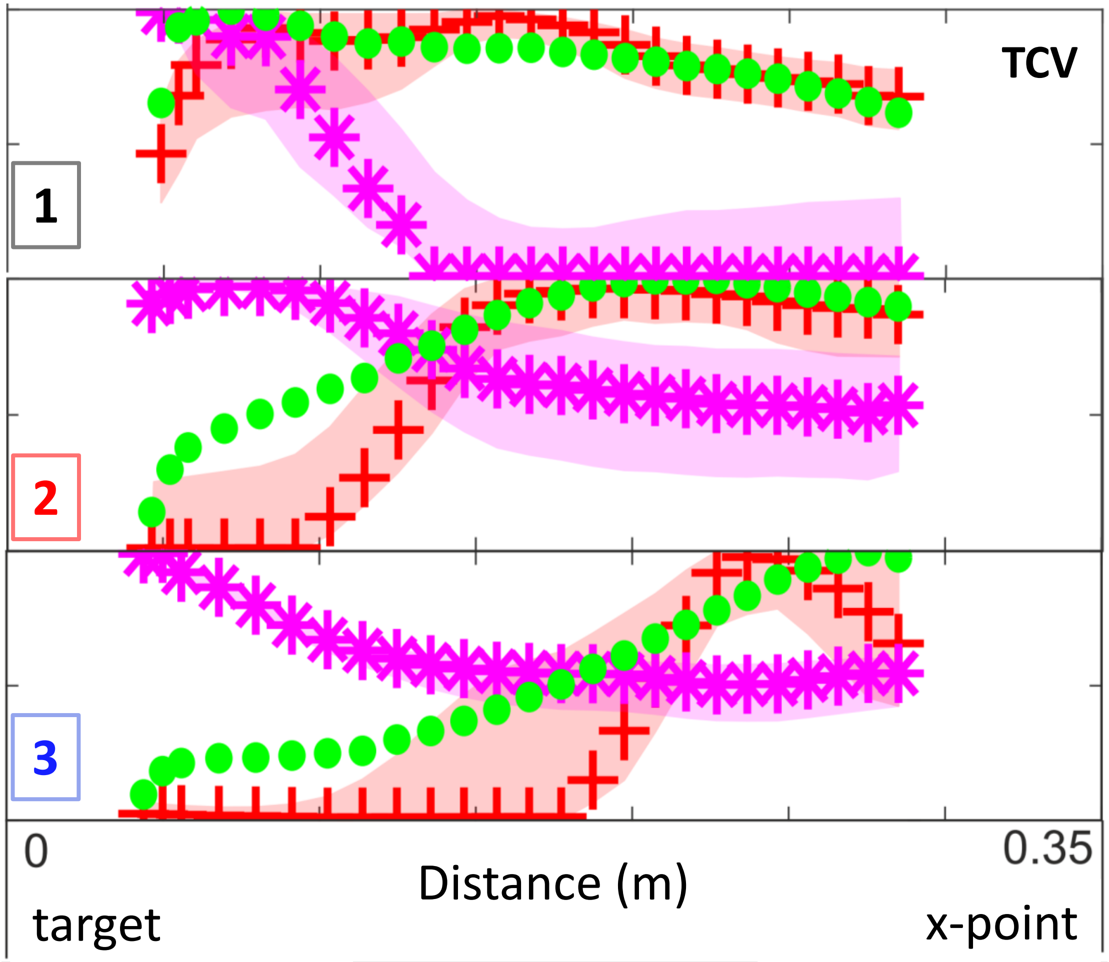
Plasma-molecule interactions along the divertor leg



Dα (H excitation)
Dα (plasma-mol. interaction)
∫ Fulcher (600-614 nm)



Normalised emission profiles



- Dα excitation (D) emission ‘detaches’ from target followed by Fulcher emission at detachment onset
- Dα (plasma-mol. inter.) ‘remains peaked at target

-> suggests different localisation D_2 dissociation and power/part. losses D_2^+

In Dα (H excitation) region
D mfp ~ 5-10 cm

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2. **Investigate how plasma-atom/molecule interactions can impact detachment through power/particle losses**

3. Investigate under which conditions plasma-molecule interactions impact detachment and how this compares to simulations

- Conclusions

How plasma-mol. interactions can impact particle balance

[Verhaegh, et al. NME 2021]

Attached:

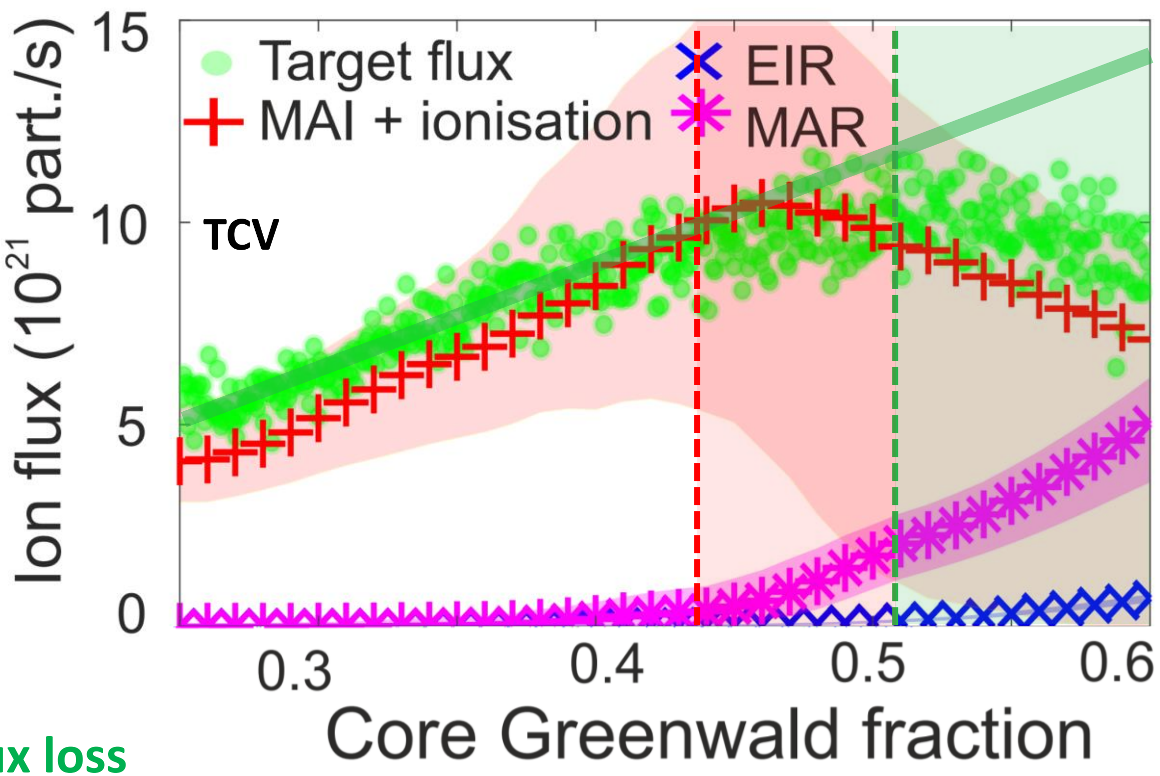
- **Ionisation + MAI** (Molecular Activated Ionisation) in agreement with **target flux**

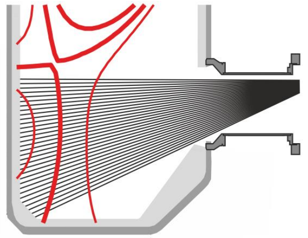
Detachment onset:

- **MAR** (Molecular Activated Recombination) starts to occur
- **Total ion source** drops

Detached

- **Electron-ion recombination (EIR)** << **MAR**
- Drop in **total ion source** and **MAR** both similar to **target flux loss**





How plasma-mol. interactions can impact particle balance

[Verhaegh, et al. NME 2021]

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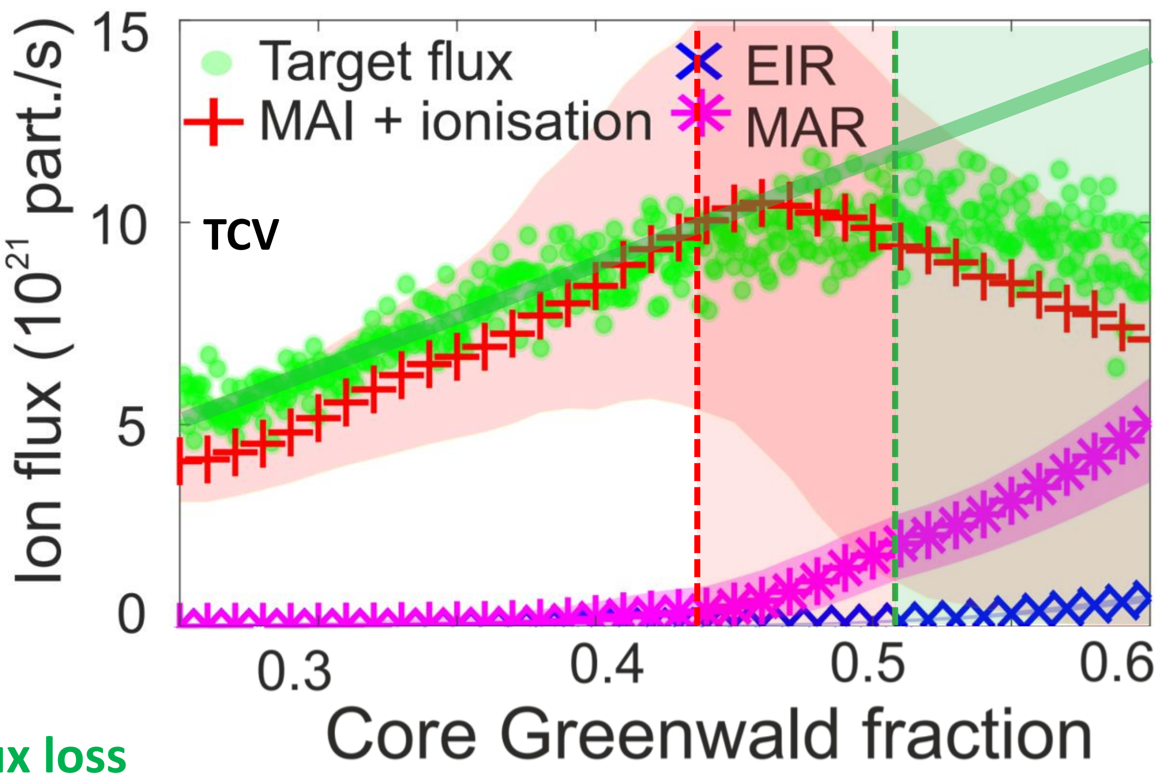
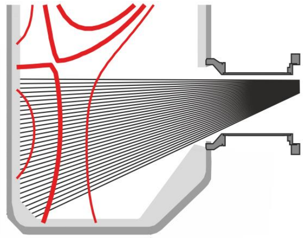
- **Total ion source** drops

Detached

- **Electron-ion recombination (EIR)** << **MAR**
- Drop in **total ion source** and **MAR** both similar to **target flux loss**

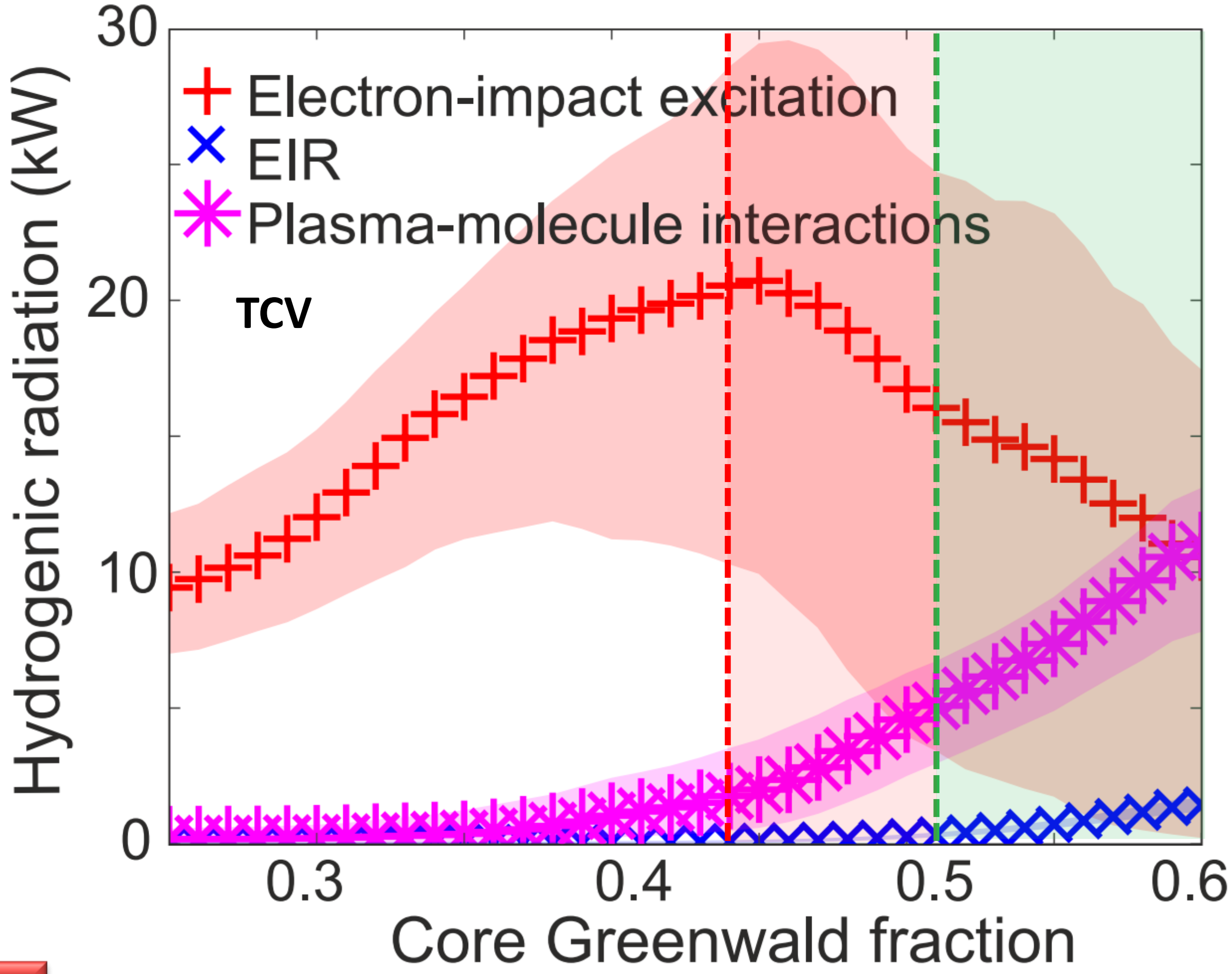


- **MAR can be an important ion sink (50% of ion target flux) during detachment**
- **For these TCV conditions MAR is more significant than EIR**

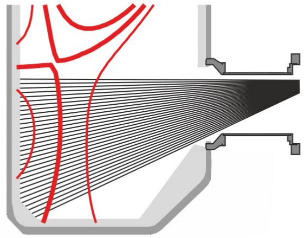


How plasma-mol. interaction can impact power balance

- Radiative loss from molecular bands negligible*
- Radiative loss from **excited atoms** after **plasma-molecule interaction** can be **significant**



- **Plasma-molecule interactions -> excited H atoms -> significant H line radiation**



* [Groth, et al. 2018 NME]

How plasma-mol. interaction can impact <u>power balance</u>

- Radiative loss from molecular bands negligible*

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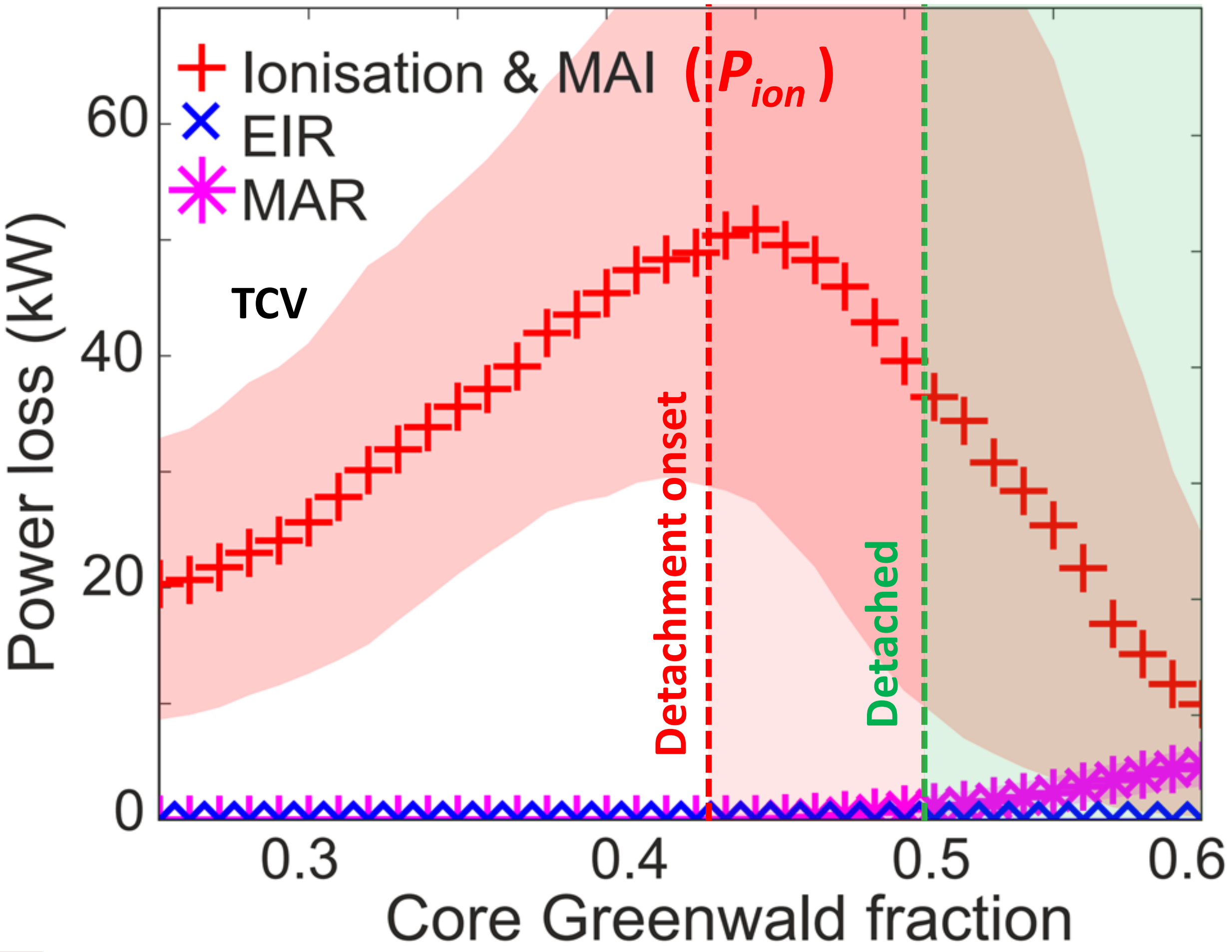
Power loss = radiation + potential ($H \rightarrow H^+$ 13.6 eV) change

- **Net power loss EIR** ~ 0
- Small **net power loss MAR** (E_{MAR} ~ 8 [5-11] eV)
- **Atomic ionisation & MAI power loss significant**

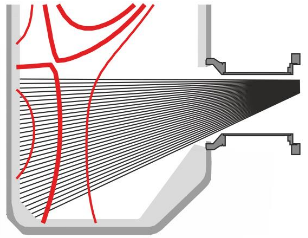
E_{ion} ~ 30-40 eV E_{ion} > 50 eV

E_X is energy loss per X reaction



- **Plasma-molecule interactions -> <u>excited H atoms</u> -> significant H line radiation**
- **Ionisation + MAI dominant hydrogenic power loss**

* [Groth, et al. 2019 NME]



Power and particle balance

Power balance model (assume $I_t = I_i$):

$$\overbrace{P_{div} - P_{rad}^{imp}}^{P_{recl}} = \overbrace{P_{ion}}^{I_t E_{ion} = \epsilon I_t + P_{rad}^{H,exc}} + \overbrace{P_{target}}^{\gamma T_t I_t}$$

Power balance:

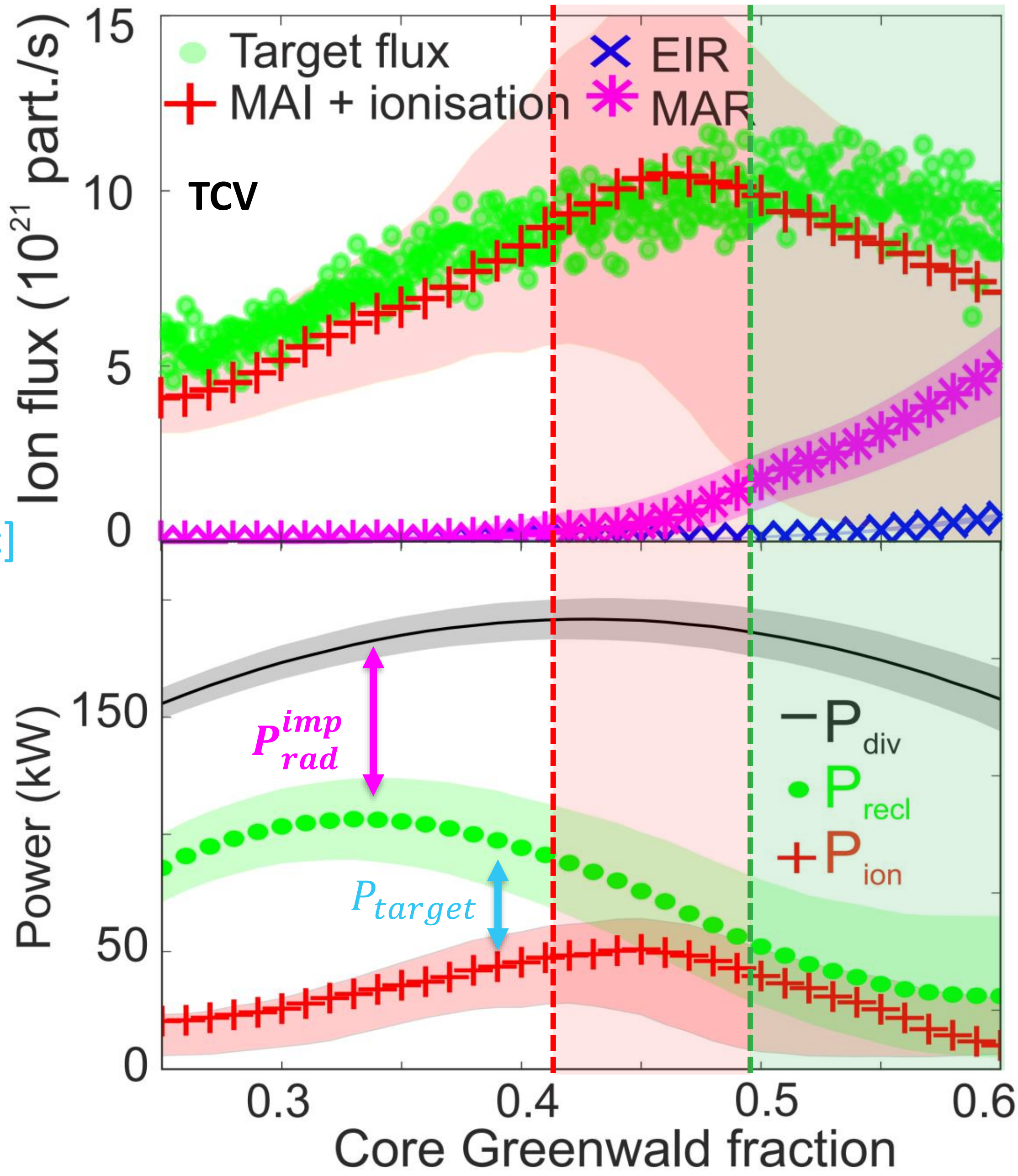
- P_{rad}^{imp} reduces **power entering recycling region (P_{recl})**
- As P_{recl} and P_{ion} come closer (P_{ion}/P_{recl} increases), P_{target} [kinetic] **(and thus the target temperature) drops, MAR starts**
- Drop in target power from both drop in surface recombination (ϵI_t) as well as kinetic ($\gamma T_t I_t$) power load

'Power limitation':

Detachment onset: P_{recl} **~ 2** P_{ion} $\quad T_t \sim \overbrace{E_{ion}/\gamma}^{4-6\ \text{eV}}$

in agreement with analytical model [Verhaegh, et al. 2019, NF]

- **Roll-over:** P_{recl} ~ P_{ion} and tracks P_{recl} $\quad T_t < E_{ion}/\gamma$



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Power balance:

- P_{rad}^{imp}
- As P_r
  (and
- Drop
  recombination (ϵI_t) as well as kinetic ($\gamma T_t I_t$) power load

The **ion source reduction**, which causes has a critical role in the target ion flux loss, **occurs as P_{ion} appears to be limited by P_{recl} : 'power limitation'**

Result (now with molecules) similar to [Verhaegh, et al. 2019, NF]

'Power limitation':

Detachment onset: P_{recl} ~ 2 P_{ion} $\quad T_t \sim \overbrace{E_{ion}/\gamma}^{4-6\ \mathrm{eV}}$

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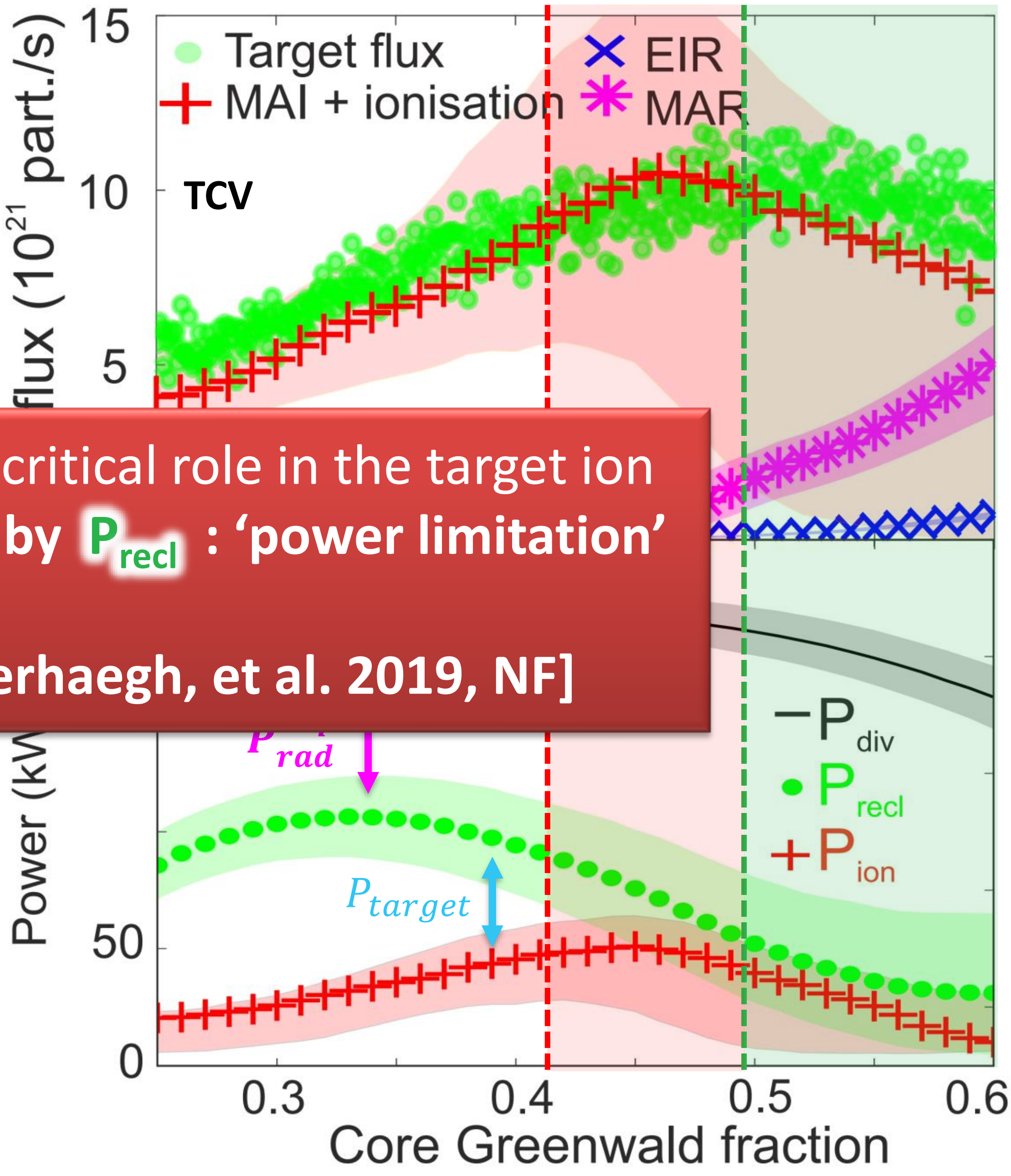


Goals and outline

- Motivation and introduction

1. Investigate how plasma-molecule interactions impact hydrogenic line emission, and how Balmer series measurements can be used to study molecular effects

2. Investigate how plasma-atom/molecule interactions can impact detachment through power/particle losses

3. **Investigate under which conditions plasma-molecule interactions impact detachment and how this compares to simulations**

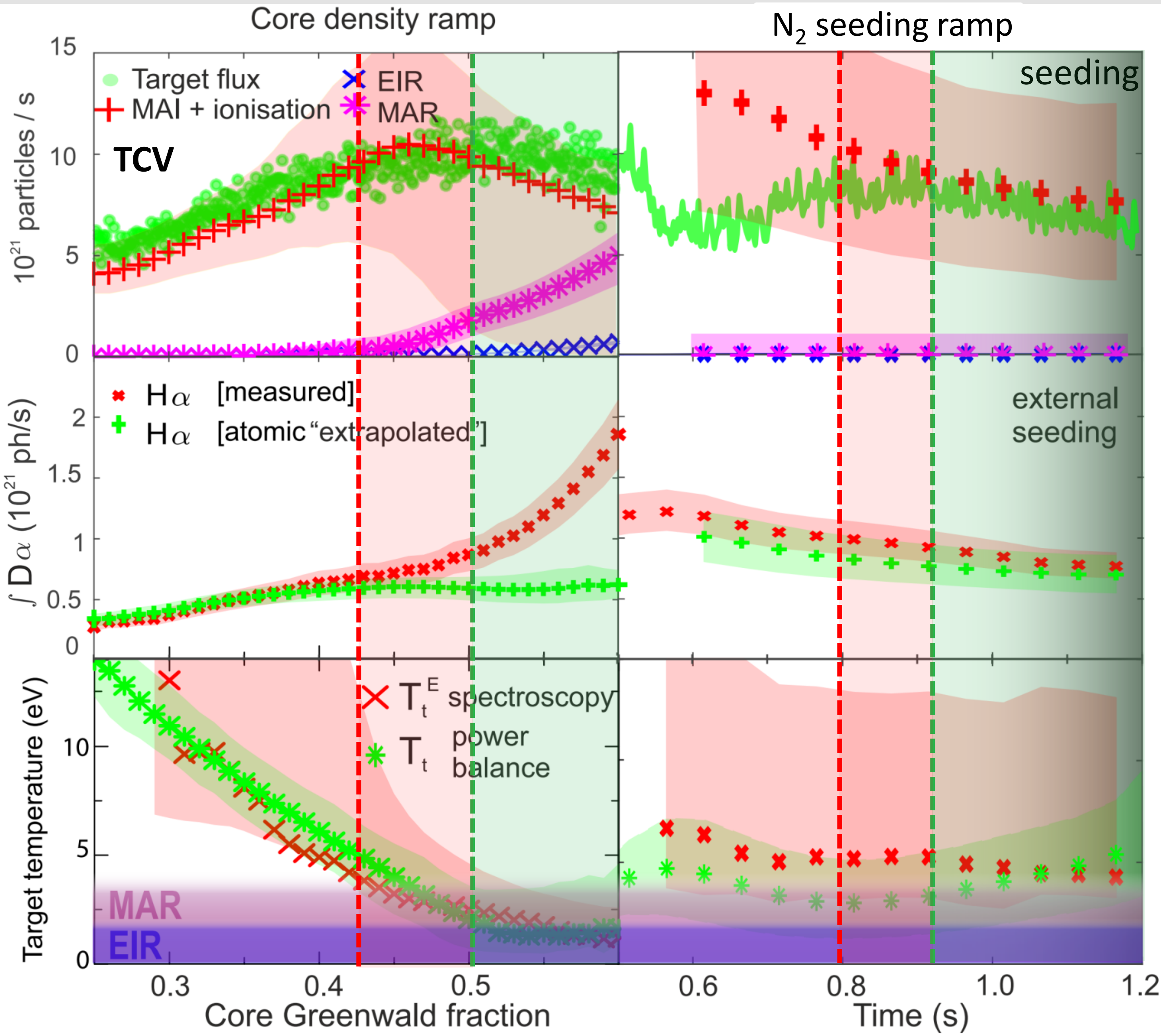
- Conclusions

Plasma-mol. interactions during a N_2 density ramp

<u>Ha behaviour different during seeding</u>

- **Atomic estimate Dα** agrees with **measured Dα** and drops with **ion source**
- Target temperature too high for **MAR** & **EIR** during seeding

- Observed for all N_2 seeded discharges (TCV), consistent with SOLPS simulations*



* TCV - [Smolders, et al. PPCF 2020]
MAST-U [Myatra, et al. in preparation]

Plasma-mol. interactions during a N_2 density ramp

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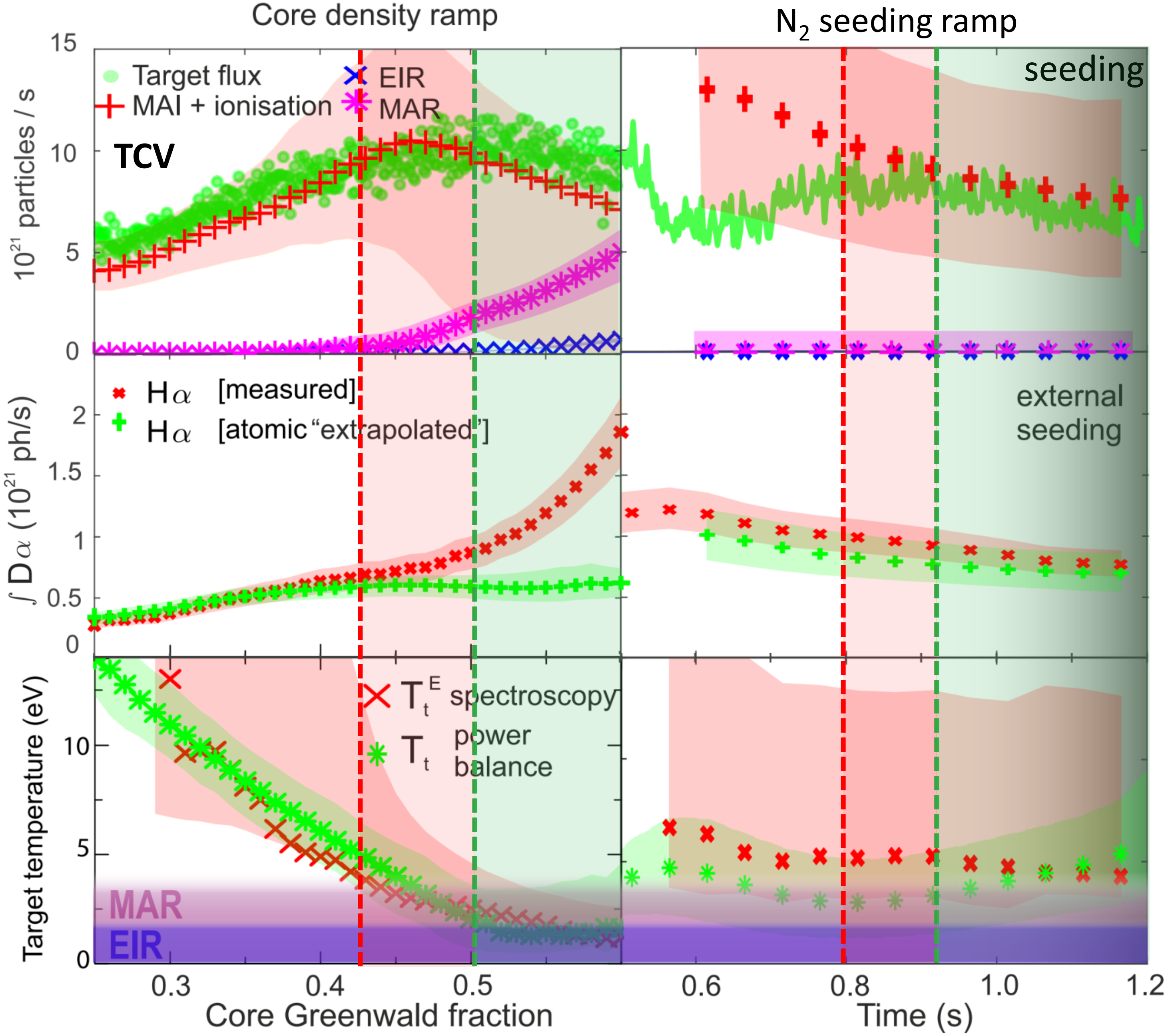
MAR and Dα from plasma-mol. inter. do not occur during N_2 seeding as target temperatures remain too high



TCV observations compared to simulations

- **Vibrational** state **unresolved**
- Experiment and simulation agree reasonably [Verhaegh, et al. NF, 2019] , except:

Differences simulation & experiment:

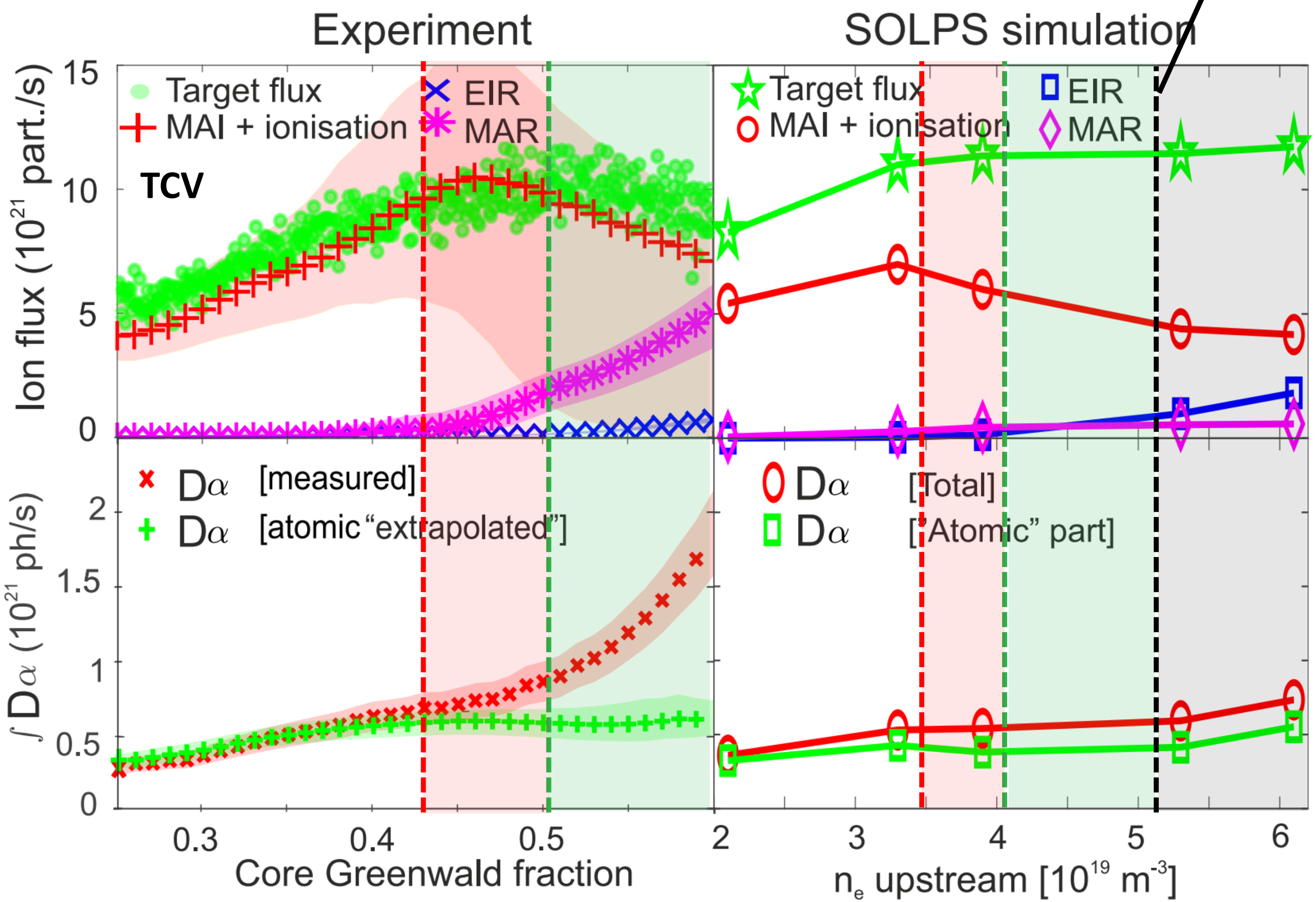
- **Dα** stays constant during detachment
- **MAR** /impact D_2^+ negligible
- No roll-over of the **ion target current**, despite roll-over **ion source** loss

The effect of D_2^+ is strongly underestimated in the simulation compared to the experiment

Simulations from [A. Fil, et al. CPP, 2018]

Default $D_2 + D^+ \rightarrow D_2^+ + D$ rate Eirene (default isotope rescaling Eirene)

experiment disrupted



D_2^+ molecular CX rates

Eirene (default:

1. averaged over vibrational states (v) – simplified model with: electron impact collisions with D_2 and E_{D2} = 0.1 eV, thermalization of molecules, then
2. *effective* Mol. CX: $D_2^+ + D^+ \rightarrow D_2^+ + D$ – mass rescaled from Hydrogen -> Deuterium

- D_2^+ static in simulations (however, D_2^+ lifetimes are short) -> model D_2^+/D_2 ratios using no transport assumptions

D_2^+ creation:

$D_2^+ + D^+ \rightarrow D_2^+ + D$

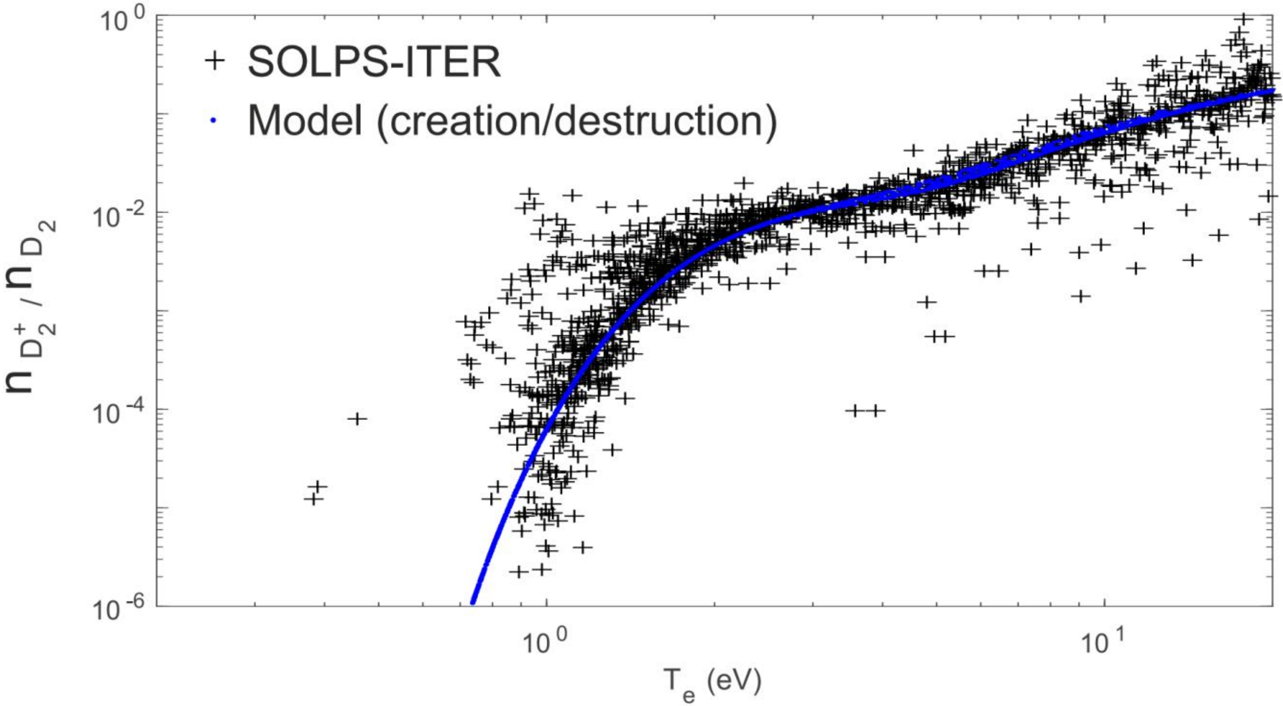
$e^- + D_2 \rightarrow 2\, e^- + D_2^+$

D_2^+ destruction

$e^- + D_2^+ \rightarrow D + D$

$e^- + D_2^+ \rightarrow e^- + D^+ + D$

$e^- + D_2^+ \rightarrow 2e^- + D^+ + D^+$



D_2^+ molecular CX rates

Eirene (default):

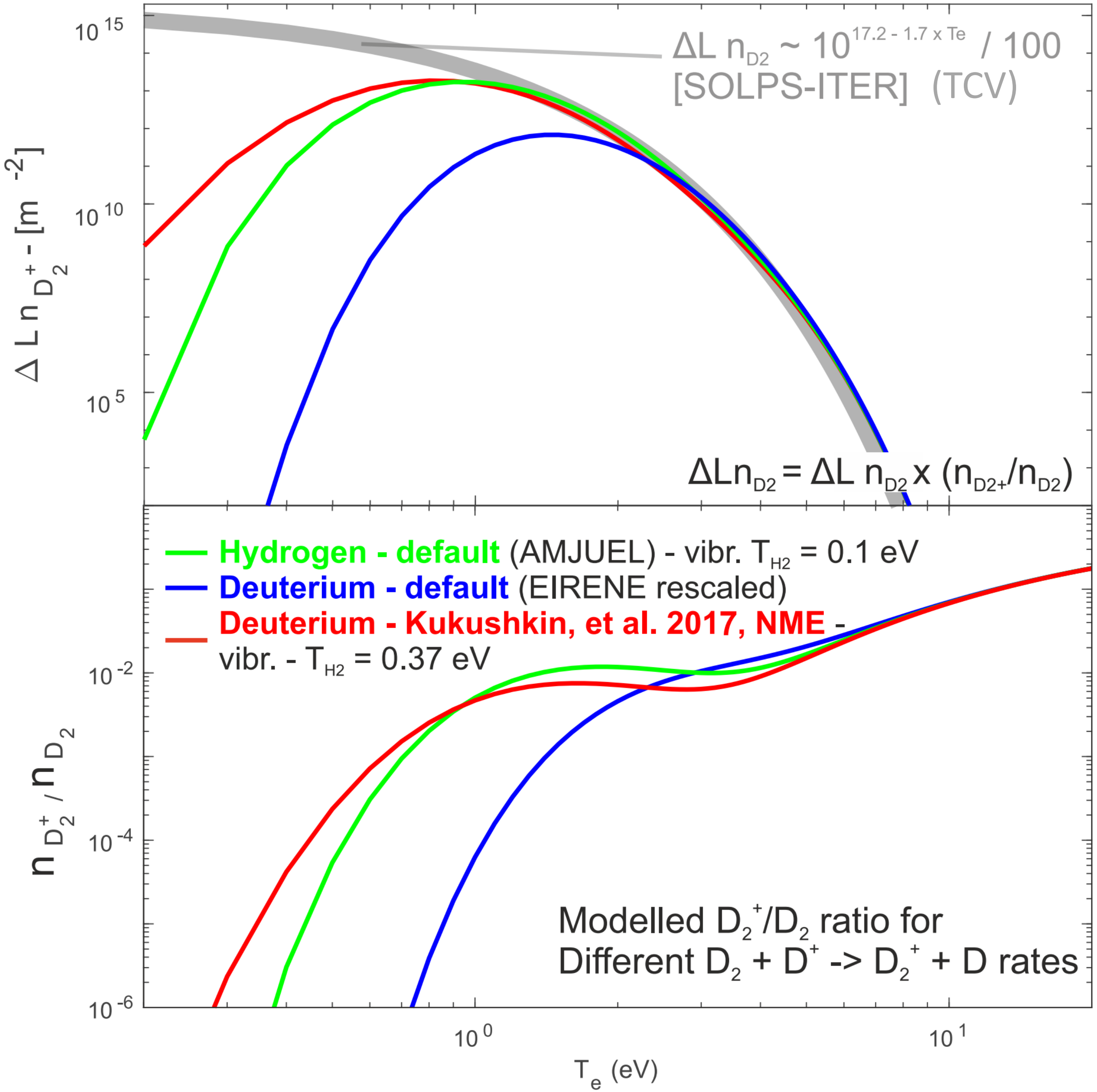
1. *averaged* over vibrational states (v), then
2. *effective* mol. CX: $D_2^+ + D^+ \rightarrow D_2^+ + D$ – mass rescaled

D_2^+/D_2 ratios modelled using different mol. CX rates:

- **Default Eirene/AMJUEL** (hydrogen rates)
- **Eirene rescaled deuterium** (default)
  [drops more strongly at lower temperatures]
- **Deuterium – Kukushkin, et al. 2017, NME**
  individual mol. CX (v) rescaled *then* averaged

- D_2 density increases at with decreasing T_e

Large difference in D_2^+ densities between the **default hydrogen** and **rescaled deuterium** rates. **Derived deuterium rate** similar to **hydrogen rate**

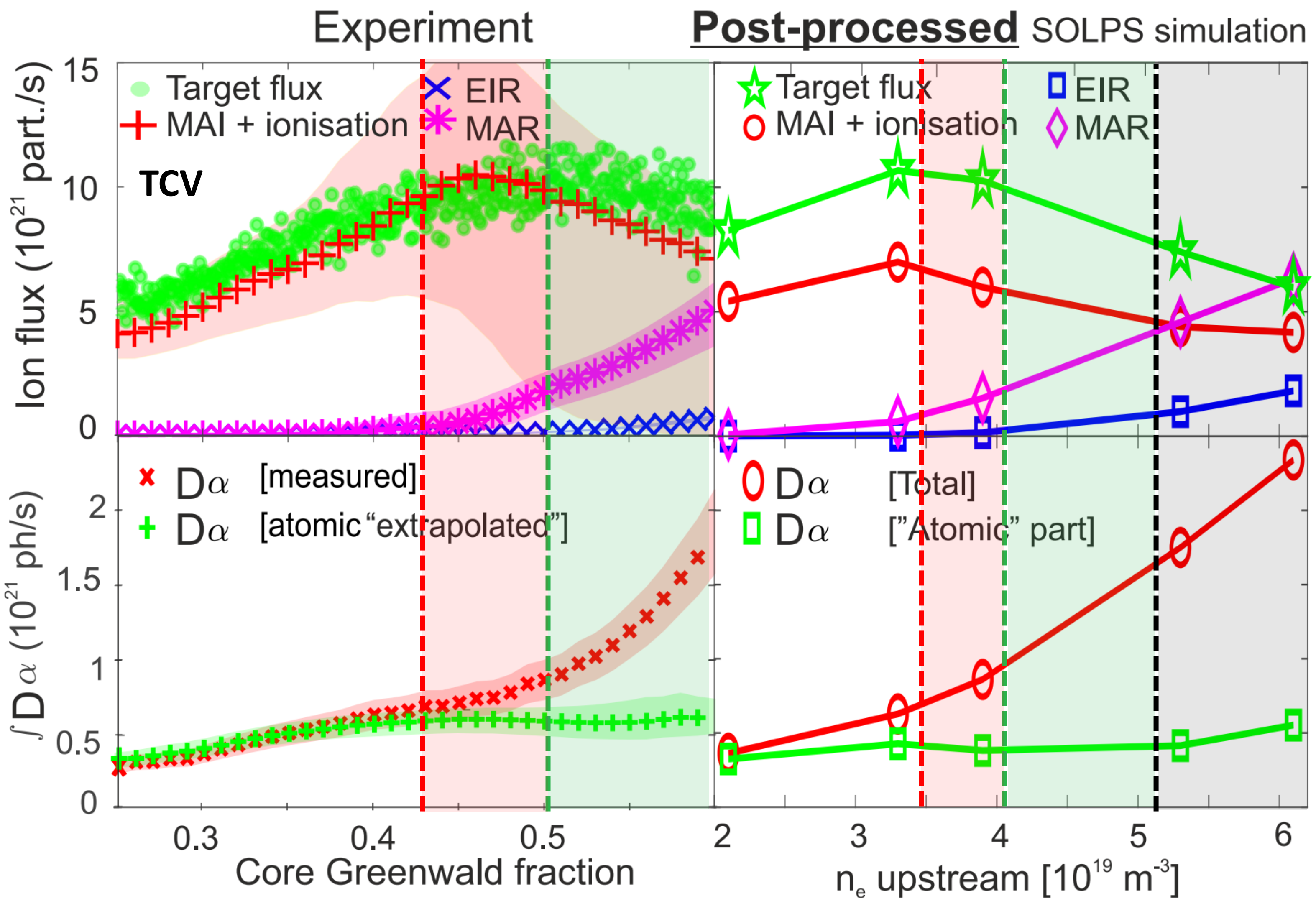


TCV observations compared to simulations

Post-processed (not strictly self-consistent) using the $D_2 + D^+ \rightarrow D_2^+ + D$ rate from **Kukushkin, et al. 2017, NME**

<u>**Agreement**</u> simulation & experiment:

- **Dα increases** during detachment
- **MAR / impact D_2^+ significant**
- **Roll-over** of the **ion target flux**, as well as **ion source**



Simulations from [A. Fil, et al. CPP, 2018]

TCV observations compared to simulations

Agreement simulation & experiment:

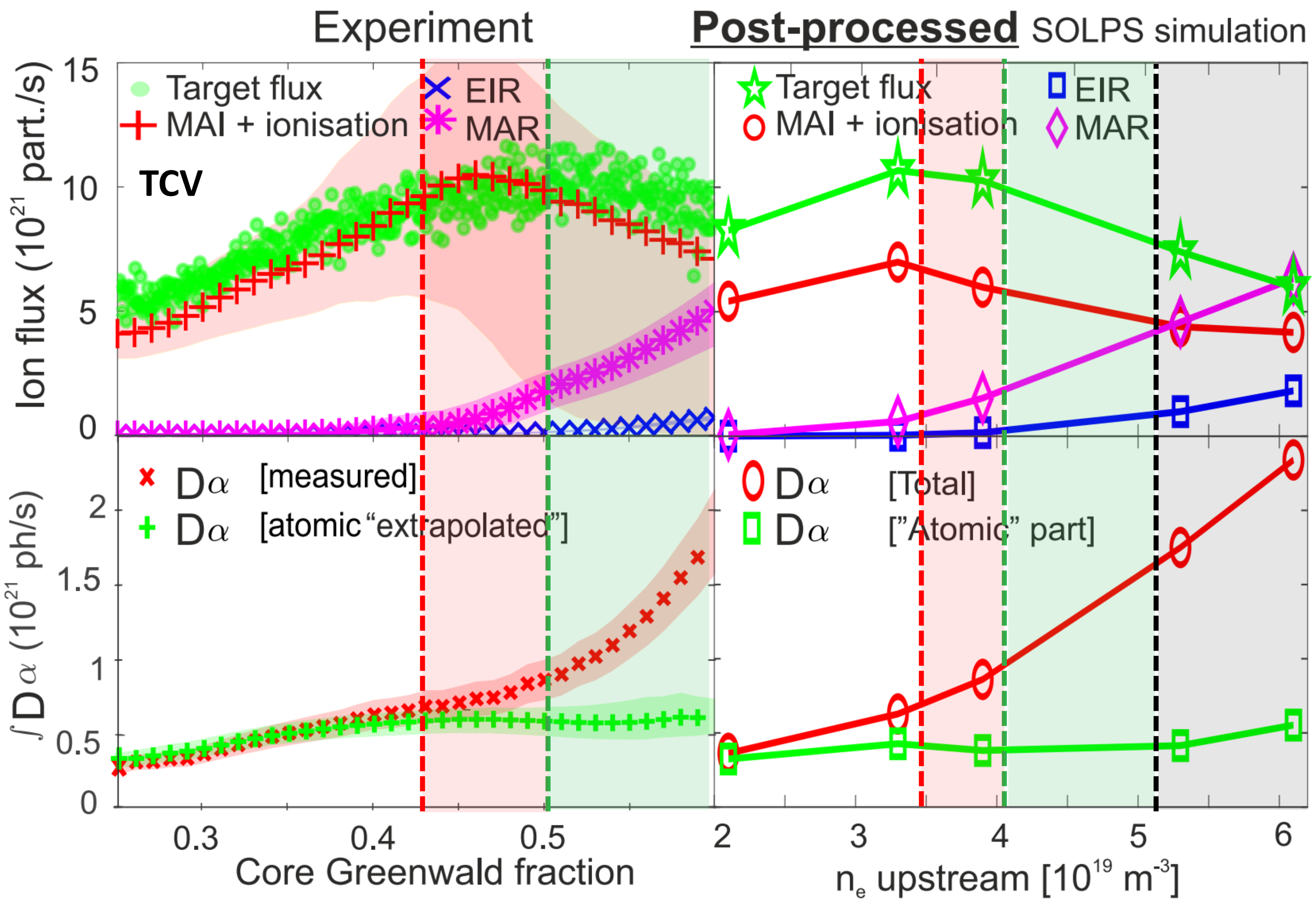
- **Dα increases** during detachment
- **MAR / impact D_2^+ significant**
- **Roll-over** of the **ion target flux**, as well as **ion source**

The effect of D_2^+ is in agreement between experiment/simulation with mol. CX rate Kukushkin, NME, 2018

- Coincidence ?
- More research required (other devices, impact wall material, impact vibrational states)

Simulations from [A. Fil, et al. CPP, 2018]

Post-processed (not strictly self-consistent) using the $D_2 + D^+ \rightarrow D_2^+ + D$ rate from **Kukushkin, et al. 2017, NME**



Conclusion and discussion

Plasma-molecule interactions result in **excited atoms**, significantly impacting (T_e = [1.5-3.5] eV):

- Hydrogenic line emission -> **implications for diagnostic analysis**
- Power balance (**50% of total H rad**.)
- Particle balance (**MAR >> EIR** for TCV)

→ **implications for detachment physics**

Such interactions are presently:

- Underestimated in SOLPS simulations
- Not accounted for in spectroscopic analysis

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Generality of these results needs to be investigated, depends on:

- The vibrationally excited levels of H_2
  - Molecular transport (depends on neutral mean free paths (5-10 cm TCV for H) / divertor shape)
  - Wall conditions (e.g. carbon vs tungsten)
- Used isotope mixture
- Temperature regime (not observed during N_2 seeding where T_t is higher)

Conclusion and discussion

Plasma-molecule interactions result in **excited atoms**, significantly impacting (T_e = [1.5-3.5] eV):

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Such interactions are presently:

- Underestimated in SOLPS simulations
- Not accounted for in spectroscopic analysis

However, the TCV results are quantitatively consistent (Hβ/Hα ratios) with DIII-D [Hollman, et al. 2005, PPCF]

JET Hα measurements also suggestive of plasma-molecule interactions [Lomanowski, et al. 2020, PPCF]

Conclusion and discussion

Plasma-molecule interactions result in **excited atoms**, significantly impacting (T_e = [1.5-3.5] eV):

- Hydrogenic line emission -> **implications for diagnostic analysis**
- Power balance (**50% of total H rad.**)
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implications for detachment physics

Such interact

- Underestin
- Not accour

Plasma-molecule interactions (on TCV) have dominant effects on hydrogenic line intensities and power and particle during detachment

Further experimental and simulation investigation required

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