CCPQ-AMO Workshop – Atomic and Molecular Data Needs for Plasma Applications, April 2021, Online

EUROfusion

Experimental investigation of the role of plasma-atom/molecule interactions on power, particle ~~and momentum~~ balance in tokamak power exhaust

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Contributors

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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

Detachment physics

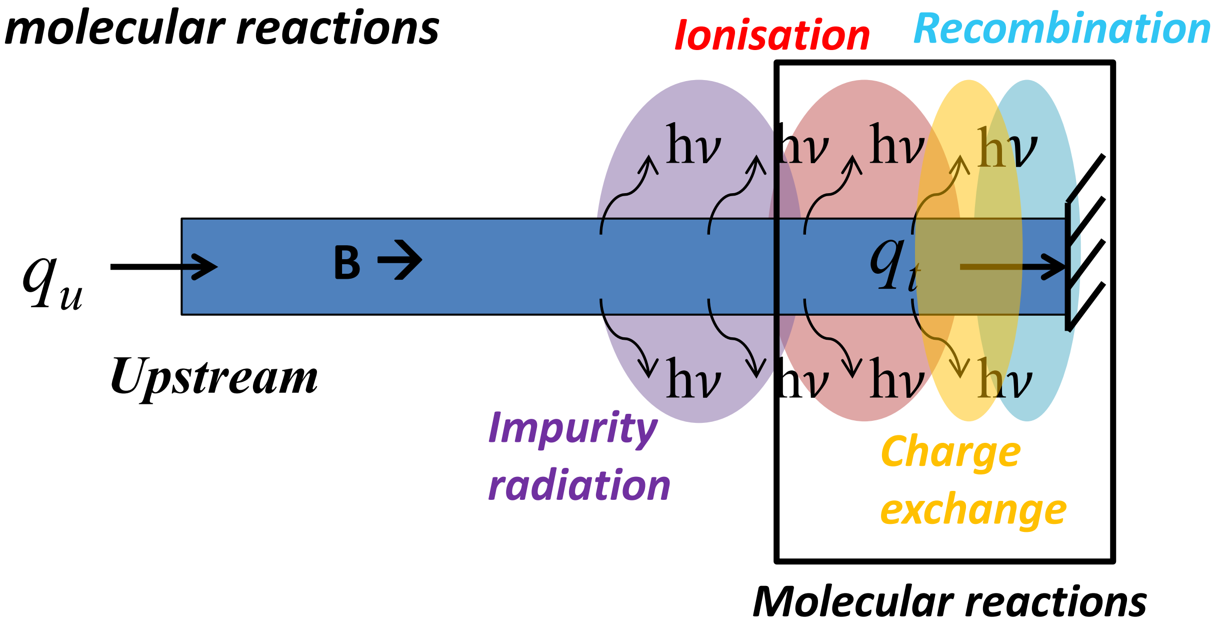
Detachment is necessary to mitigate power exhaust for ITER/DEMO:
reduces target particle and heat load

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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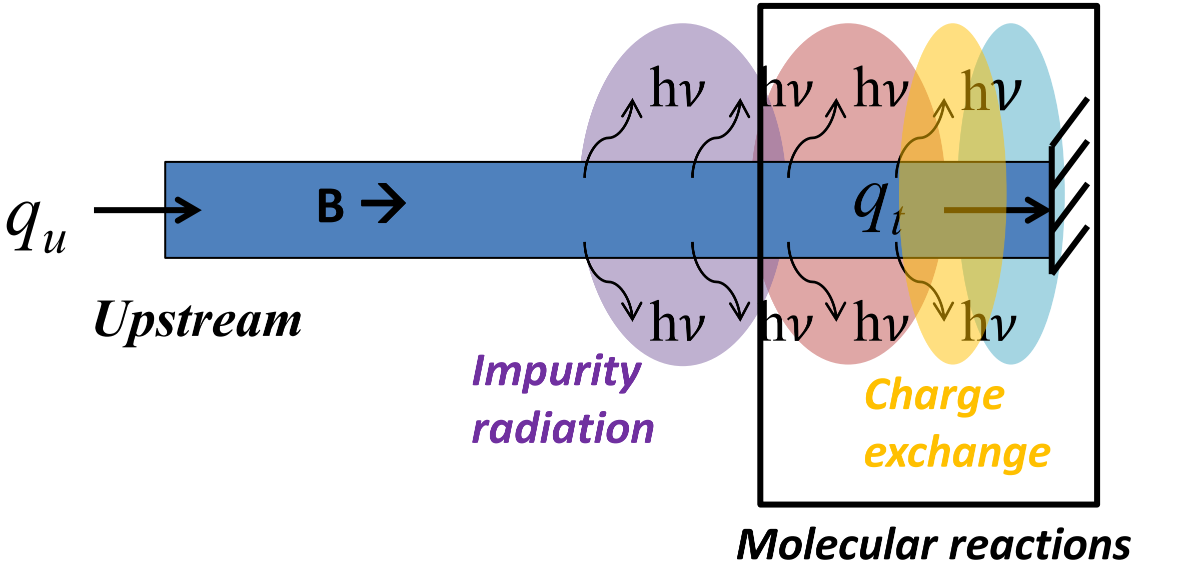


Detachment is driven by atomic/molecular reactions through dependencies between power, particle and momentum balances

***Plasma-molecule* interactions alter all three of these balances.**

In this work we <u>investigate these interactions experimentally</u> to estimate:

- **impact on detachment (power/particle balance)**
- **impact on diagnostic interpretation**
- **agreement experiment and SOLPS-ITER modelling**

‘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 D_2**

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

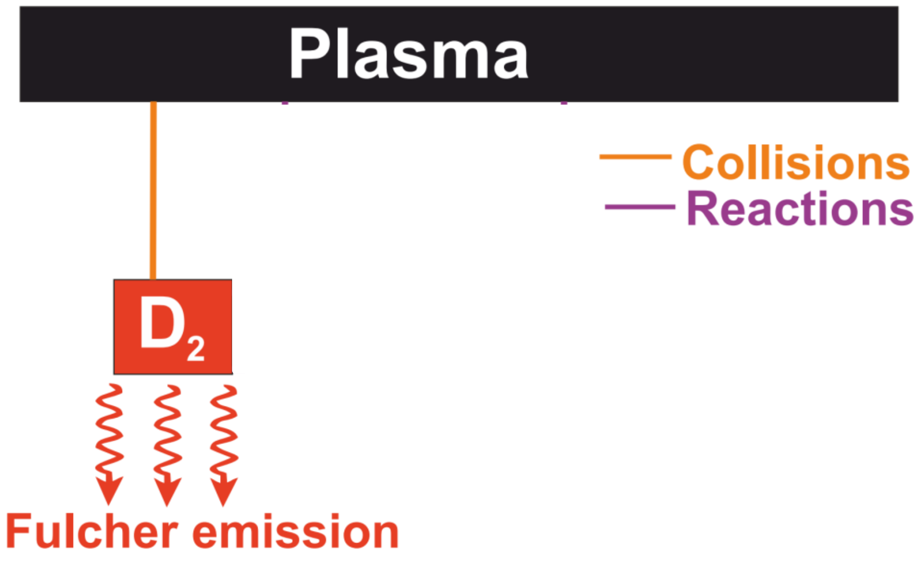
‘Detachment’ and plasma-molecule interactions

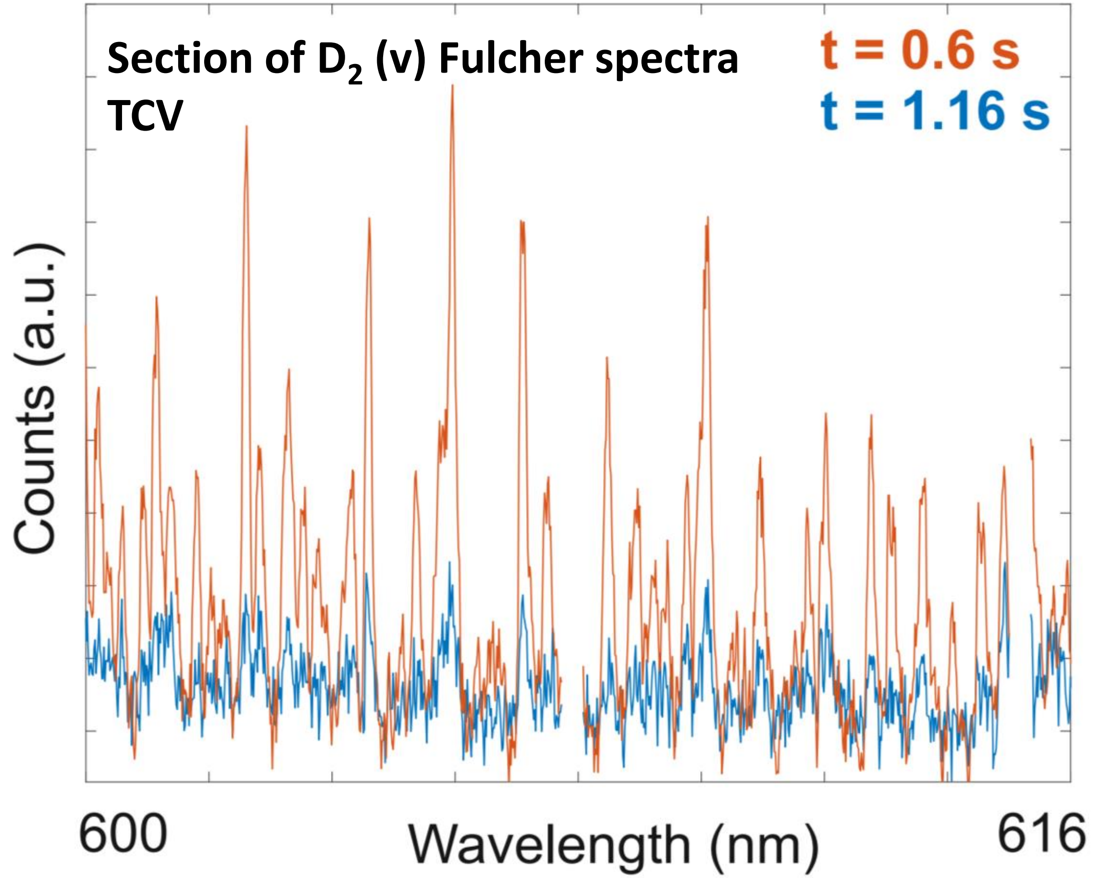
Detachment requires:
- Power loss
- Momentum loss
- Particle loss

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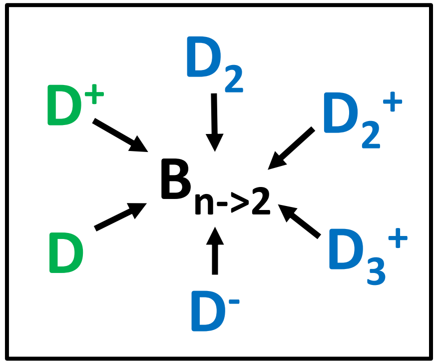
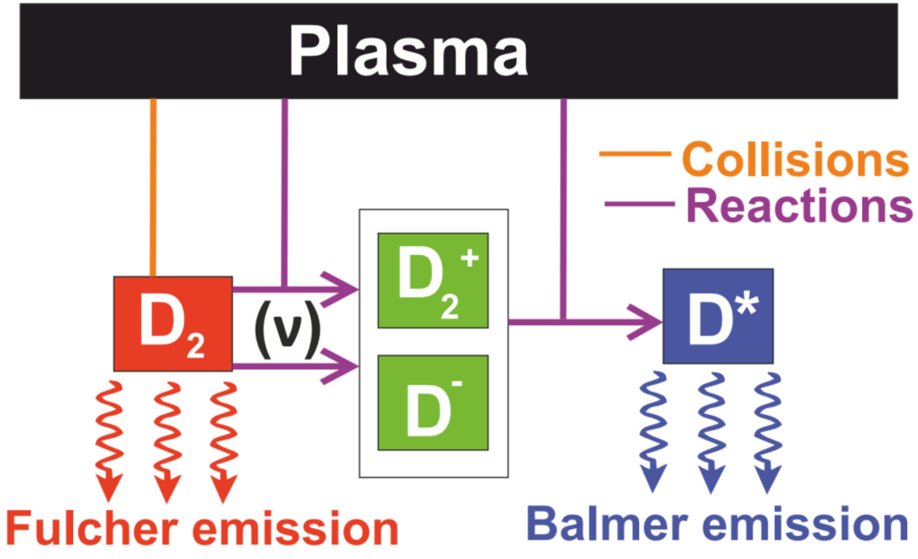
   For instance: $D_2 + D^+ \rightarrow D_2^+ + \mathbf{D}$; $D_2^+ + e^- \rightarrow \mathbf{D^*} + \mathbf{D^*}$
   [Molecular Activated Recombination (**MAR**)]
   a) Impacts particle (MAR & MAI) and momentum balance
   b) Leads to ***excited (*) hydrogen atoms*** -> **atomic line emission & radiation**

[Wünderlich, et al. Yacora, 2020]



‘atomic’
‘molecular species’



Hydrogen Balmer spectrum

‘Detachment’ and plasma-molecule interactions

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

<u>In this work:</u> we investigate this and use it as a diagnostic (passive spectroscopy – Balmer line emission).

Detachment requires:

- Power loss
- Momentum loss
- Particle loss

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

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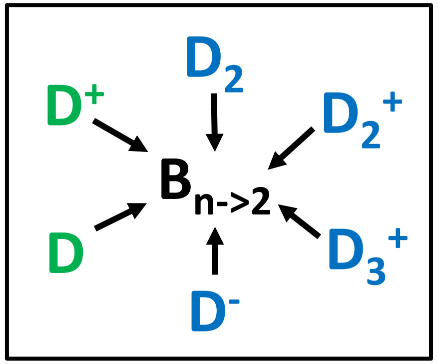

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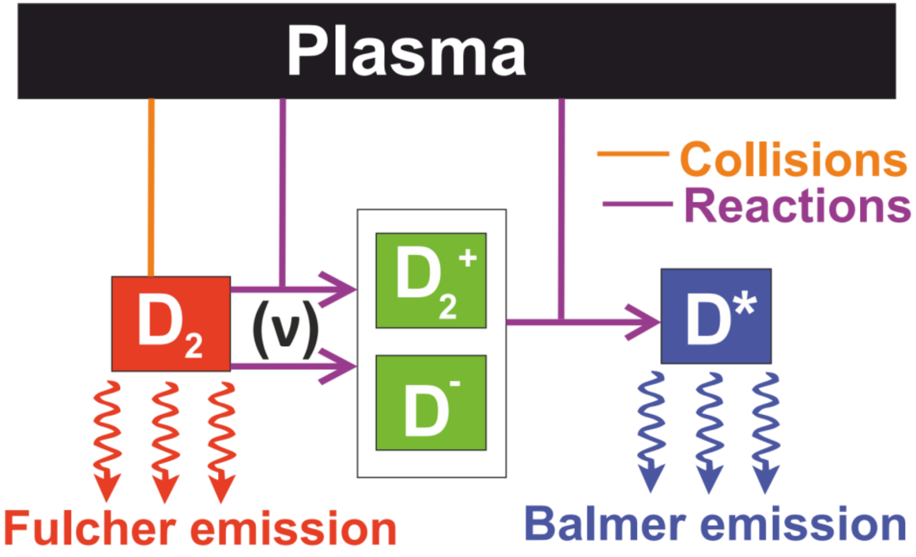


Hydrogen Balmer spectrum

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

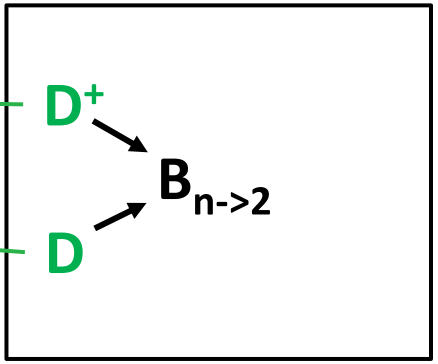
3. Investigate how the presented experimental inferences compare to plasma-edge modelling

- Conclusions

TCV tokamak (**carbon** wall): Ohmic (400 kW, Ip = 340 kA) L-mode core **density ramp**, reversed field (unfavourable for H-mode), open (conventional) divertor, outer divertor studied

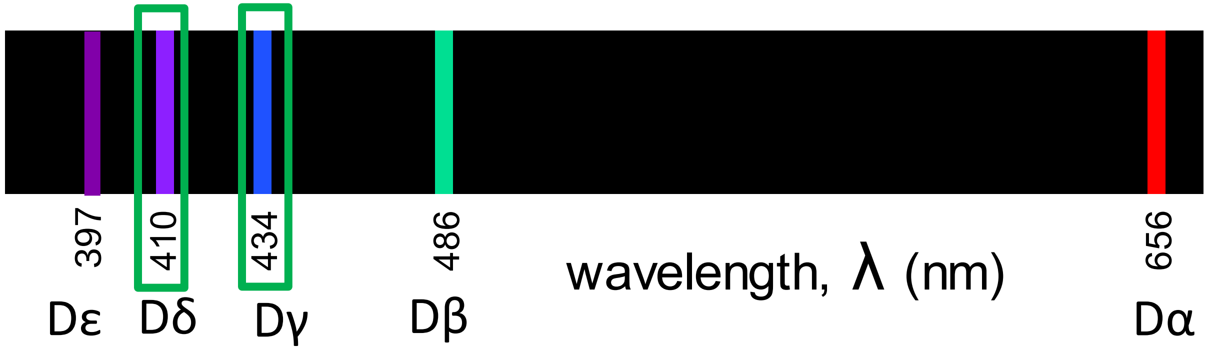
$D\alpha$ emission and molecules

- 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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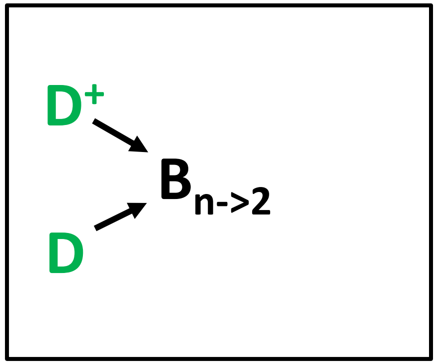
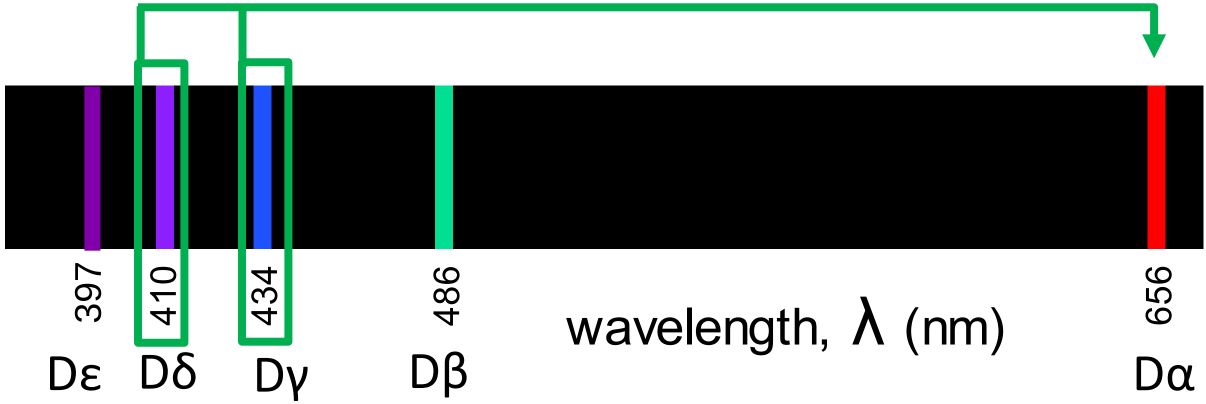


- Lower-n Balmer lines are less influenced by EIR -> ‘effectively’ more influenced by plasma-molecule interactions (-> avoid using this for the ‘atomic analysis’)

<u>Spectroscopic analysis:</u>

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

Hydrogen Balmer spectrum

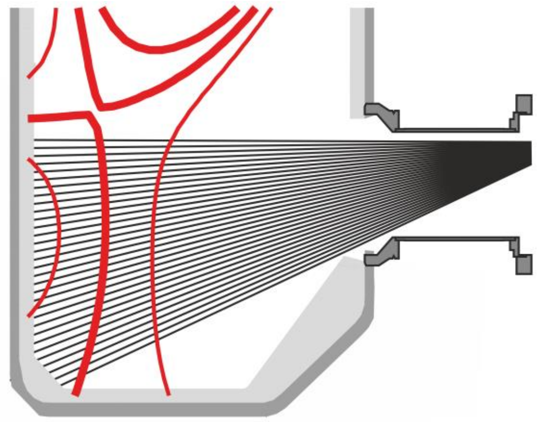


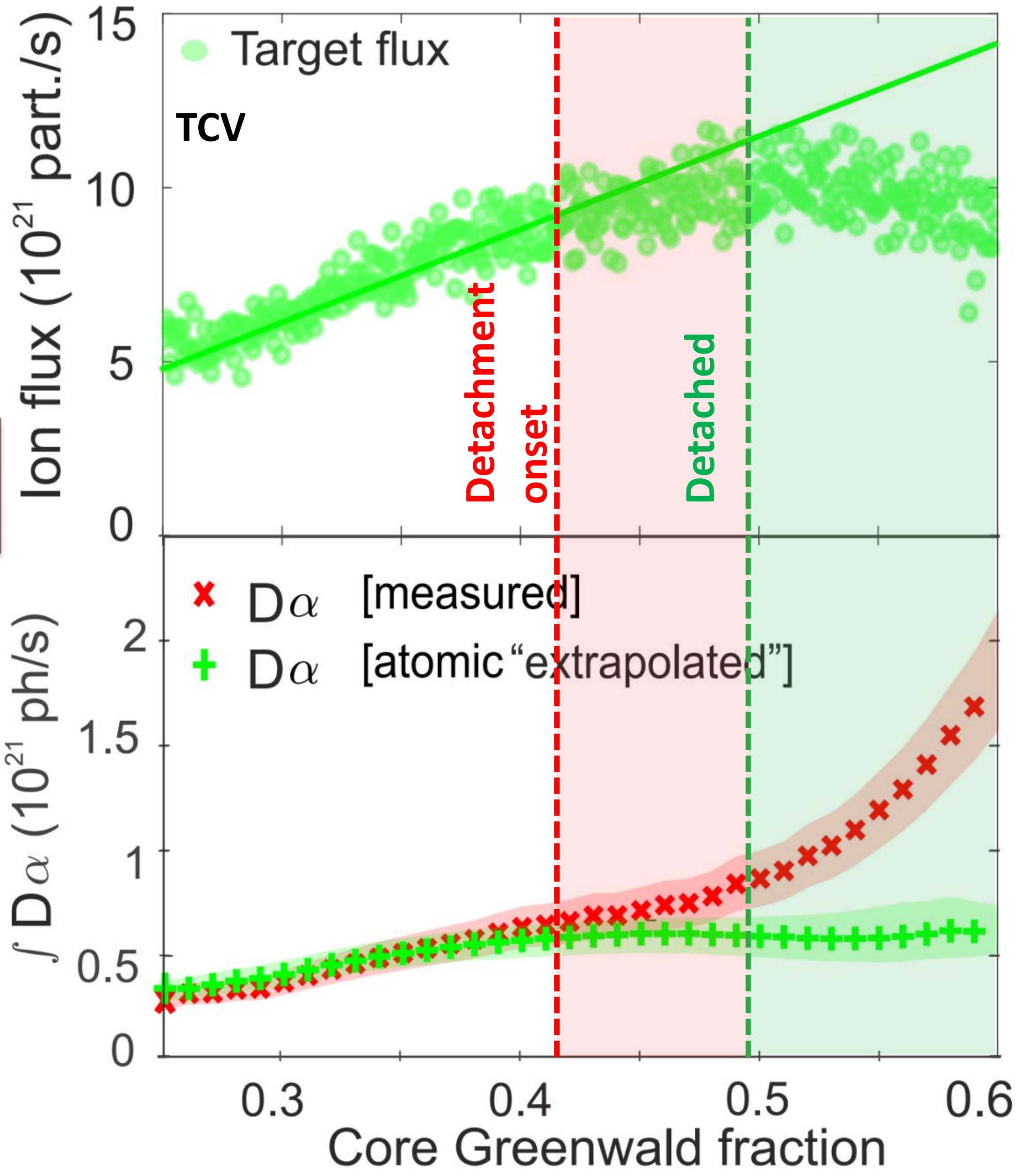
$D\alpha$ emission and molecules - results

[Verhaegh, Thesis, 2018]

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

Increase measured Dα during detachment **consistent with observations on other devices** (JET, DIII-D, …)





$D\alpha$ emission and molecules - results

[Verhaegh, Thesis, 2018]

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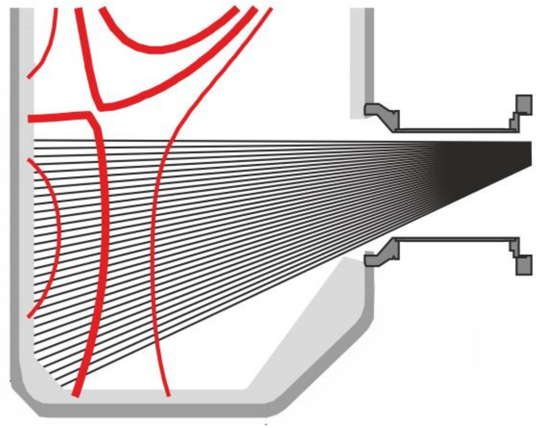
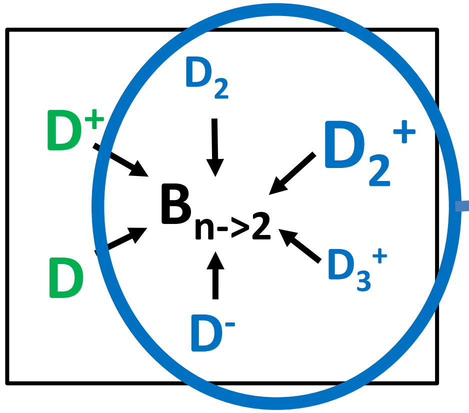
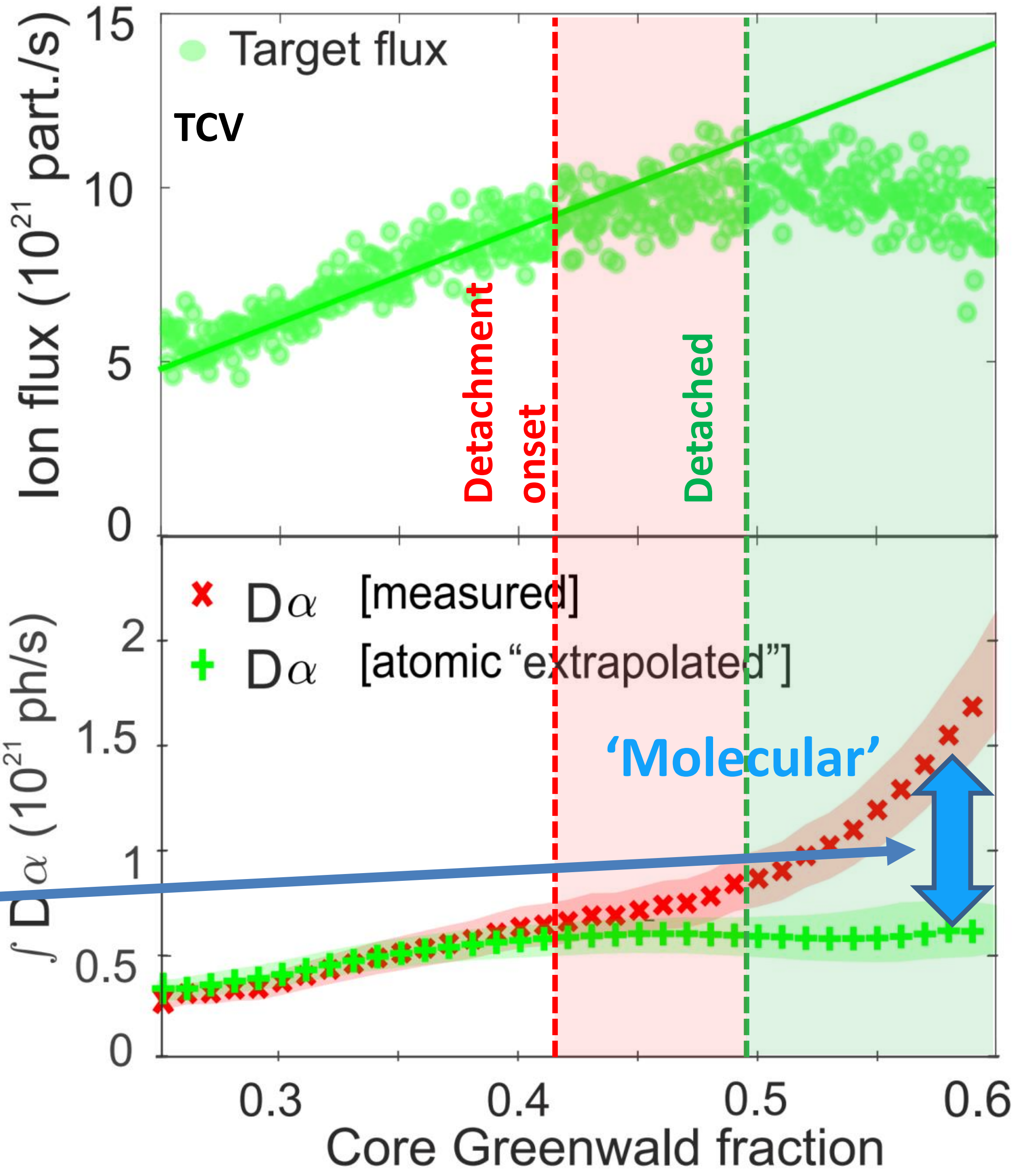
  -> $D\alpha$ from excited atoms after plasma-molecule interactions







$D\alpha$ emission and molecules - results

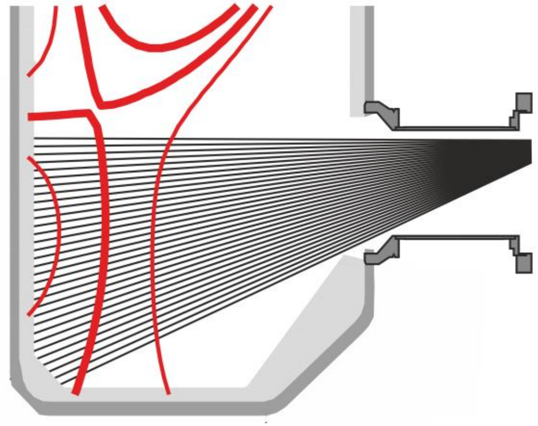
[Verhaegh, Thesis, 2018]

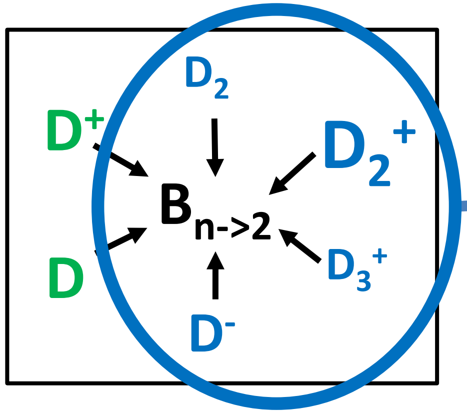
- **Measured $D\alpha$ emission** increases during detachment beyond **$D\alpha$ emission expected purely on the basis of atomic reactions**
  - **-> $D\alpha$ from excited atoms after plasma-molecule interactions**

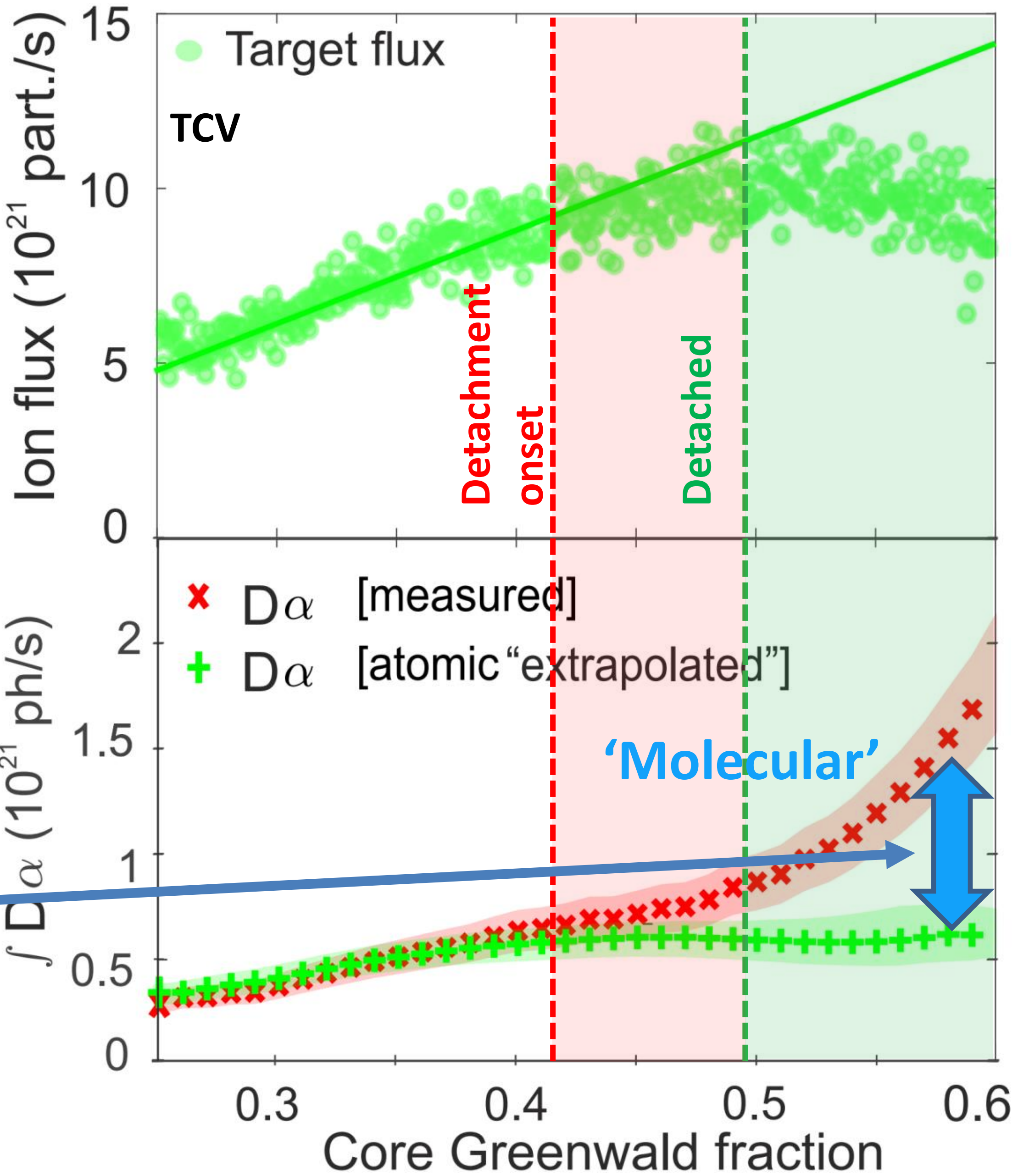
This mismatch of Dα is an indicator for:

1. **Particle losses through MAR**
2. **Power losses from D* after plasma-mol. interactions**
3. **Strong contribution plasma-mol. inter. Balmer lines**

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





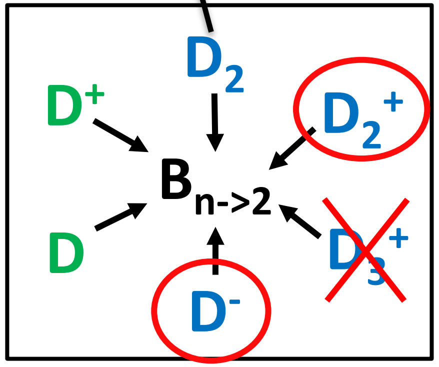


Novel Balmer line spectra analysis - BaSPMI

<u>**Spectroscopic analysis**</u>: [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**

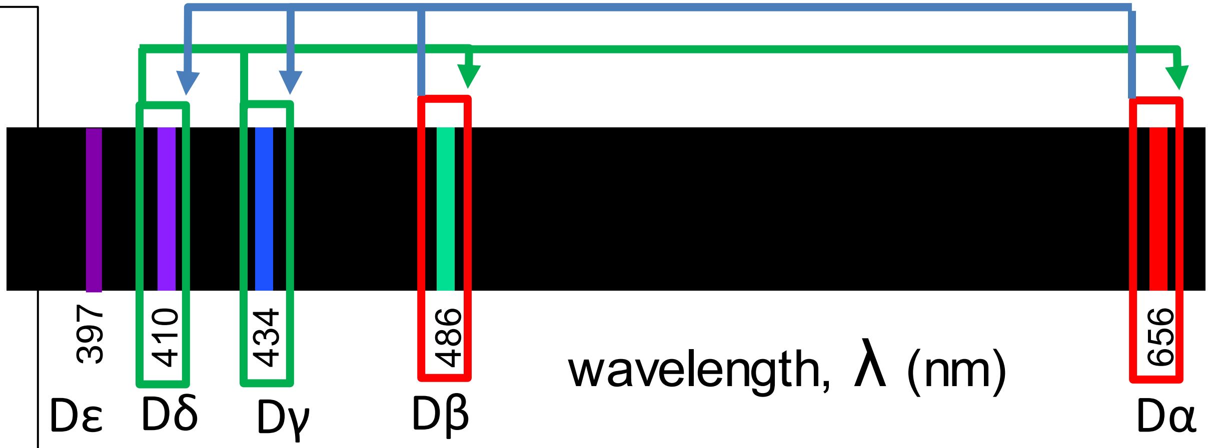
Negligible impact, estimated with SOLPS



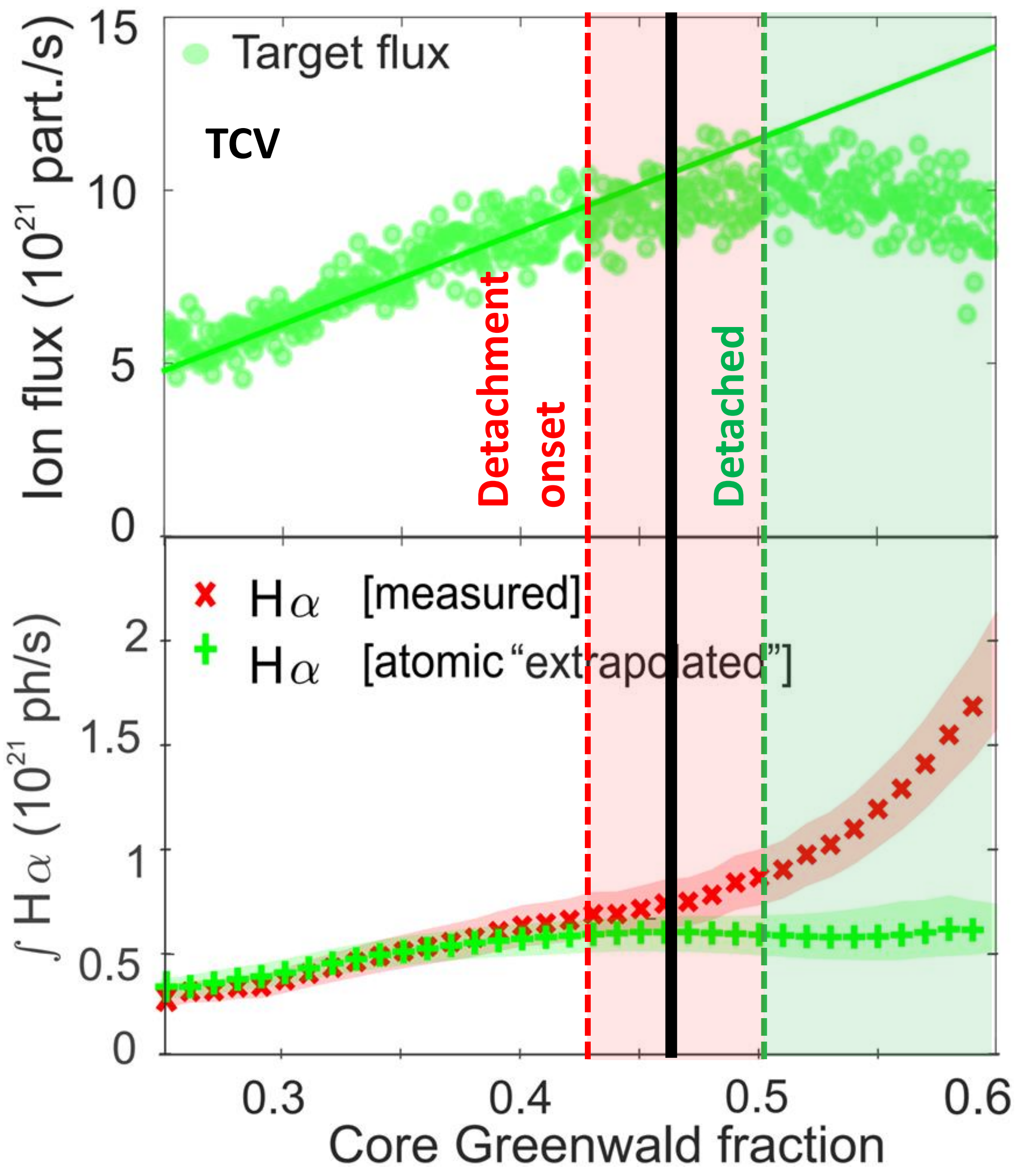
[Wünderlich, et al. Yacora]

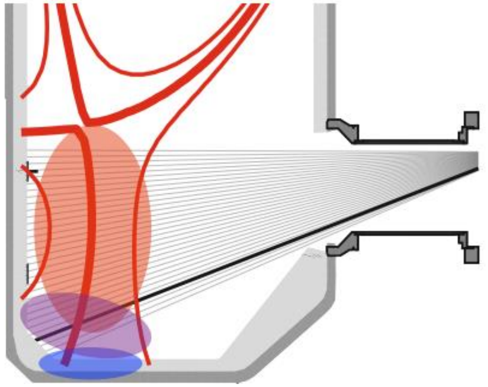
- Uses <u>**hydrogen CR**</u> model (Yacora online –Wünderlich, et al., 2020) results for MAR/MAI and population coefficients (**applied <u>to deuterium</u> plasma**)
- Does not rely on creation cross-sections for D_2^+ and D^-
- Monte Carlo **uncertainty** propagation (line ratios (13%), brightnesses (18%), ... 12.5/25% **atomic/molecular coefficients**)

Hydrogen Balmer spectrum



How plasma-mol. interaction impacts hydrogenic line emission

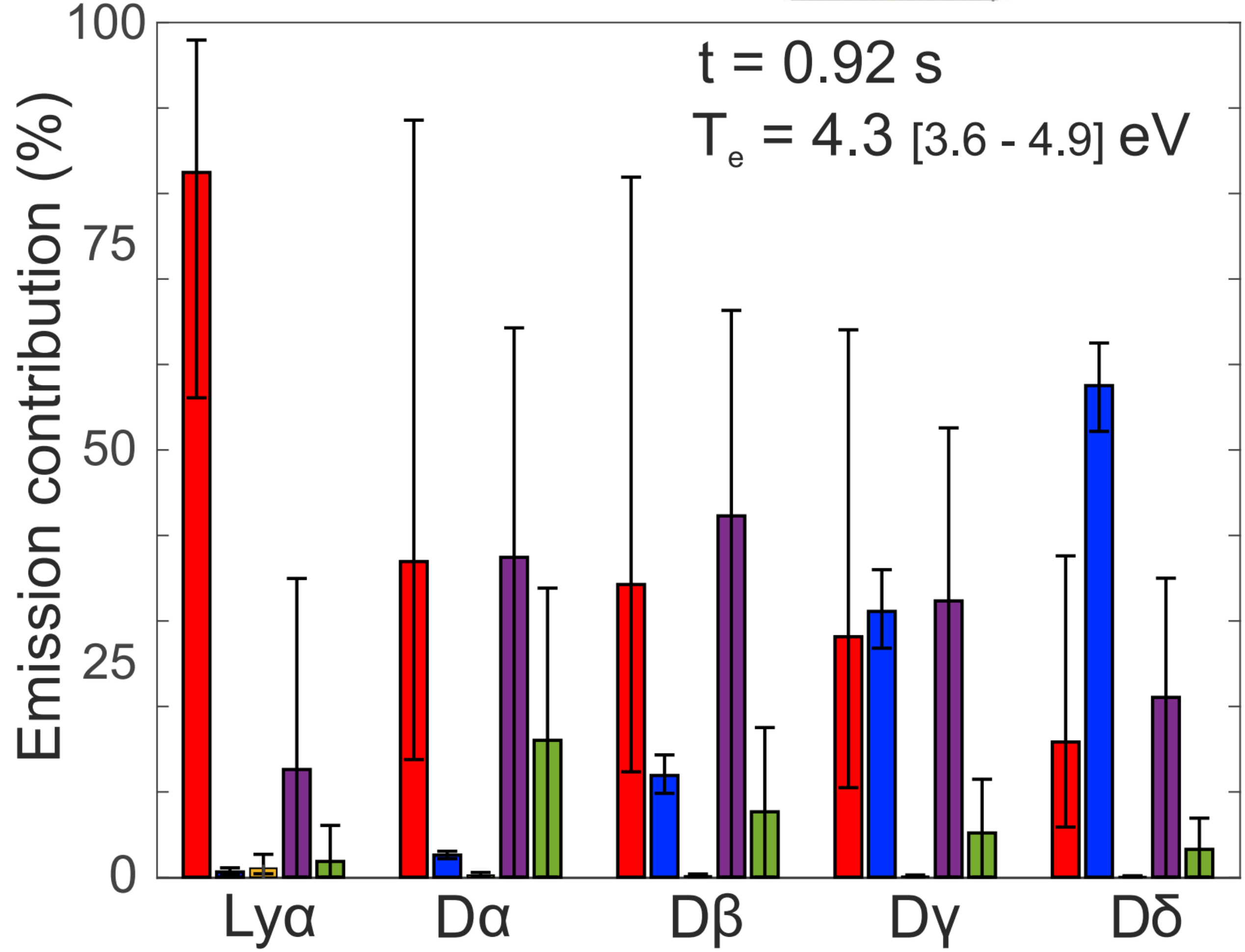




Excitation (D)

EIR – (D^+)

Molecules (D_2^+, D_2, D^-)



[Verhaegh, et al. 2021, PPCF]

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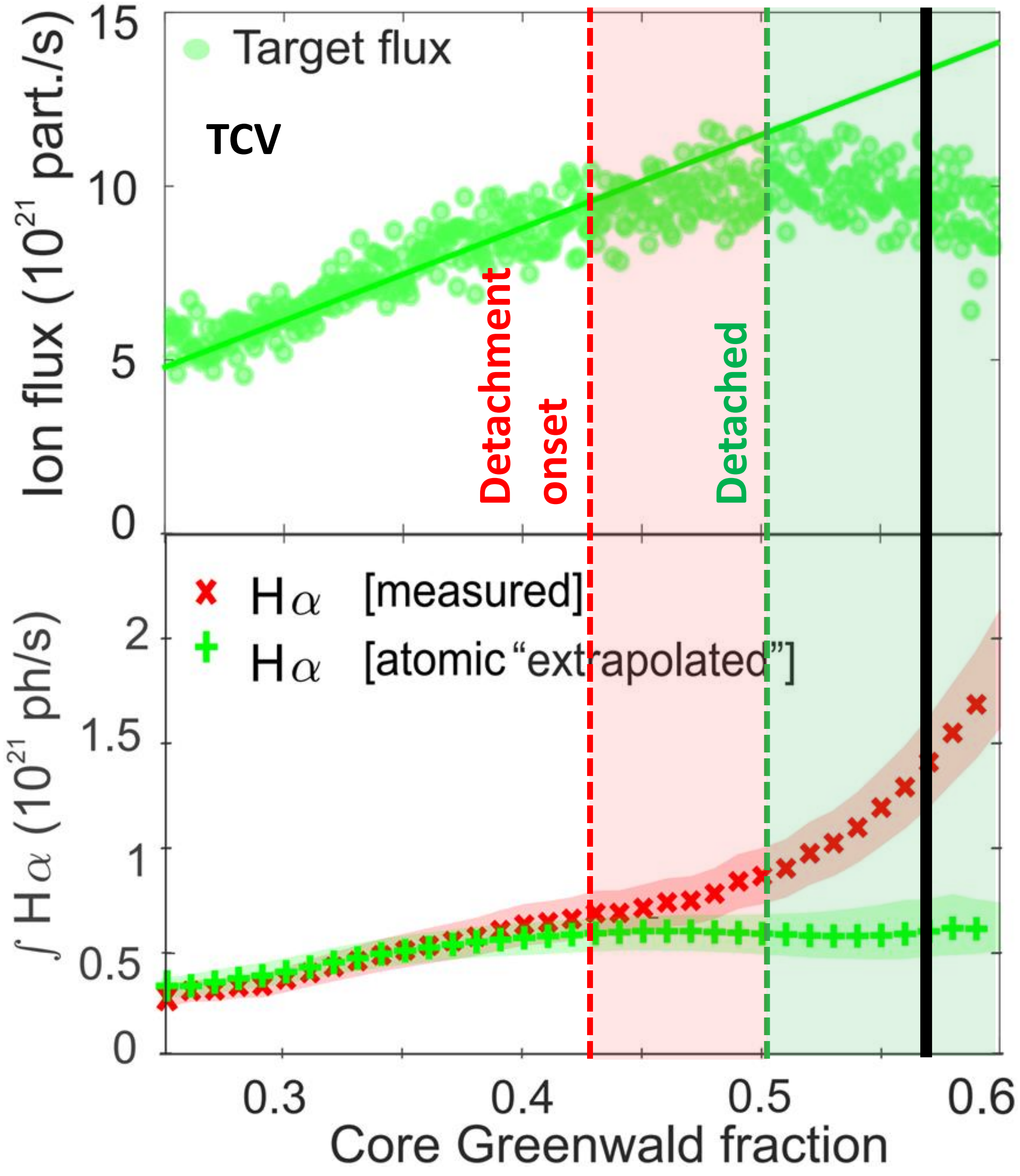
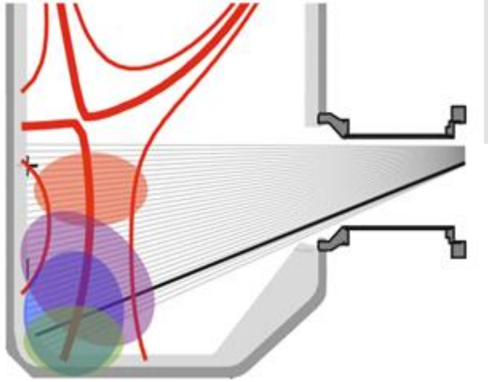
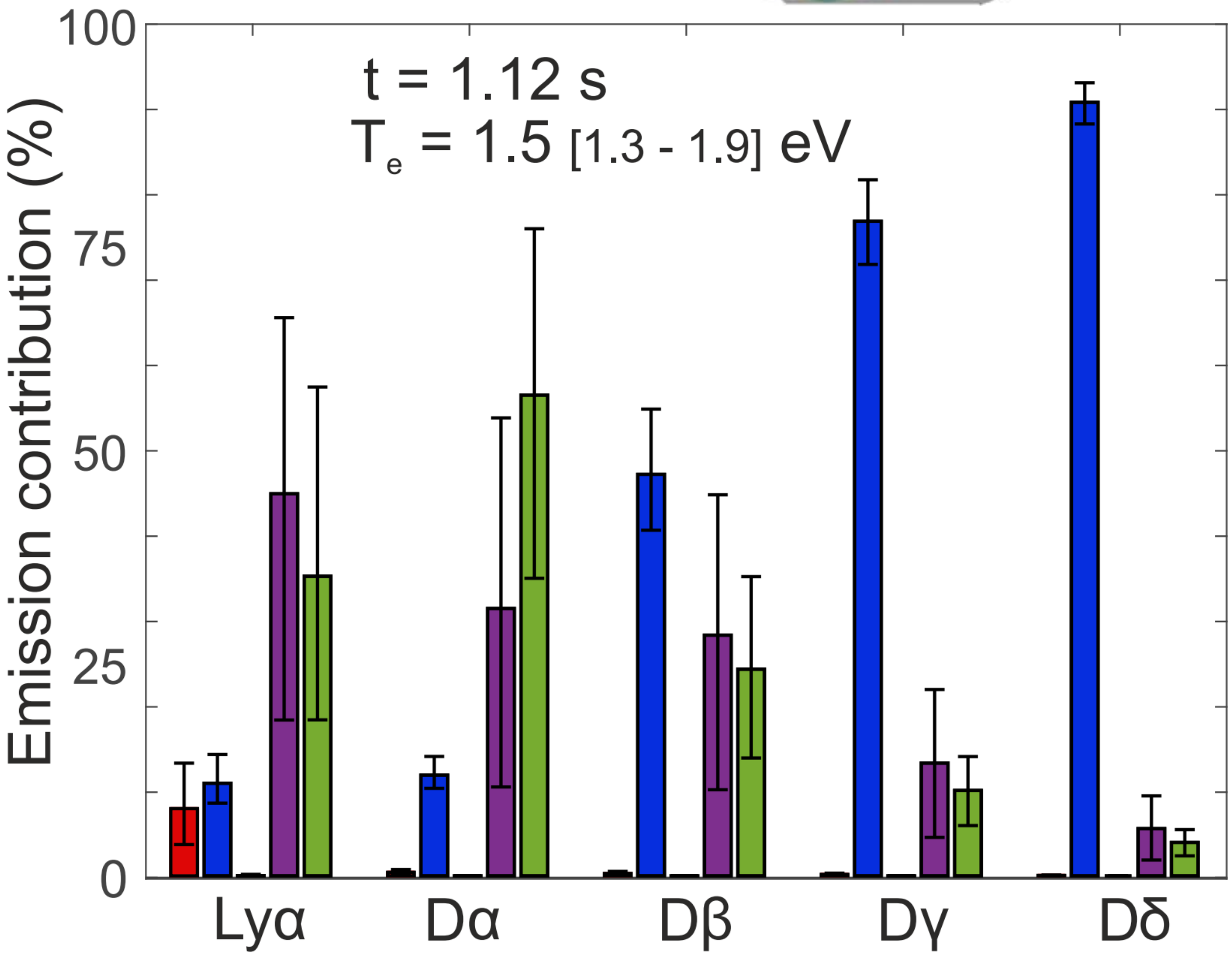






[Verhaegh, et al. 2021, PPCF]

How plasma-mol. interaction impacts hydrogenic line emission

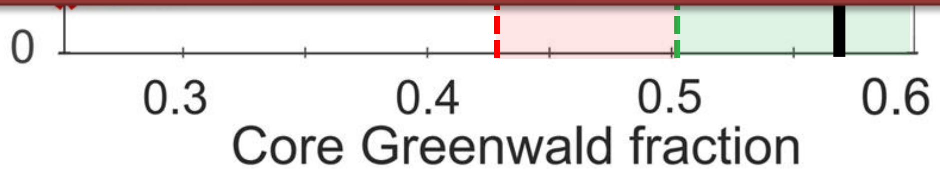
Plasma-molecule interactions:

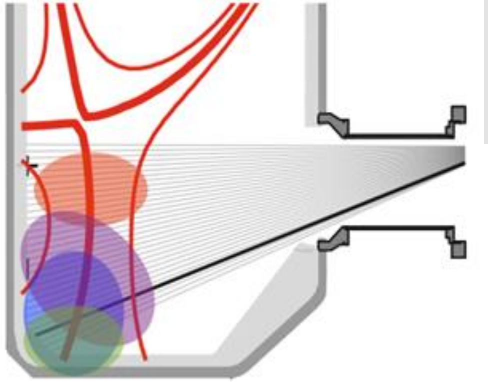
- Impact the hydrogenic spectra during detachment
- Have a non-negligible impact on medium-n Balmer lines (<40%, needs to be accounted for ionisation estimates)

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





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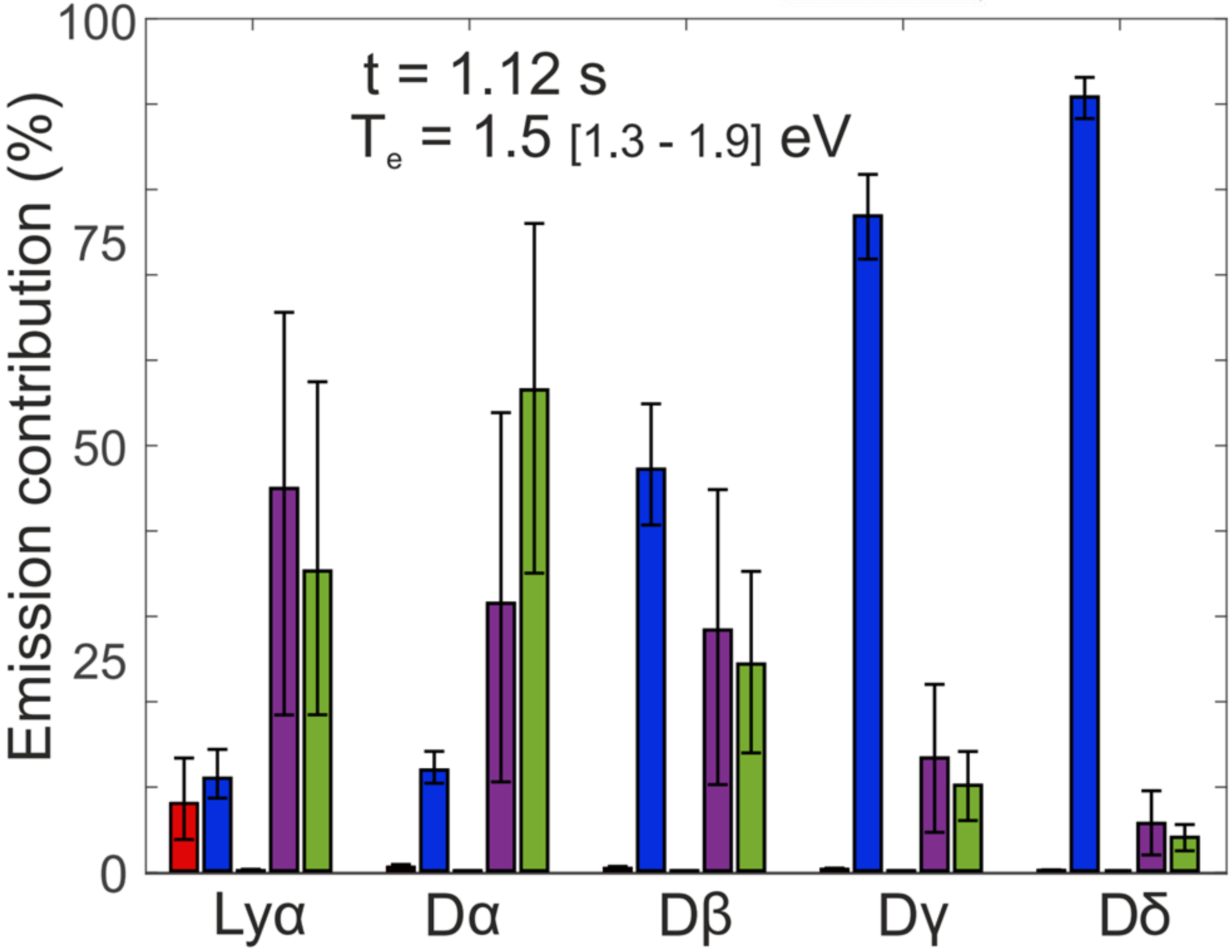
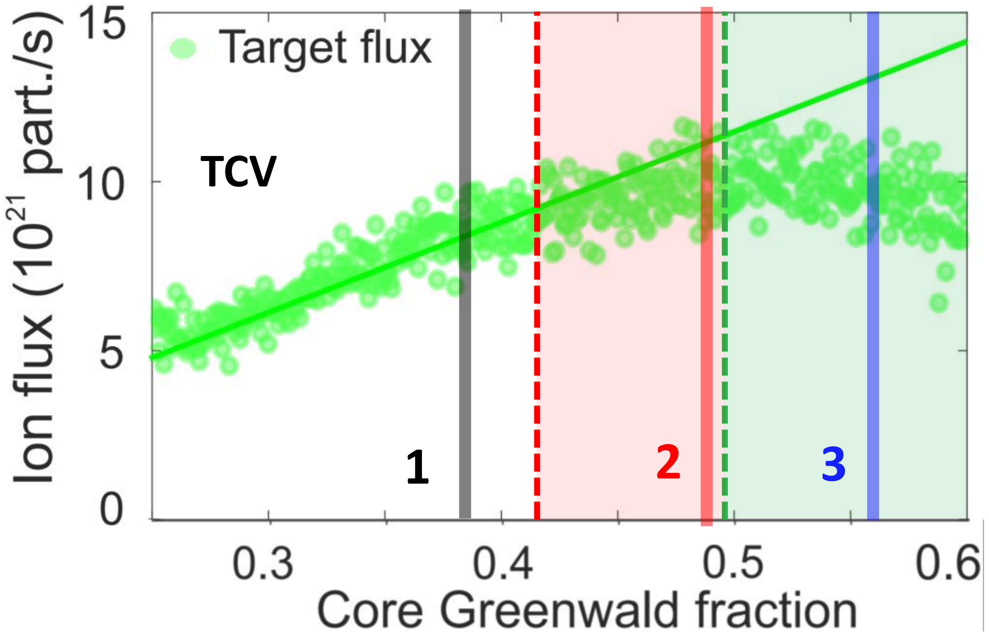
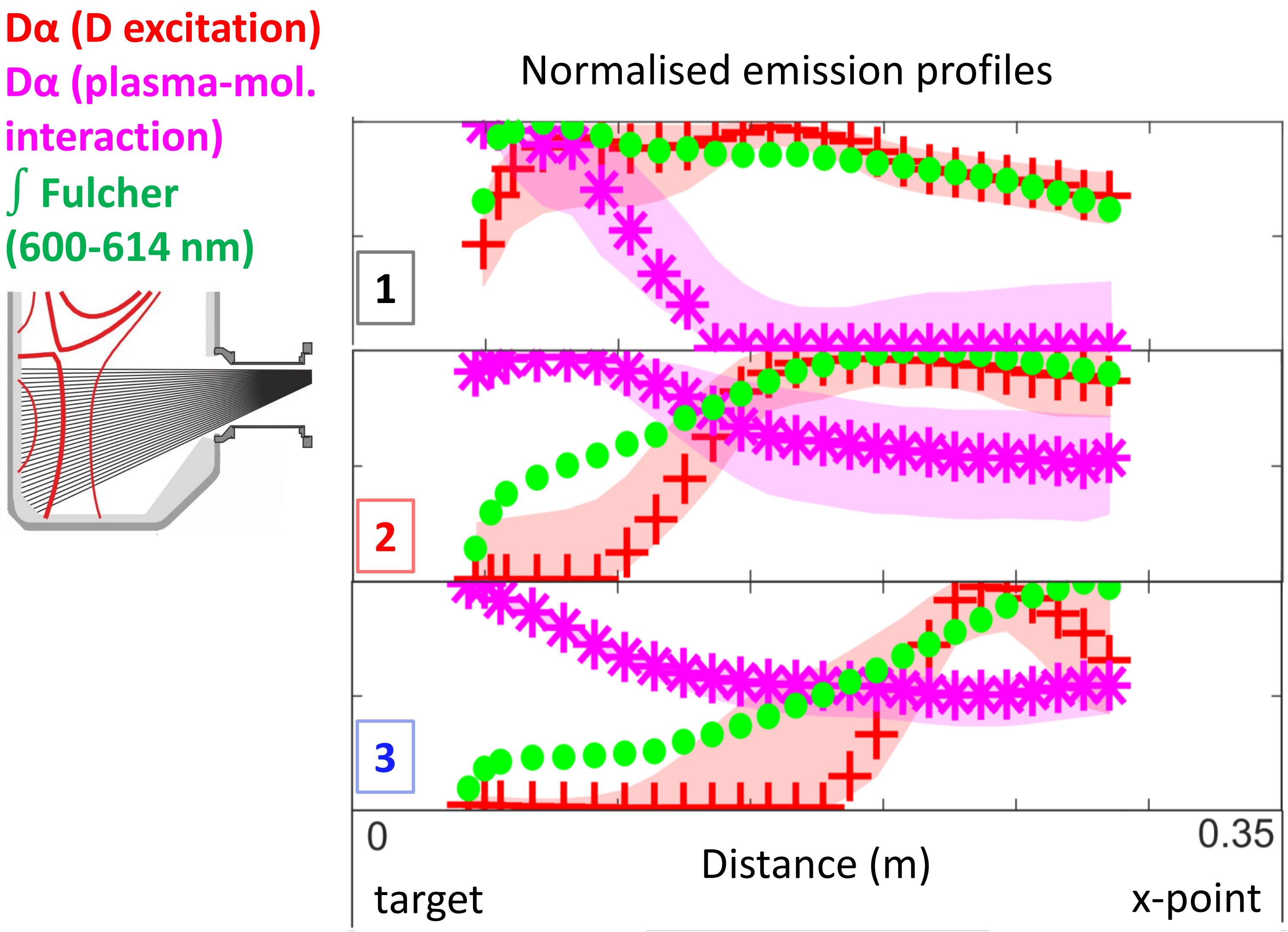


[Verhaegh, et al. 2021, PPCF]

Plasma-molecule interactions along the divertor leg



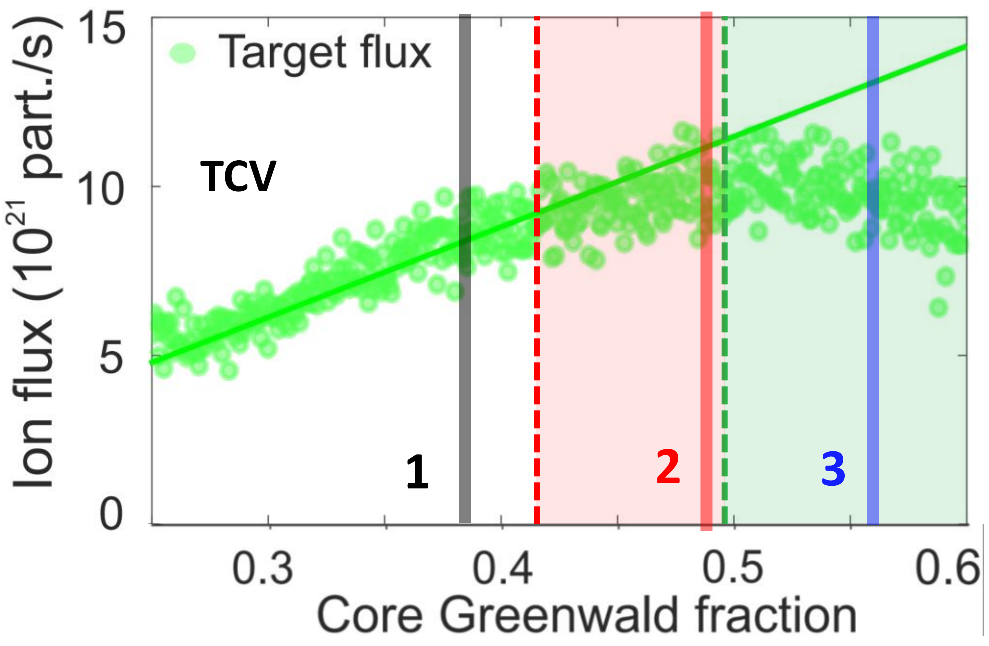


[Verhaegh, et al. NME 2021]

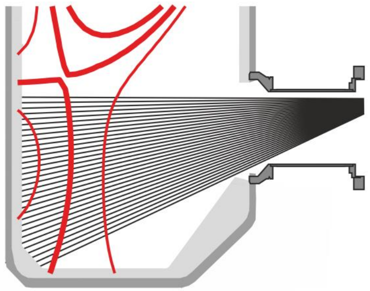
In Dα (D excitation) region

D mfp ~ 5-10 cm

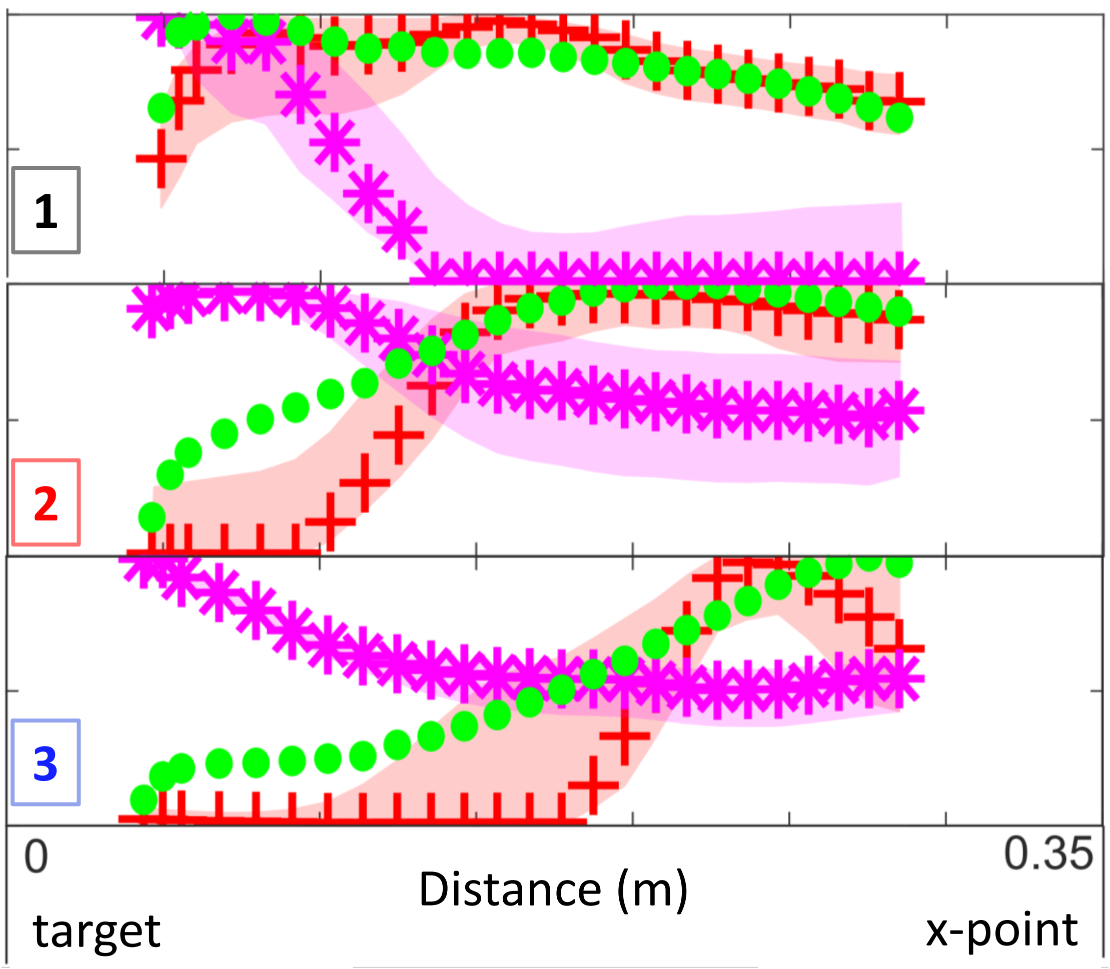
Plasma-molecule interactions along the divertor leg



Dα (D 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

-> raises questions on diagnosing MAR using Fulcher band measurements

[Verhaegh, et al. NME 2021]

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

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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 how the presented experimental inferences compare to plasma-edge modelling

- Conclusions

How plasma-mol. interactions can impact particle balance

Attached:

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

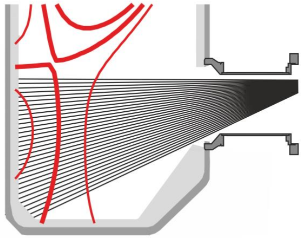
Detachment onset:

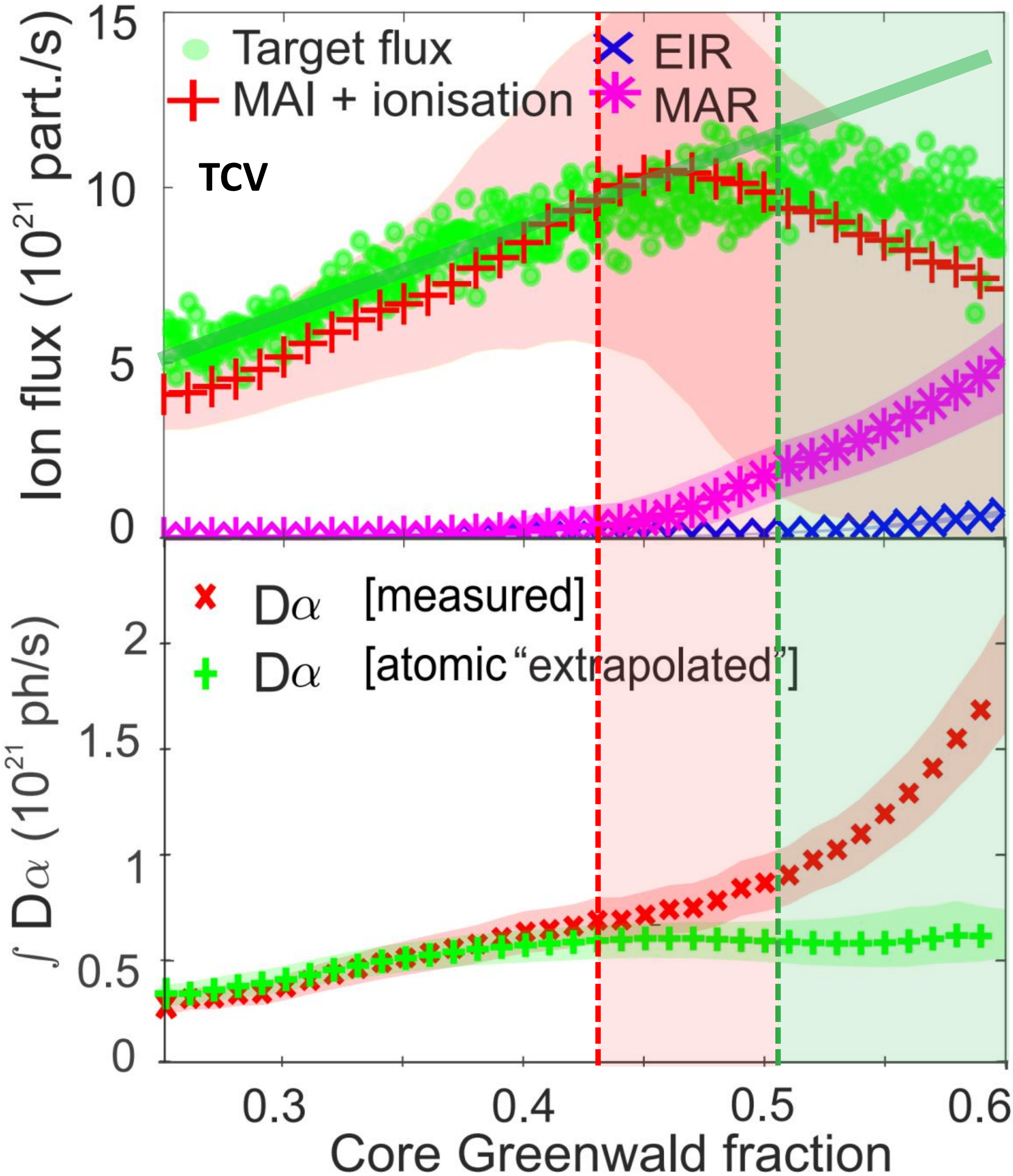
- **MAR** (Molecular Activated Recombination) starts to occur
- **Total ion source** drops

Detached

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

[Verhaegh, et al. NME 2021]





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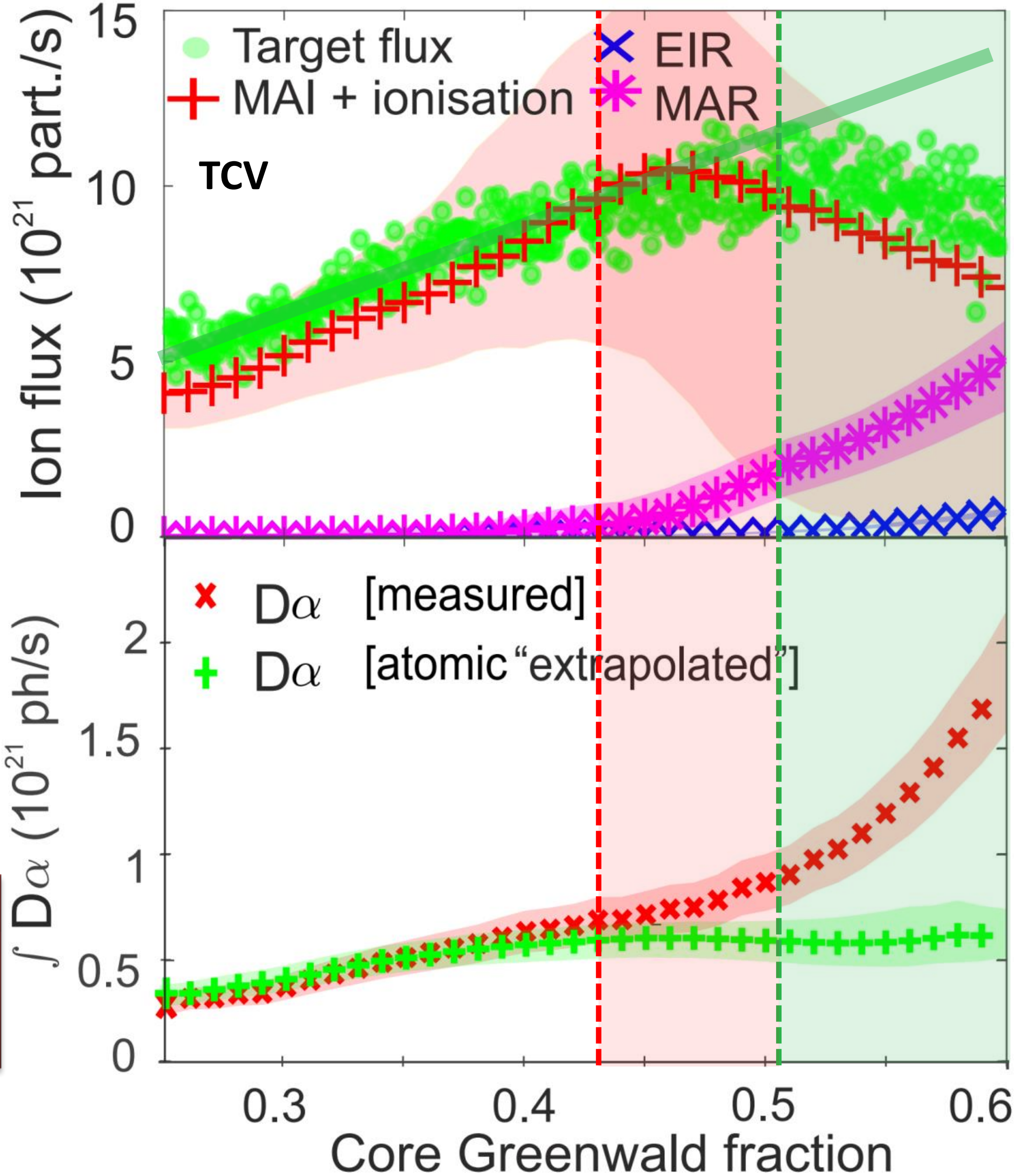


MAR – can be an important ion sink (50% of ion target flux) during detachment; and is more significant than EIR (for these TCV conditions, n_e = 10^{20} m^{-3})

How plasma-mol. interaction can impact power balance

- Radiative loss from molecular bands negligible*

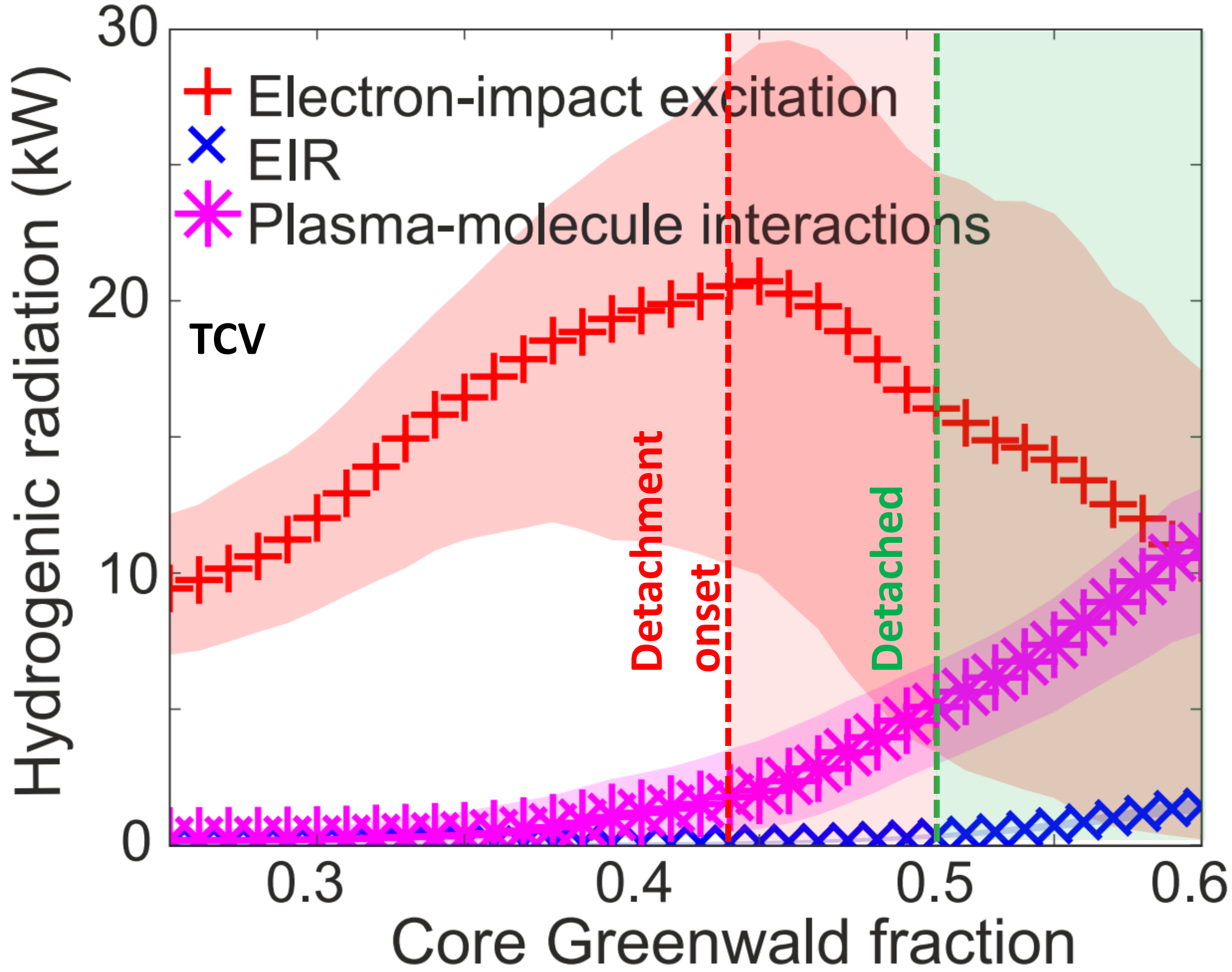
* [Groth, et al. 2018 NME]

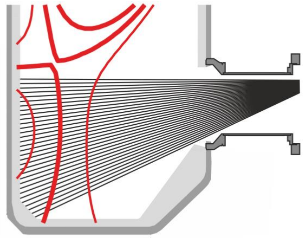
- Radiative loss from **excited atoms** after **plasma-molecule interaction** can be **significant**

Plasma-molecule interactions -> excited D atoms
-> significant D line radiation

Net power loss depends on **potential energy conversions**

- **Net** power loss **MAR** small (~8 eV per ion/6 kW)





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TCV observations compared to simulations

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

<u>Differences</u> 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

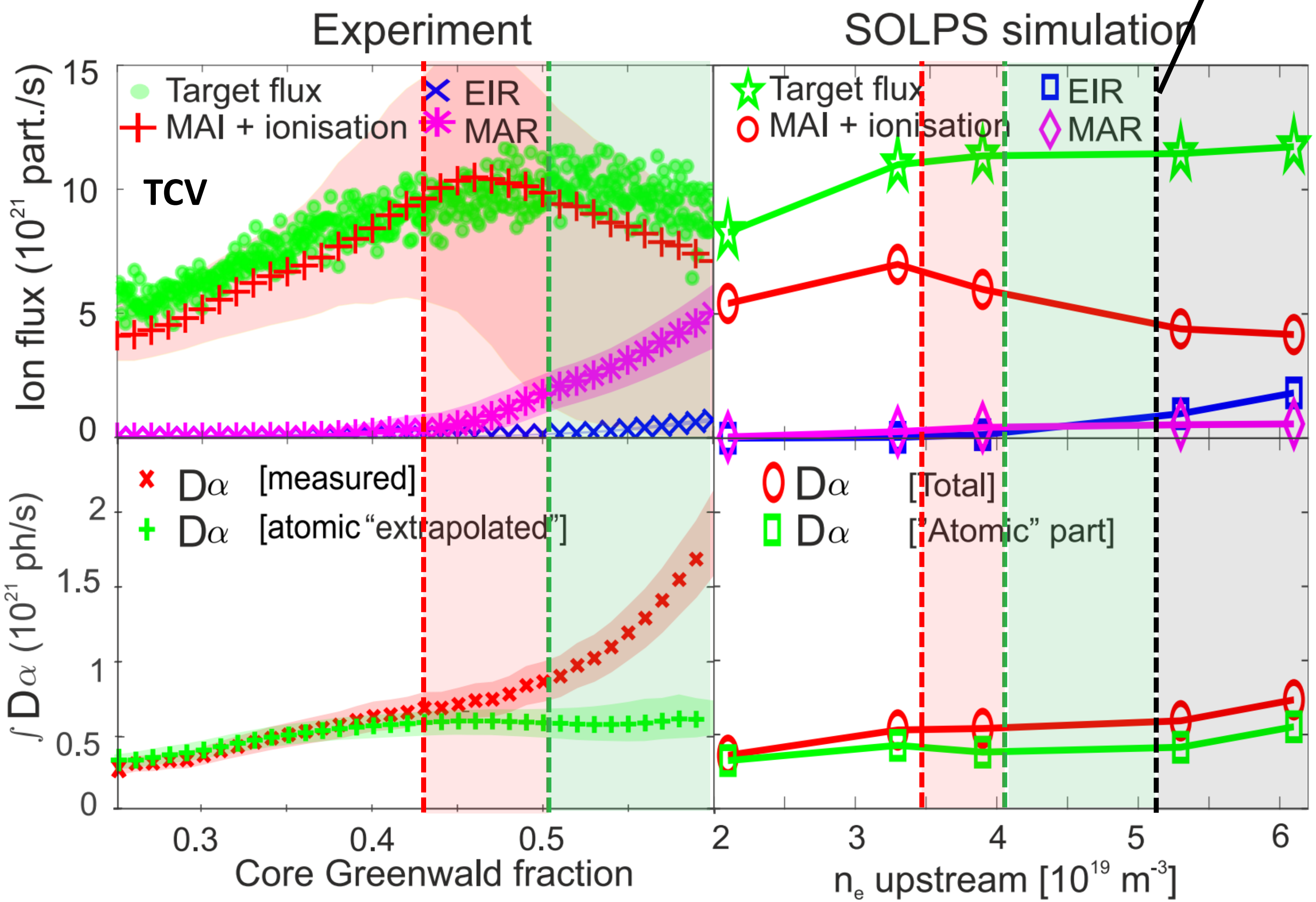
The effect of D_2^+ is strongly underestimated in the simulation compared to the experiment

In agreement with JET results

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

Vibrational state **unresolved** (default):

1. averaged over vibrational states (v) – simplified model with:
   electron impact collisions with D_2 vibrational-vibrational exchange (E_{H2} = 0.1 eV)
2. *effective* mol. CX: $D_2 + D^+ \rightarrow D_2^+ + D$ – mass rescaled from Hydrogen -> Deuterium ($T_e/2$)

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

D_2^+ creation:

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

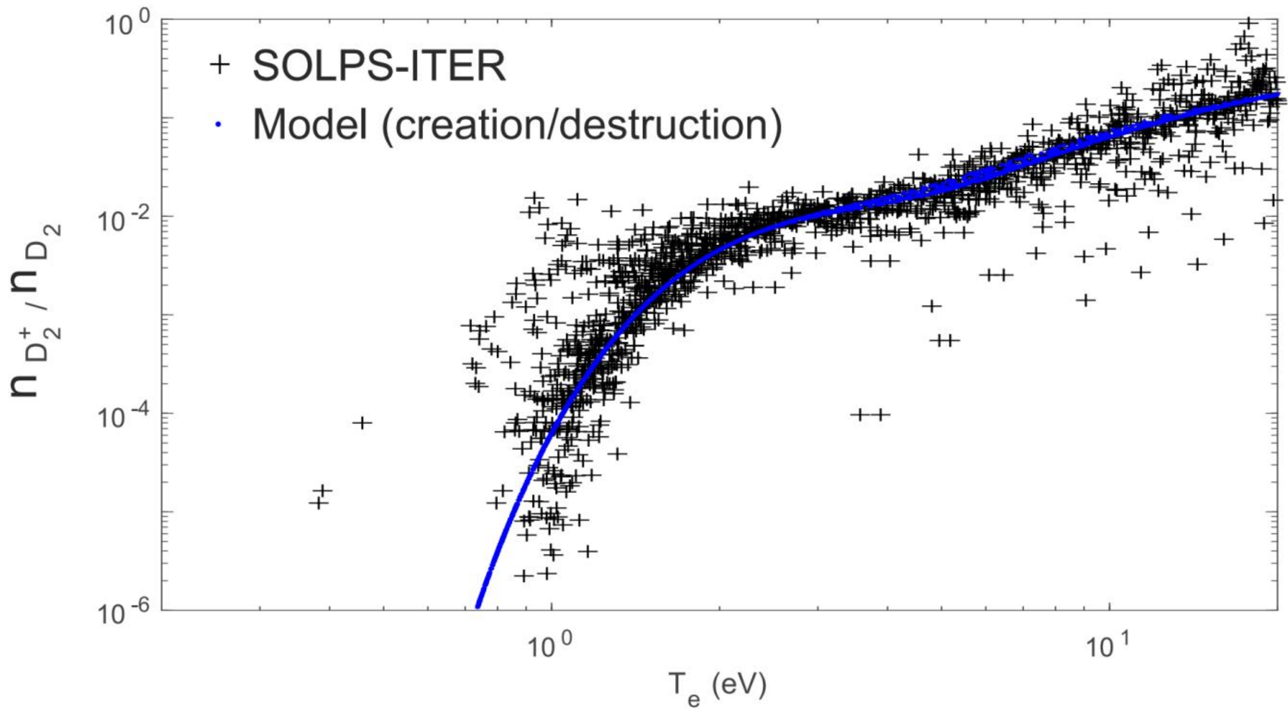
$e^- + D_2 \rightarrow 2\,e^- + D_2^+$

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

Vibrational state **unresolved** (default):

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

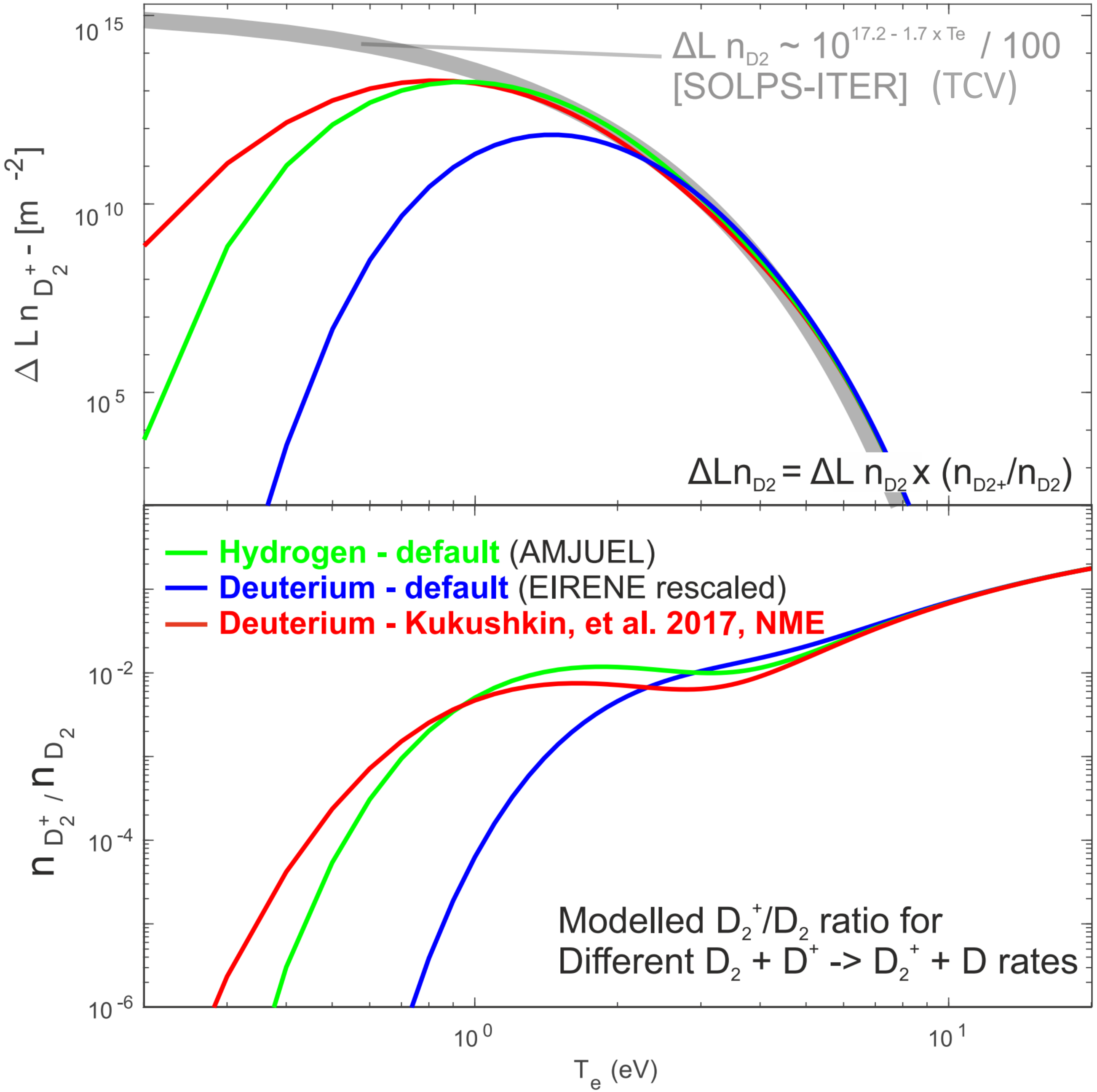
D_2^+/D_2 ratios modelled using different mol. CX rates:

- **Default Eirene/AMJUEL** (hydrogen rates) ($E_{H2} = 0.1$ eV)
- **Eirene rescaled deuterium** (default)
  [drops more strongly at lower temperatures]
- **Deuterium – Kukushkin, et al. 2017, NME** ($E_{H2} = 0.4$ eV)
  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

Caveat: Rates by Kukushkin, et al. under discussion
[Reiter, Jül-4411 report]

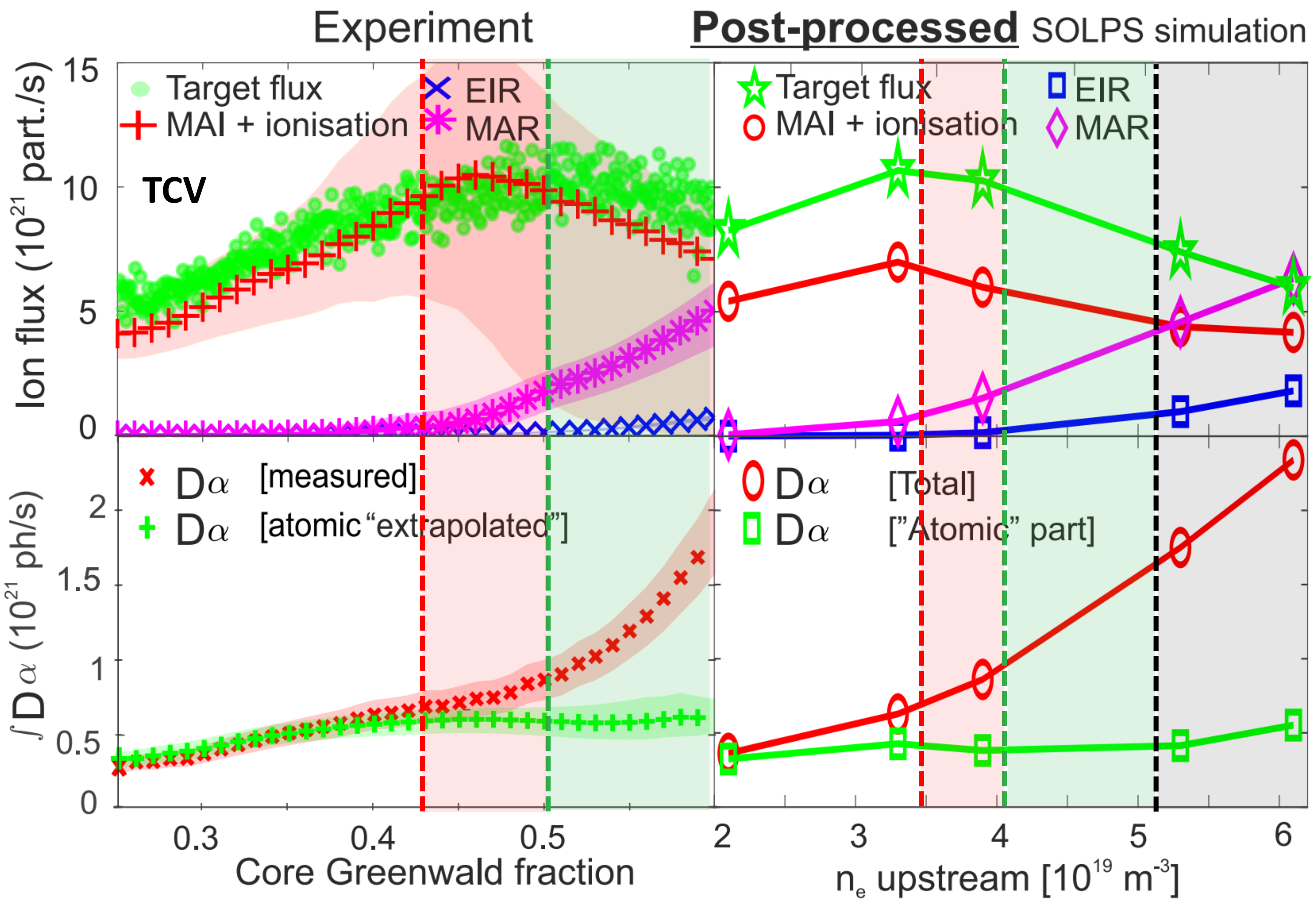


TCV observations compared to simulations

Post-processed (not strictly self-consistent) using the $D_2 + D^+ \rightarrow D_2^+ + D$ rate from Kukushkin, PSI/NME, 2018

Agreement 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

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

- **Dα increase**s during detachment
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- **Roll-over** of the **ion target flux**, as well as **ion source**

The effect of D_2^+ is <u>in agreement</u> 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]

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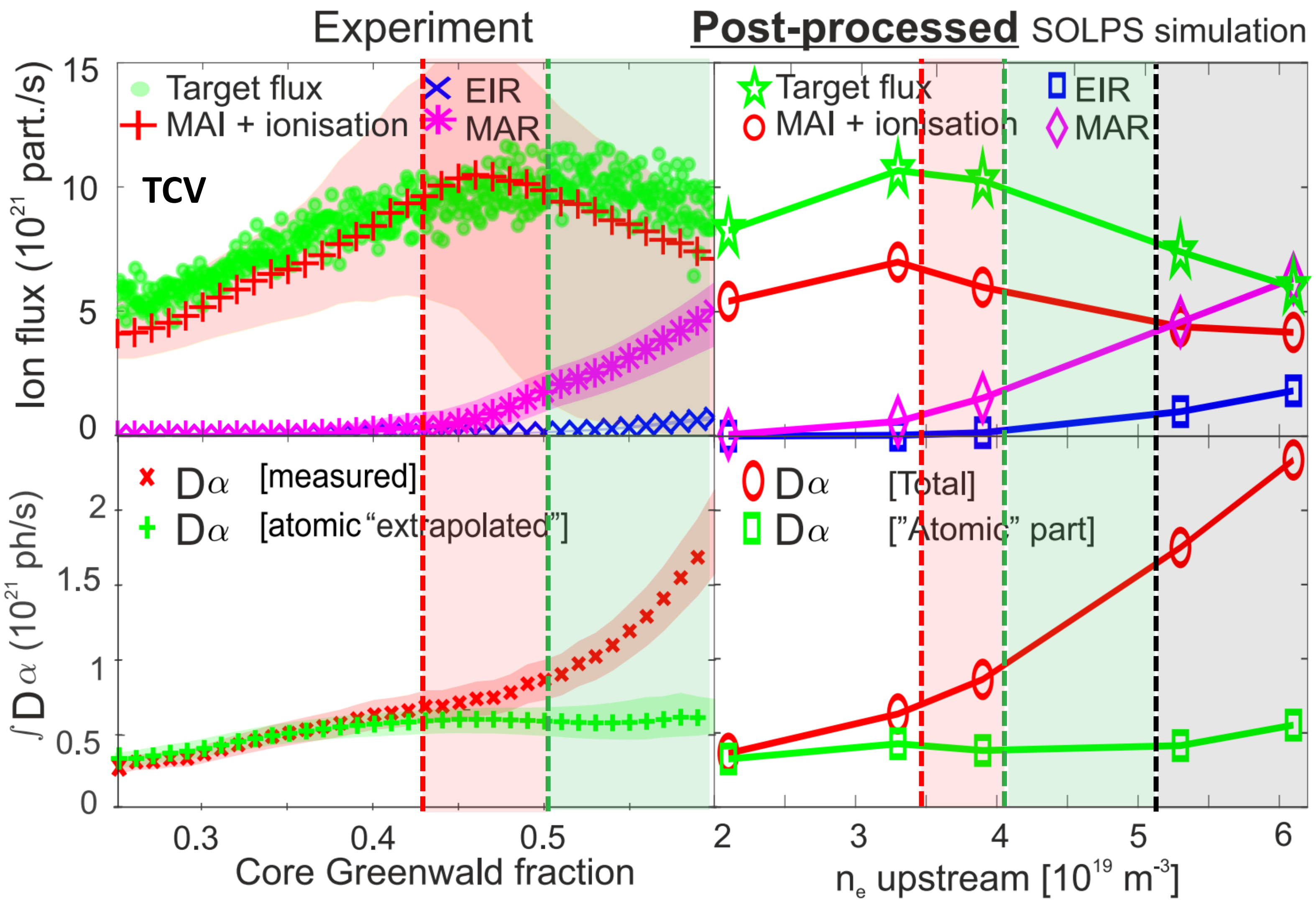

Conclusion

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**

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

Further experimental and simulation investigation required

Discussion

Caveats:

- Hydrogen CR models models used for deuterium plasma
- Line integrated measurements, however the detachment process is 2D -> towards multi-wavelength imaging [C. Bowman, A. Perek, …]

This work raises **questions** about:

- The **isotope rescaling used in Eirene**, particularly for molecular charge exchange
- **Spectroscopic analysis**; requires accounting for plasma-molecule interactions
- Dα(/Lyβ) enhancements may have implications for **diagnosis** of **photon opacity**

Generality of this work needs to be **investigated**, depends on:

- The vibrationally excited levels of D_2
  - Molecular transport (depends on neutral mean free paths (5-10 cm TCV for D) / divertor shape)
  - Wall conditions (e.g. carbon vs tungsten – reflection vs absorption)
- **More studies needed** (Fulcher band spectroscopy vs vibrationally resolved simulations)

Discussion

However, these **TCV results** are **consistent** with **results** from **DIII-D** [Hollman, et al. 2005, PPCF] as well as **JET** [Lomanowski, et al. 2020 PPCF] - spectroscopic analysis needed for other devices

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