An experimental analysis of the impact of plasma-molecule interactions on power/particle losses, atomic line emission; and comparisons against simulations

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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 requires:
• Power loss
• Momentum loss
• Particle loss (↓ ionisation and/or ↑ ion sink)

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

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

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

Detachment requires:
• Power loss
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Detachment induced by chain of **atomic and molecular reactions**

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

In this work we investigate these interactions experimentally to estimate:
• impact on detachment (power/particle balance)
• impact on diagnostic interpretation
• agreement experiment and SOLPS-ITER modelling
‘Detachment’ and plasma-molecule interactions

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

1. **Collisions** between the plasma and D$_2$
   a) Transfers momentum/power plasma $\rightarrow$ molecules,
   b) Excites D$_2$ (v) $\rightarrow$ **Molecular spectra** (negligible radiation)

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

Studied experimentally in tokamaks

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**Plasma**

- Collisions
- Reactions

**Fulcher emission**

**Section of D$_2$ (v) Fulcher spectra**

TCV

<table>
<thead>
<tr>
<th>Time (s)</th>
<th>Counts (a.u.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>t = 0.6 s</td>
<td></td>
</tr>
<tr>
<td>t = 1.16 s</td>
<td></td>
</tr>
</tbody>
</table>

**Graph:**

- Wavelength (nm)
- Counts (a.u.)
‘Detachment’ and plasma-molecule interactions

1. **Collisions** between the plasma and D₂
   a) Transfers momentum/power plasma -> molecules,
   b) Excites D₂ (v) -> Molecular spectra (negligible radiation)

2. **Reactions** between the plasma and ‘molecular species’
   For instance: D₂ + D^+ -> D₂^+ + D; D₂^+ + e^- -> D* + D*
   [Molecular Activated Recombination (MAR)]
   a) Impacts particle (MAR & MAI) and momentum balance
   b) Leads to **excited (*) hydrogen atoms** -> atomic line emission & radiation

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

[Wunderlich, et al. Yacora, 2020]

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'Detachment' and plasma-molecule interactions

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

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

For instance: \( \text{D}_2 + \text{D}^+ \rightarrow \text{D}_2^+ + \text{D} \); \( \text{D}_2^+ + \text{e}^- \rightarrow \text{D}^* + \text{D}^* \)

[Molecular Activated Recombination (MAR)]

a) Impacts particle (MAR & MAI) and momentum balance
b) Leads to **excited (*) hydrogen atoms** -> atomic line emission & radiation

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

[Wünderlich, et al. Yacora]

Hydrogen Balmer spectrum

- \( \text{D}_\varepsilon \)
- \( \text{D}_\delta \)
- \( \text{D}_\gamma \)
- \( \text{D}_\beta \)
- \( \text{D}_\alpha \)

wavelength, \( \lambda \) (nm)

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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 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
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**

- \( \text{D}^+ \) to \( B_{n\rightarrow2} \)
- \( \text{D} \) to \( B_{n\rightarrow2} \)

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Kevin Verhaegh | IAEA Technical Meeting | 29-03-2021 | Molecules & Balmer line emission | Page 3a/14
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- **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’)

**Spectroscopic analysis:**
1. Apply atomic analysis to medium-n Balmer line pair
2. Use result to estimate atomic contribution $D\alpha$, compare against measurement
**Dα emission and molecules - results**

- Measured *Dα* emission increases during detachment beyond *Dα* emission expected purely on the basis of atomic reactions

Increase measured *Dα* during detachment consistent with observations on other devices (O. Groth, previous talk)
**$D\alpha$ emission and molecules - results**

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

  \[-D\alpha \text{ from excited atoms after plasma-molecule interactions}\]

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Kevin Verhaegh | IAEA Technical Meeting | 29-03-2021 | Molecules & Balmer line emission | Page 4b/14
**Dα emission and molecules - results**

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

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

This **mismatch of $D\alpha$** 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 $D\alpha$, $D\beta$, $D\gamma$, $D\delta$ (BaSPMI - [Verhaegh, et al. PPCF, 2021])

![Graph showing $D\alpha$ flux vs. core Greenwald fraction](image)
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** \( D_\alpha, D_\beta \)
3. **Measured** \( D_\alpha, D_\beta = \text{‘Atomic’ + ‘Molecular’ emission} \)
4. Iterate to **self consistent separation** \( D_\alpha, D_\gamma, D_\delta \) (and \( D_\beta \) for \( D_2^+, D^- \) separation)
5. Multiply **separate brightnesses** with ‘**reaction/radiation per photon** per photon’ ratios to obtain:
   1. **Particle sinks/sources** (MAR, MAI, ionisation, electron-ion recombination)
   2. **Radiative power losses**

- Uses **hydrogen CR** model (Yacora online – Wünderlich, et al., 2020) 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**)

Negligible impact, estimated with SOLPS
How plasma-mol. interaction impacts hydrogenic line emission

Excitation (D)

EIR – (D⁺)

Molecules (D₂⁺, D₂, D⁻)

[Verhaegh, et al. 2021, PPCF]
How plasma-mol. interaction impacts hydrogenic line emission

Excitation (D)
EIR – (D\(^+\))
Molecules (D\(_2^+\), D\(_2\), D\(^-\))

Verhaegh, et al. 2021, PPCF
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\textsuperscript{-} may be present despite low cross-section for D [Krishnakumar, et al. PRL, 2011]

If D\textsuperscript{-} is not accounted for, D\beta would be overestimated by 34 [25-44]% near the target

MAR/power losses similar (given the uncertainties) whether D\textsuperscript{-} is accounted for or not
Plasma-molecule interactions along the divertor leg

\[ \text{D}_\alpha (\text{D excitation}) \]
\[ \text{D}_\alpha (\text{plasma-mol. interaction}) \]
\[ \int \text{Fulcher (600-614 nm)} \]

In the \( \text{D}_\alpha (\text{D excitation}) \) region, \( \text{D mfp} \approx 5-10 \text{ cm} \)

[Verhaegh, et al. NME 2021]
Plasma-molecule interactions along the divertor leg

- \( \text{D} \alpha \text{ (D excitation)} \) emission 'detaches' from target followed by Fulcher emission at detachment onset (consistent with JET – see talk M. Groth)
- \( \text{D} \alpha \) (plasma-mol. interaction) 'remains peaked at target

-> raises questions on diagnosing MAR using Fulcher band measurements

[Verhaegh, et al. NME 2021]

In \( \text{D} \alpha \) (D excitation) region

\( \text{D mfp} \sim 5-10 \text{ cm} \)
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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]
How plasma-mol. interactions can impact particle balance

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

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

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

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

**Differences** simulation & experiment:
- $D_\alpha$ 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 previous talk

Simulations from [A. Fil, et al. CPP, 2018]
D_{2}^{+} molecular CX rates

• Mol. CX: D_{2}^{+} + D^+ -> D_{2}^{+} + D – mass rescaled by Eirene from Hydrogen -> Deuterium (T_e/2)

• Vibrational states - Boltzmann distribution T_{D_2} = 0.1 eV

• 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^+ -> D_{2}^{+} + D
e^- + D_2 -> 2 e^- + D_{2}^{+}

D_{2}^{+} destruction
e^- + D_{2}^{+} -> D + D
e^- + D_{2}^{+} -> e^- + D^+ + D
e^- + D_{2}^{+} -> 2e^- + D^+ + D^+
D$_2^+$ molecular CX rates

- Mol. CX: D$_2^+$ + D$^+$ -> D$_2^+$ + D – mass rescaled by Eirene

- Vibrational states - Boltzmann distribution

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. 2018, NME

- 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

Modelled D$_2^+/D_2$ ratio for Different D$_2$ + D$^+$ -> D$_2^+$ + D rates
Agreement simulation & experiment:
- $D\alpha$ increases during detachment
- MAR / impact $D_2^+$ significant
- Roll-over of the ion target flux, as well as ion source

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

Simulations from [A. Fil, et al. CPP, 2018]
Agreement simulation & experiment:

- $\text{D} \alpha$ increases during detachment
- MAR / impact $\text{D}_2^+$ significant
- Roll-over of the ion target flux, as well as ion source

The effect of $\text{D}_2^+$ 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]
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
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, A. Karhunen, ...]

This work raises questions about:

- The isotope rescaling used in Eirene, particularly for molecular charge exchange
- Spectroscopic analysis; requires accounting for plasma-molecule interactions
- $\text{Da}/(\text{Ly}\beta)$ enhancements may have implications for diagnosis of photon opacity (see S. Wiesen talk)

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)
- More studies needed (Fulcher band spectroscopy vs vibrationally resolved simulations)
However, these **TCV results** are *consistent* with results from DIII-D [Hollman, et al. 2005, PPCF] as well as JET [M. Groth, previous talk; Lomanowski, et al. 2020 PPCF] - spectroscopic analysis needed for other devices

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- Da(/Lyβ) enhancements may have implications for **diagnosis of photon opacity** (see S. Wiesen talk)

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