EUROfusion

Study of molecular hydrogen data and their impact on CRMs and exhaust simulations for detached plasmas

Kevin Verhaegh, Stefan Mijin, David Moulton, et al.

kevin.verhaegh@ukaea.uk

UK Atomic Energy Authority

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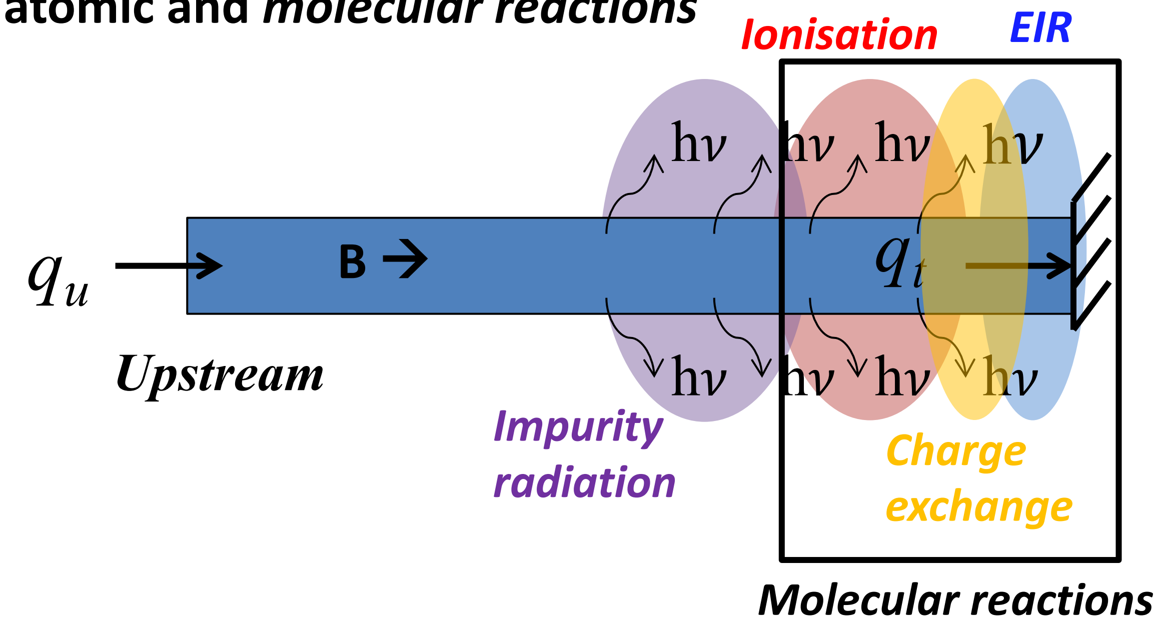
Detachment physics & plasma-molecular interactions

Detachment requires:

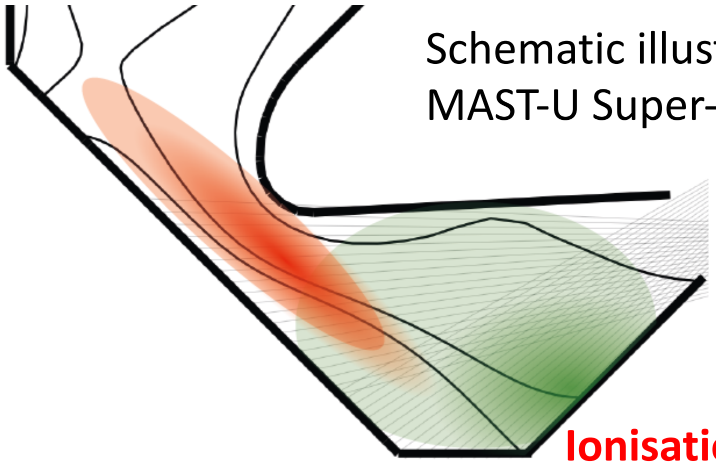
- **Power loss**
- **Momentum loss**
- **Particle loss** (↓ ionisation and/or ↑ ion sink)

Detachment (< ~ 5 eV) induced by chain of **atomic and *molecular reactions***



High molecular density can build up in detached conditions:

- **Ionisation region detached from the target ->** build-up of neutral atoms & **molecules below**
- As T_e drops, molecular density rises strongly



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

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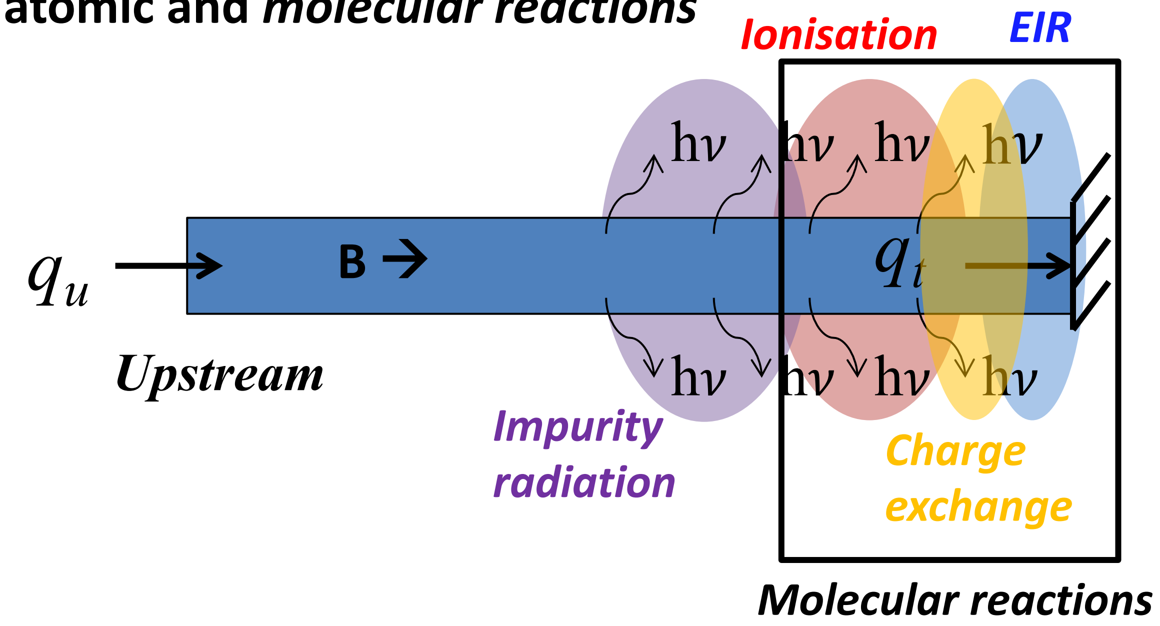
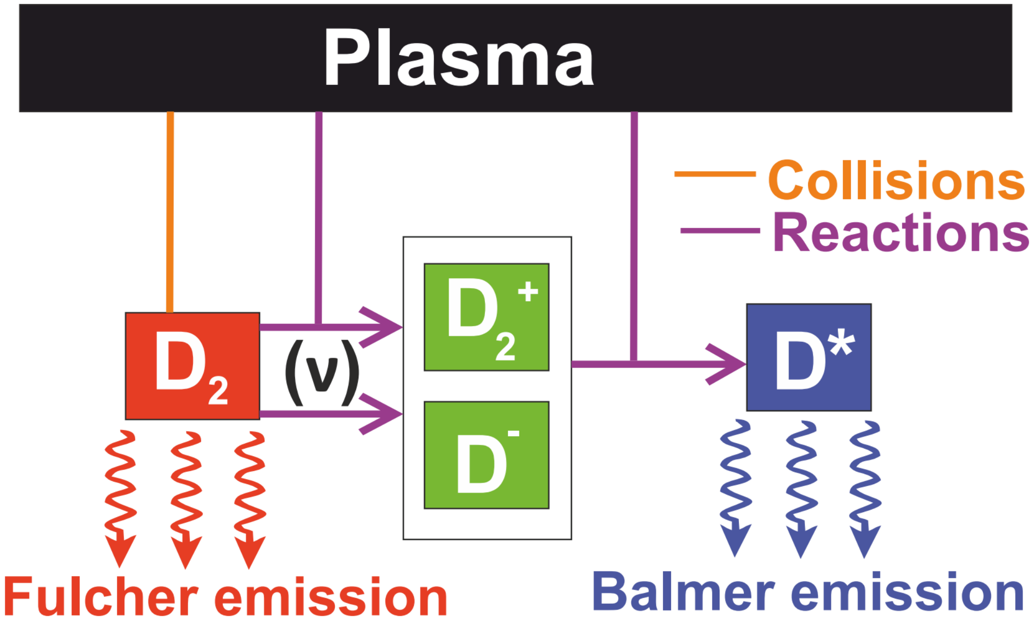


Detachment is driven by atomic/molecular reactions through dependencies between power, particle and momentum balances

Plasma-molecular interactions impact power, particle and momentum balance:

- **Collisions -> momentum & power dissipation, rovibrational excitation of molecules**
- **Plasma-chemistry: molecular ions formed -> react with the plasma -> Power, particle & momentum loss**

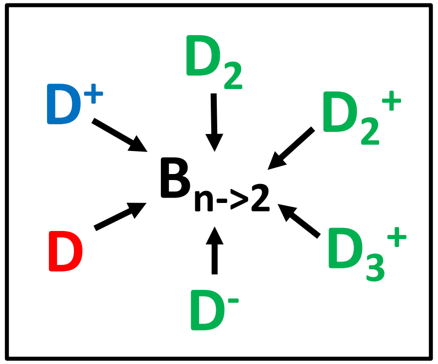


Plasma-molecular chemistry with molecular ions

Molecular ions can impact detached state and plasma diagnostics. Examples:

$D_2 + D^+ \rightarrow D_2^+ + \mathbf{D}$;	$D_2^+ + e^- \rightarrow \mathbf{D} + \mathbf{D^*}$	[Molecular Activated Recombination (**MAR**)]
D2 + D+ -> D2+ + D;	D2+ + e- -> e- + D+ + D*	[Molecular Activated Dissociation (**MAD**)]
e- + D2 -> D2- -> D- + D;	D- + D+ -> D + **D***	[MAR]

- Impacts **particle balance** (MAR)
- Provides **additional dissociation chains** (MAD) -> **power losses**, raises atom/molecule ratio, ….
- Leads to **excited (*) hydrogen atoms** -> atomic line emission & radiation



[Wünderlich, et al. Yacora, 2020]

Use Balmer lines to diagnose plasma-neutral interactions:

D* from 'plasma-molecular reactions' emission (PMR) ~ MAR / MAD

D* electron-impact excitation (EIE) emission ~ Ionisation

D* electron-ion recombination (EIR) emission ~ EIR

Deuterium Balmer spectrum

Example – MAR/D on MAST-U

Detachment evolution:

[Verhaegh, 2023, ArXiV, 2311.08580]

- **Ionisation** detached from target, **MAR** appears downstream
- Peak **MAR** detaches & **EIR** appears near target ($T_e \leq 0.2$ eV)
- **MAR remains significant** even at strong **EIR** ($T_e \leq 0.2$ eV)

MAR significant before Electron-Ion Recombination (EIR) and remains dominant

MAD is the dominant dissociation mechanism!

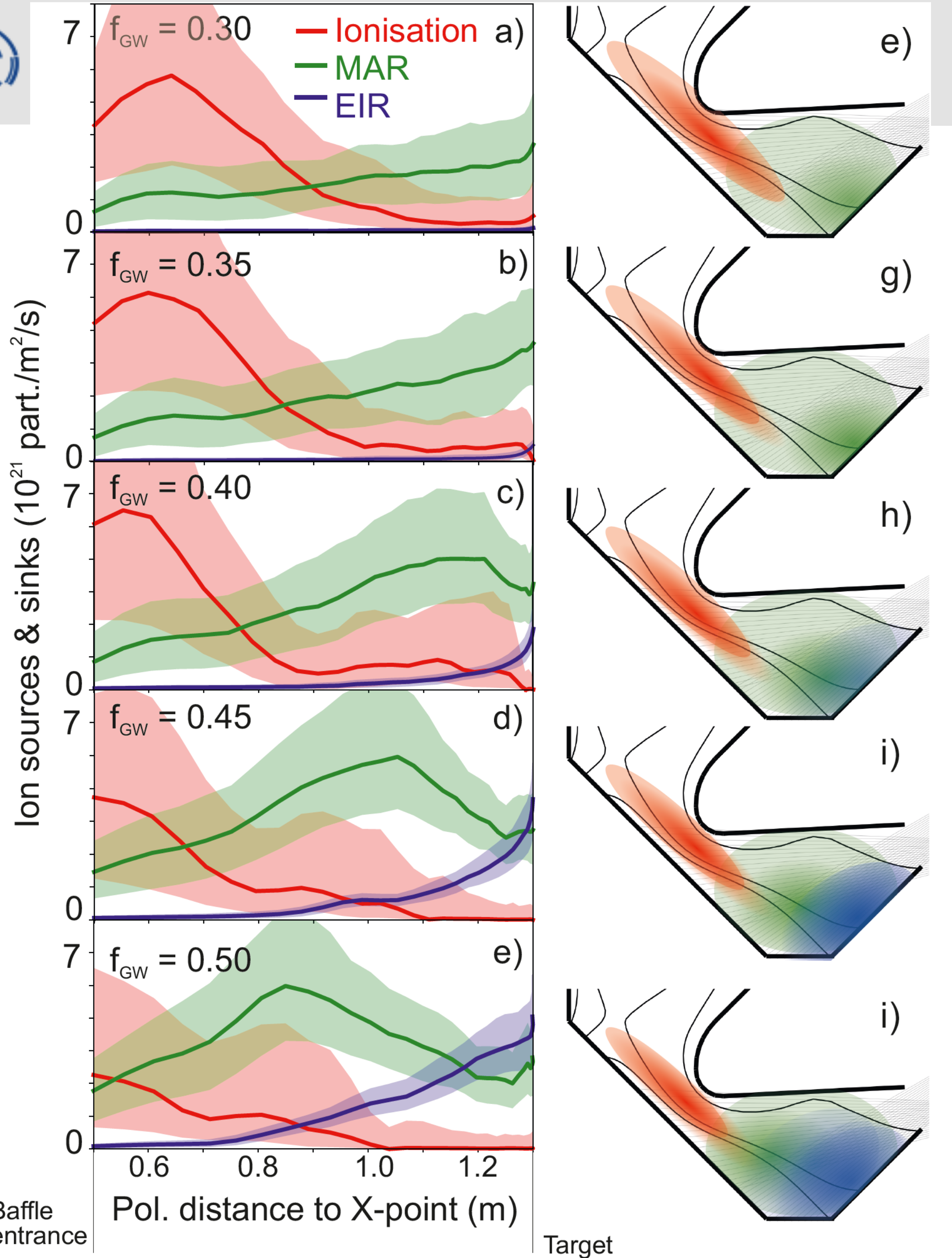
-> Can lead to significant divertor power dissipation (10-20% of power into divertor)

Ionisation

Electron-Ion Recombination (EIR)

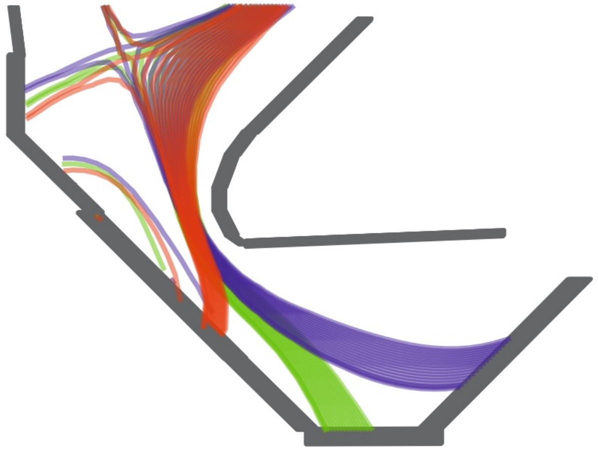
Molecular Activated Recombination (MAR)

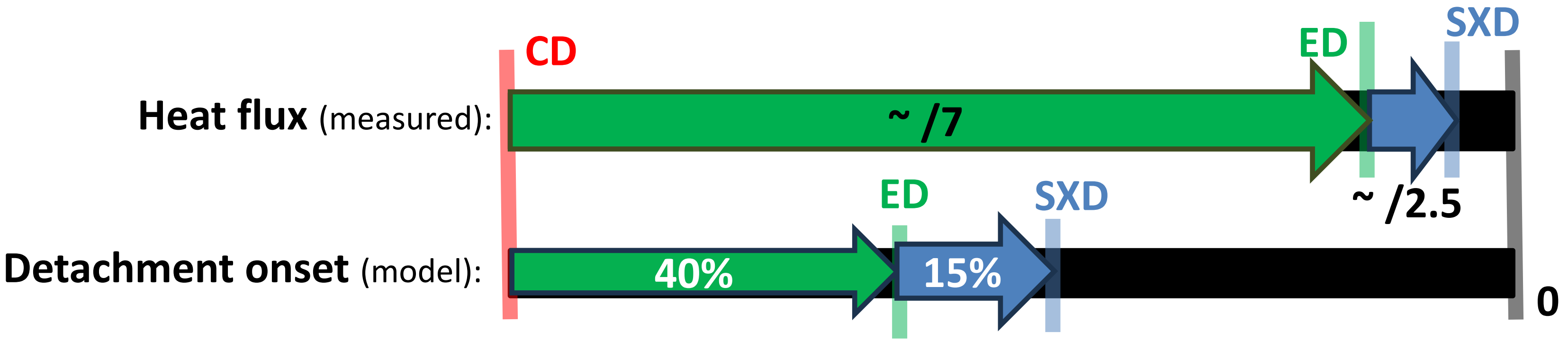
67% increase in density



The importance of MAR in baffled, long-legged divertors

Exhaust performance Super-X divertor (SXD) over Conventional Divertor (CD) retained in Elongated Divertor (ED)

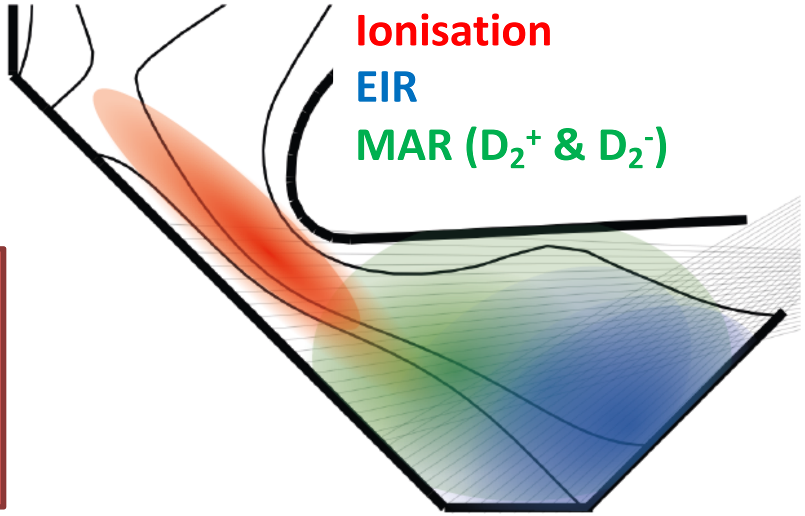




Modest shaping improves exhaust – consistent with predictions (model & simulations) without adverse core impact

What drives the physics of strongly baffled long-legged divertors?

- **More volume** available below front **ED** & **SXD** for **detachment processes**
  - ➢ **Plasma-molecular chemistry (MAR, …) -> particle & power sinks**

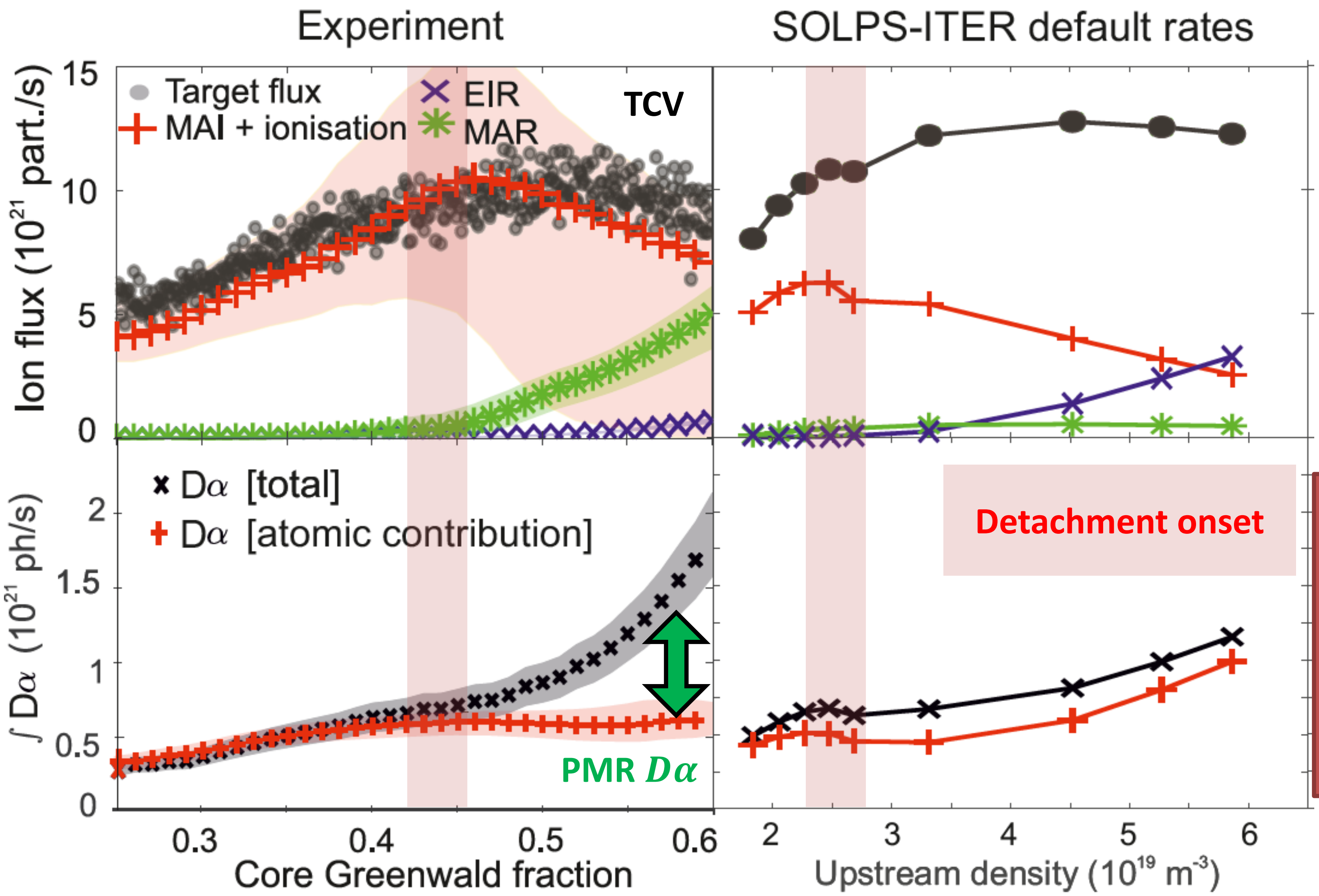


Plasma-molecule interactions crucial detachment driver in MAST-U.
Underestimated in modelling -> improved rates required
They can be relevant for reactors with tightly baffled alternative divertors

Example – no MAR in interpretive simulations (TCV)

TCV tokamak - #56567 – L-mode, Ohmic, 340 kA, single null conventional non-baffled, 2016-2018

SOLPS-ITER: [A. Fil, et al. 2018, CPP]



Experiment & simulation disagree on plasma-mol. interactions:

1. **No MAR simulation**
2. **Negligible PMR $D\alpha$ simulation**
3. **No ion flux roll-over simulation**

Why does MAR not appear in simulations, in contrast to experiments ?

Inaccuracies implementation molecules in plasma exhaust codes (!)

[K. Verhaegh, et al. 2021, NF]

MAR: $D_2 + D^+ \rightarrow D_2^+ + D$; $D_2^+ + e^- \rightarrow D^* + D$

Molecular rate modifications & exhaust modelling

Eirene $D^+ + D_2 \rightarrow D_2^+ + D$ rate (see details [K. Verhaegh, 2023, NF, 076015])

- Incorrect rescaling vibrationally resolved rates -> **underestimated @ T < 1.5 eV**
- Account for lower velocity ion of heavier isotopes -> **exacerbates underestimation for D, T**

Eirene, H

Eirene (D -> T/2)

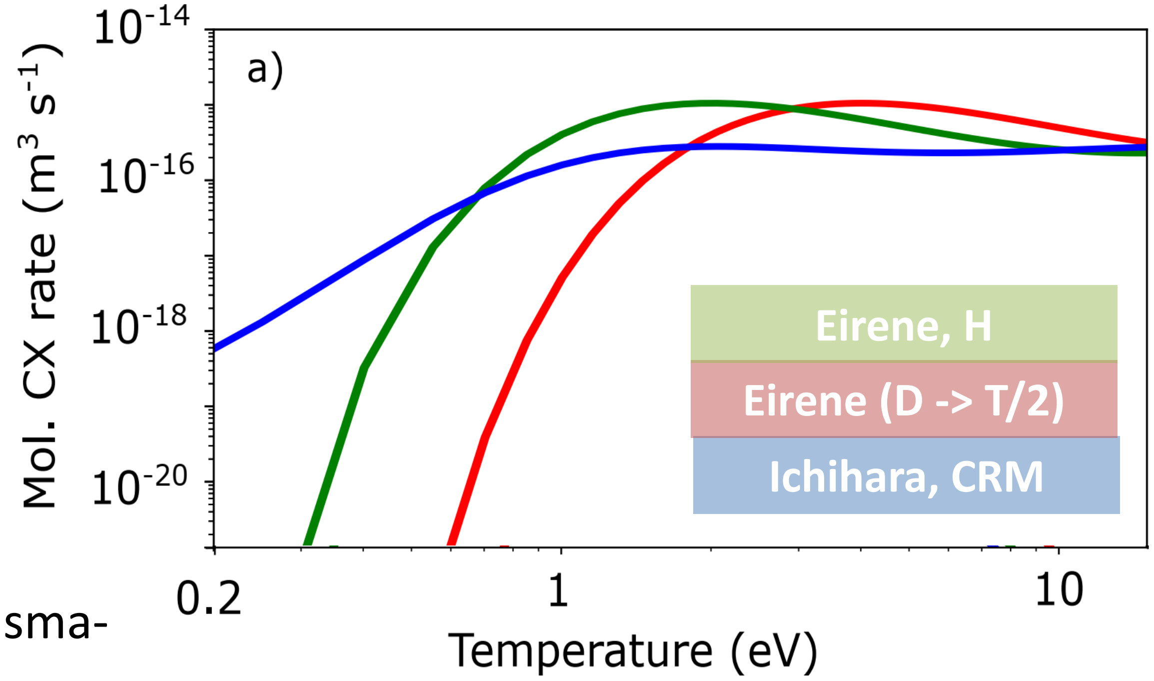
Collisional-radiative modelling

- $D_2(v)$ model with **vibr. Resolved** ab initio **mol. CX rates** [A. Ichihara, 2000, JPhysB]
- Keep all other interactions the same as Eirene

Ichihara, CRM

Courtesy of S. Kobussen, MSc. Internship project, 2023, arxiv:2311.16732

'Tip of the iceberg': many inaccuracies plasma-molecular interactions in Eirene



Underestimation of molecular CX expected at Te < 2 eV -> MAR underestimated in detachment

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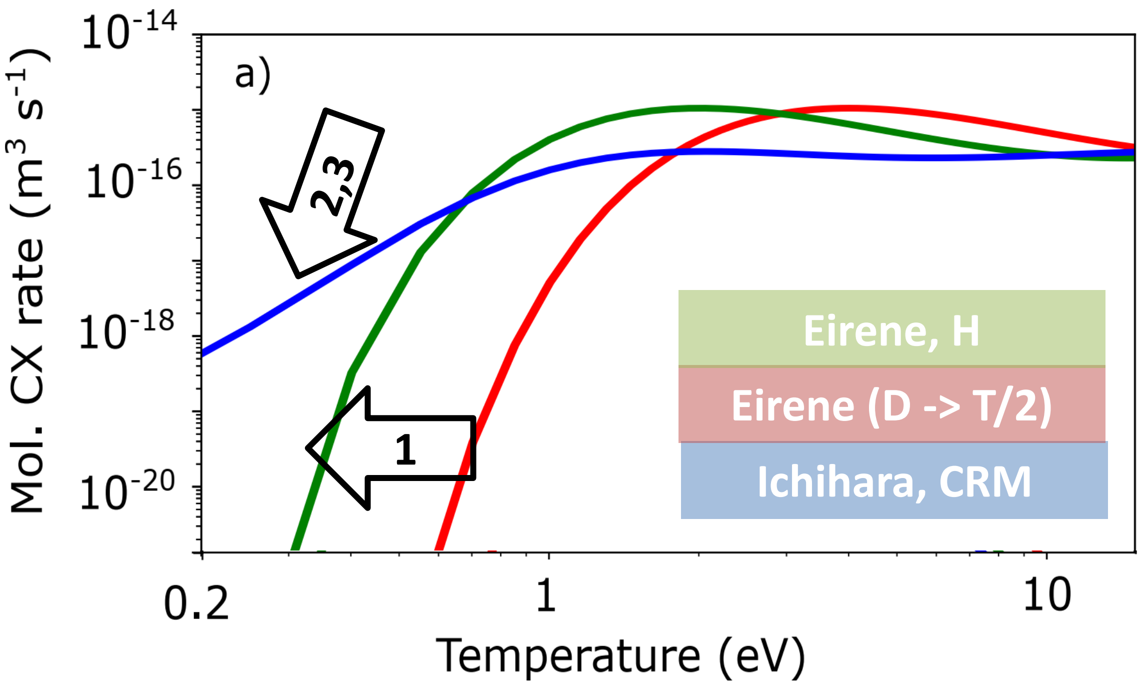
1. **Sensitivity study TCV tokamak: disable mass rescaling** [K. Verhaegh, 2023, NF, 076015] — Eirene, H
   Improved agreement with experiment !
2. **Post-process** converged **reactor-scale simulations with** Ichihara, CRM
3. **Self-consistent simulations with** Ichihara, CRM
   (see later)



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Role plasma-mol. interactions in reactors

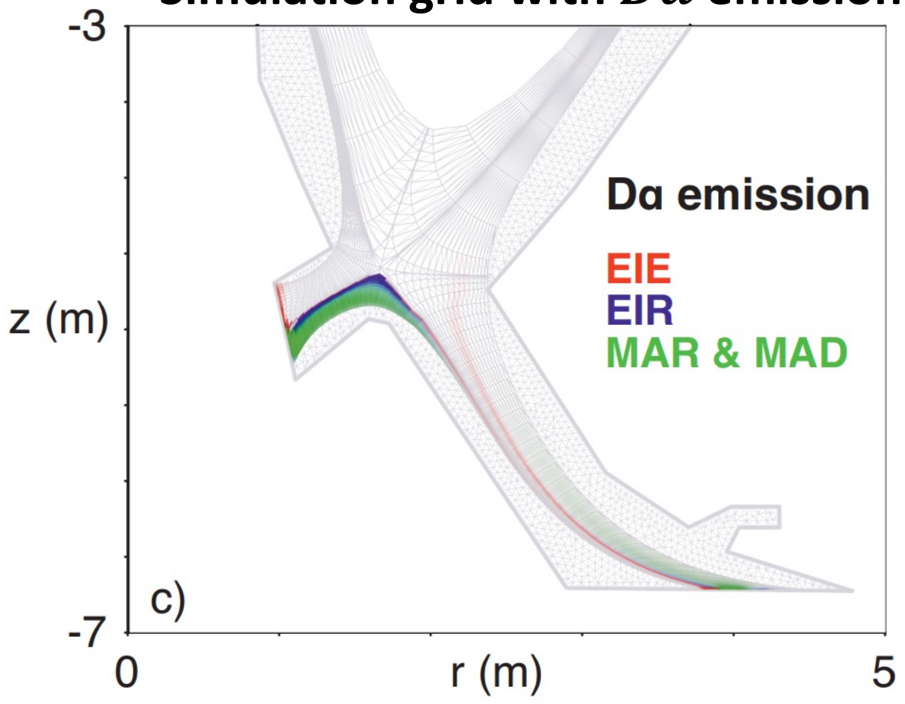
Post-processing cannot account for changes in the plasma solution

Reactor-relevant simulations for STEP (see [R. Osawa, 2023, NF; A. Hudoba, 2023, NME])

- **Tightly baffled** double null **Alternative Divertor** (Elongated / X-Divertor - outer / inner target)
- **P_{SOL} ~ 80 MW**, D fuelled, Ar seeding

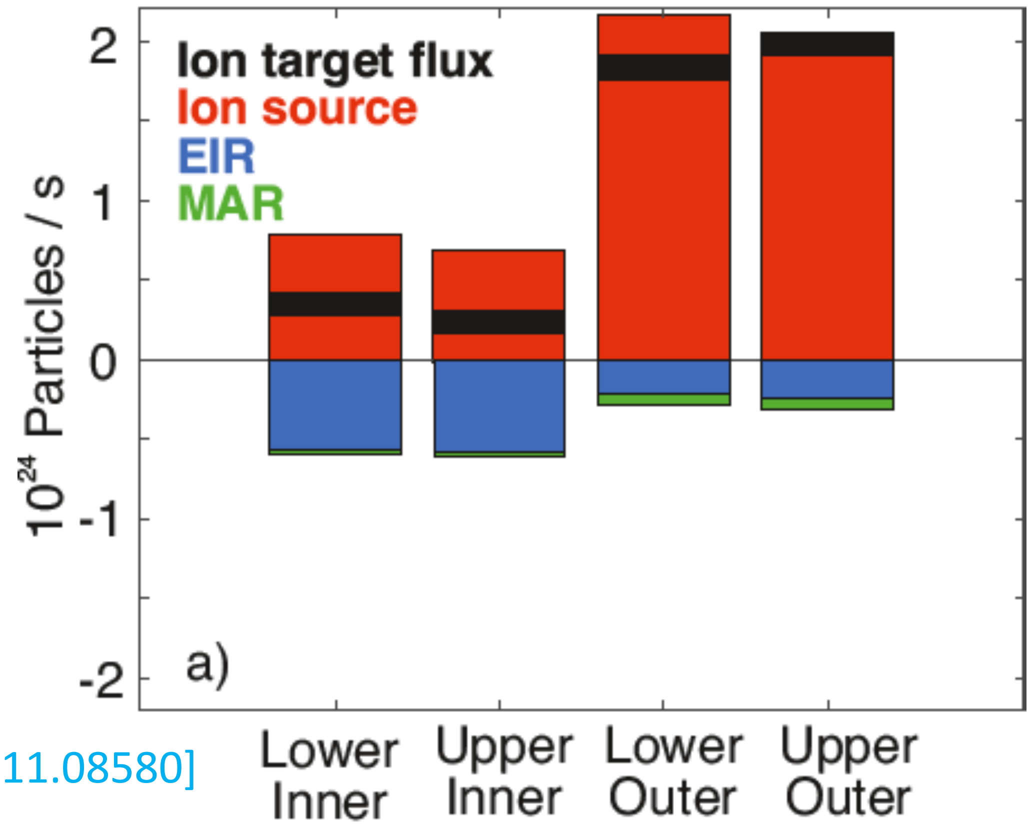
Post-process: SOLPS-ITER simulation result → **Ichihara, CRM** → D_2^+ changes → $D\alpha$, MAR, MAD changes … (assuming n_e, T_e, … remains constant)

Simulation grid with $D\alpha$ emission (post-processed)



Simulation near detachment onset (ionisation near target)

Particle balance *before* post-processing



[K. Verhaegh, 2023, ArXiV:2311.08580]

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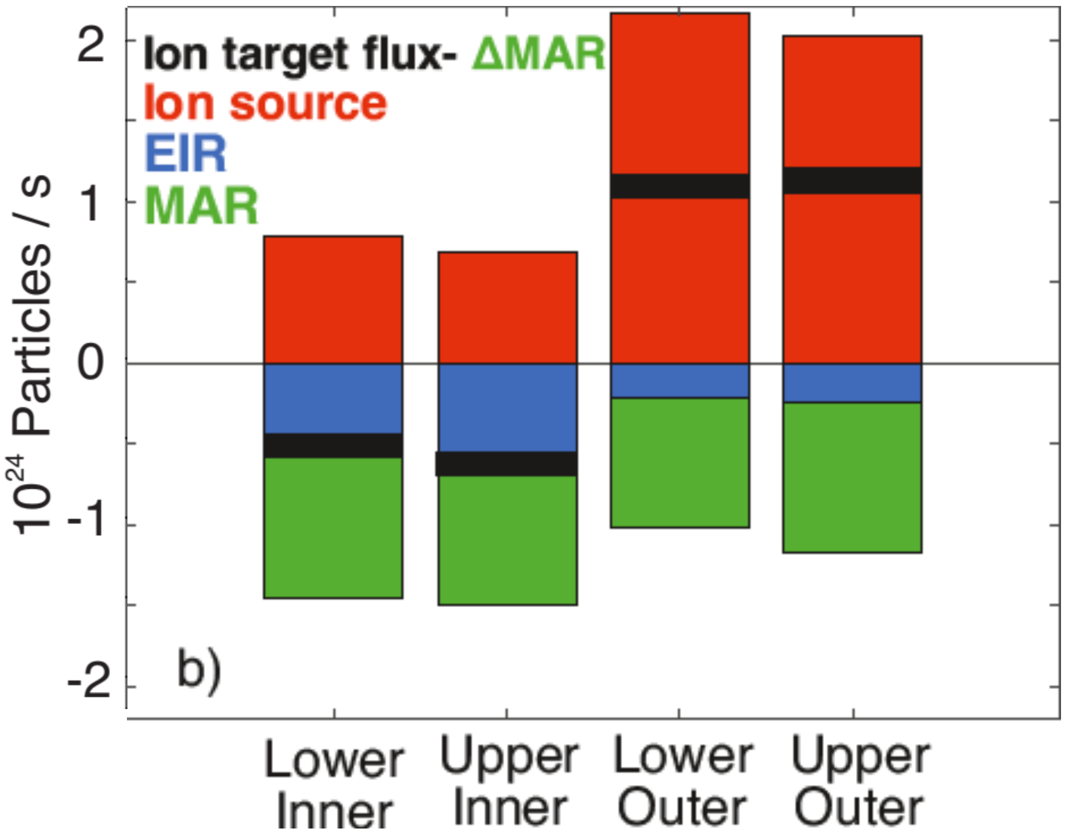
- **MAR > EIR ion sinks** (despite $n_e \sim 10^{21}$ m^{-3})
- **MAR > inner target ion flux**
- **MAD -> power losses** (> 10% of P_{SOL}) & **dissociation** (x2-x8)

Plasma-chemistry can play a role at the reactor scale !

New simulations with improved rates required to investigate **full impact**

Particle balance *after* post-processing



Role molecular chemistry during divertor detachment ?

1. **Can lead to significant atomic hydrogen emission from excited atoms after plasma-molecule interactions**
   - Can fully dominate Da emission -> additional visible emission & complicates photon opacity diagnosis
   - Complicates hydrogen emission interpretation & detachment control strategies
   - **Inaccuracies in simulations ->** wrong estimates for diagnostic design & control

2. **Dominant effective dissociation mechanism in detached conditions**
   - Dissociation from MAD >>> electron-impact dissociation (detachment increases D_2 density)
   - Dissociation can lead to significant power losses
   - **Inaccuracies in simulations** -> inaccuracies in molecule to atom ratio, underestimated power loss

3. **Can be a dominant ion sink mechanism**
   - Occurs at higher Te than EIR (<2.5 eV)
   - Can be crucial for reducing the ion target flux
   - **Inaccuracies in simulations** -> lack of 'roll-over' (cannot simulate detachment) overestimated particle flux

Summary: plasma-molecular chemistry can play an important role in the divertor during detachment:

1. **D* emission**
2. **Drives dissociation (MAD)**
3. **Ion sinks (MAR)**

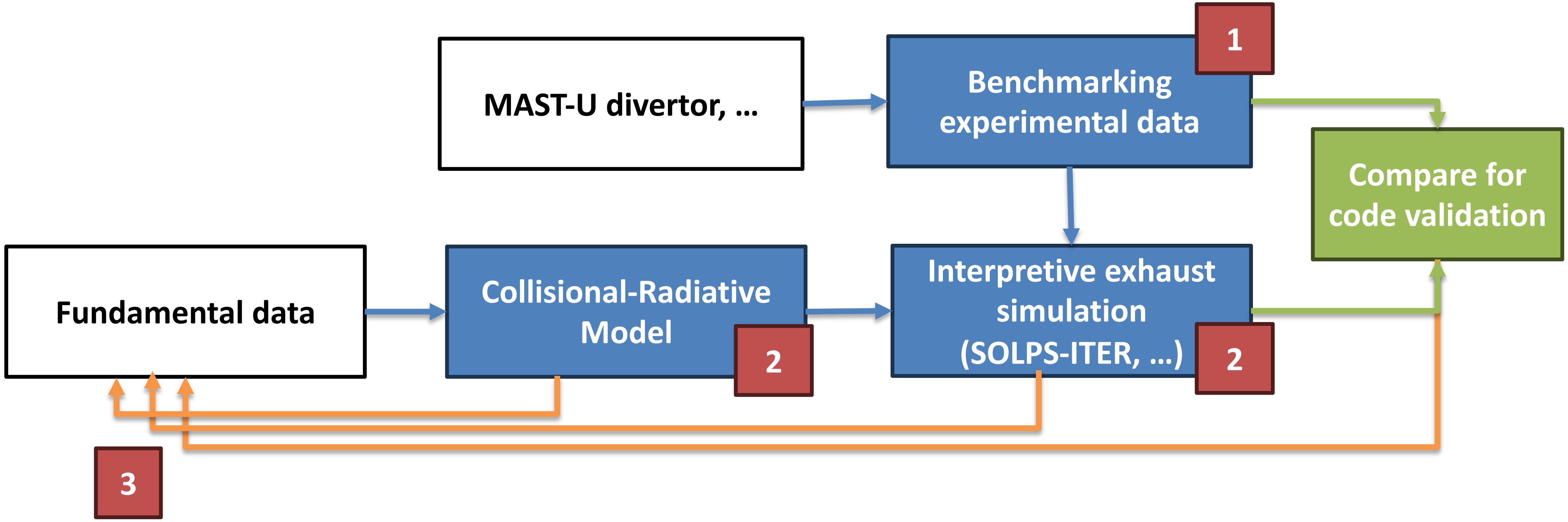
Can also be important for reactors (!)

CRP - objectives

1 Compilation of experimental data for plasma-molecular interactions in tokamak divertors

2 Evaluation of Effective Molecular Rates through Collisional-Radiative Modelling and their impact on the divertor state through Plasma-Edge Modelling

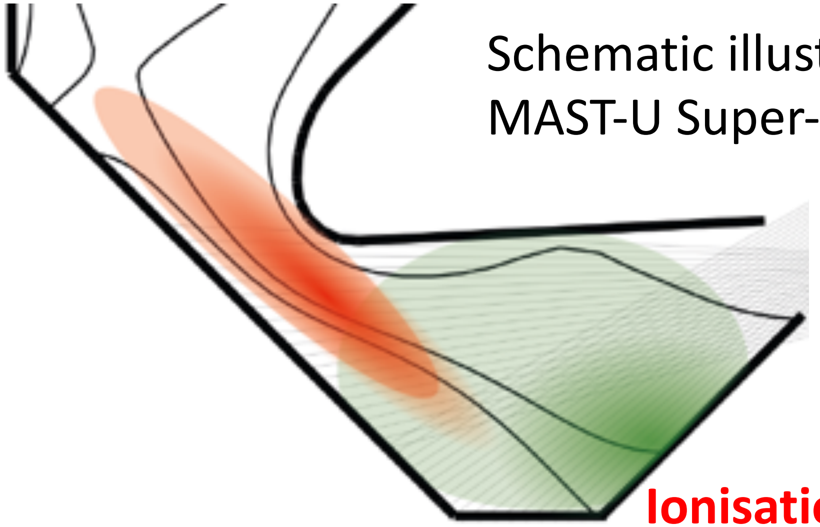
3 Assessment of Molecular Hydrogen Data for Interpreting Tokamak Divertor Experiments and Simulations



1. Experimental data for benchmarking

MAST-Upgrade Super-X divertor

- **Strongly baffled, long divertor leg** -> **deep detached operation** -> **<u>plasma-molecular interaction intensified</u>**
- Published data with advanced diagnostics & diagnostic repeats:
  - Divertor spectroscopy -> D_2 Fulcher and **Balmer line analysis**
  - Imaging diagnostics -> 2D emission distribution (D2 Fulcher + Balmer)
  - Coherence imaging spectroscopy -> 2D ne, Tn, … profile
  - Integrated Data Analysis (in progress) -> 2D ne, Te, …. Profile



Schematic illustration example MAST-U Super-X divertor

Ionisation

Plasma-molecular interactions

MAST-U divertor, … → Benchmarking experimental data [1]

[Verhaegh, et al. 2023, Nucl. Fusion, 63 016014]
[Verhaegh, et al. 2023, Nucl. Fusion, 63 126023]
[Wijkamp, et al. 2023, Nucl. Fusion]
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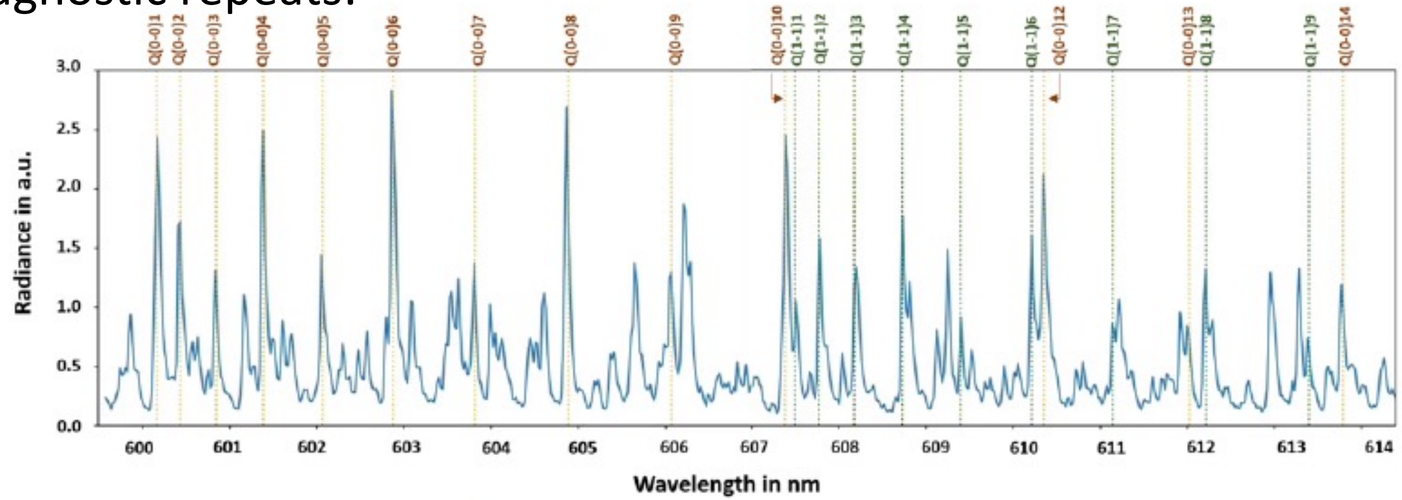
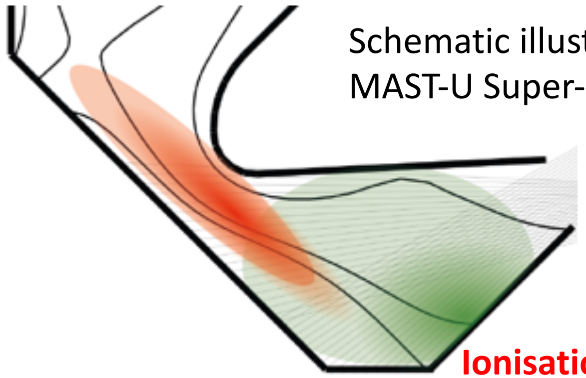


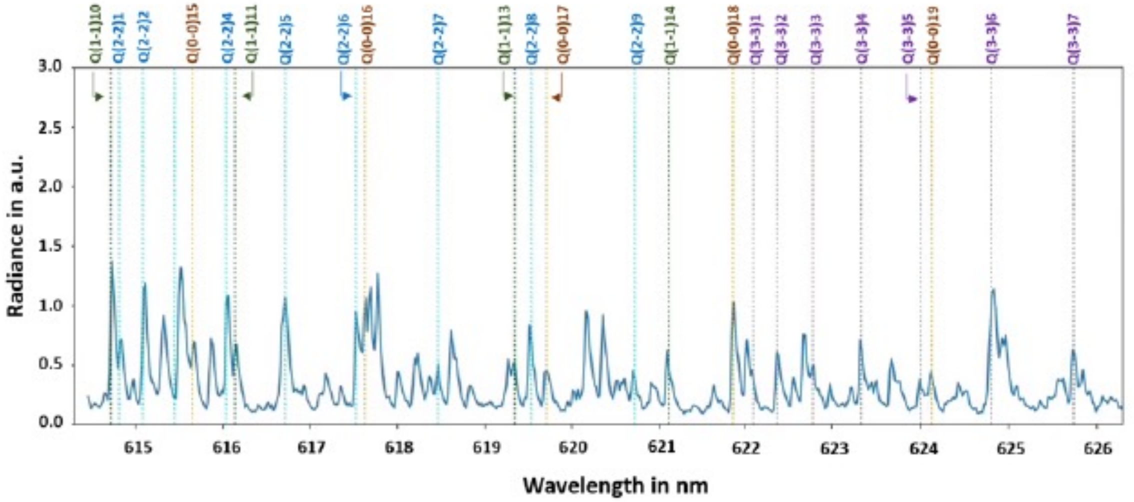


Schematic illustration example MAST-U Super-X divertor

Ionisation

Plasma-molecular interactions

[Osborne, et al. 2023, arxiv]



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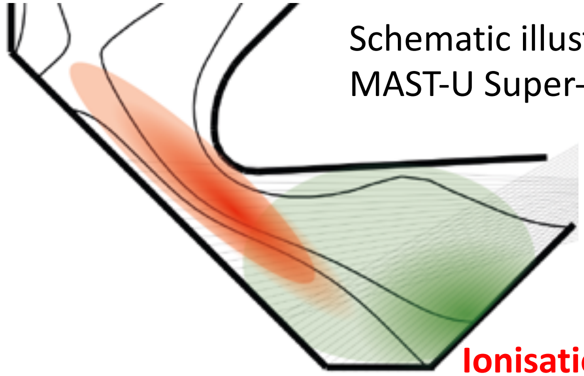

Schematic illustration example MAST-U Super-X divertor

Ionisation
Plasma-molecular interactions

Example – density ramp discharge

- **D2 Fulcher (600-605 nm) recedes further during deeper detachment**
- Balmer emission beneath D2 Fulcher -> **MAR & MAD**

Multi-wavelength imaging diagnostic [T. Wijkamp, et al. 2023, Nucl. Fusion]

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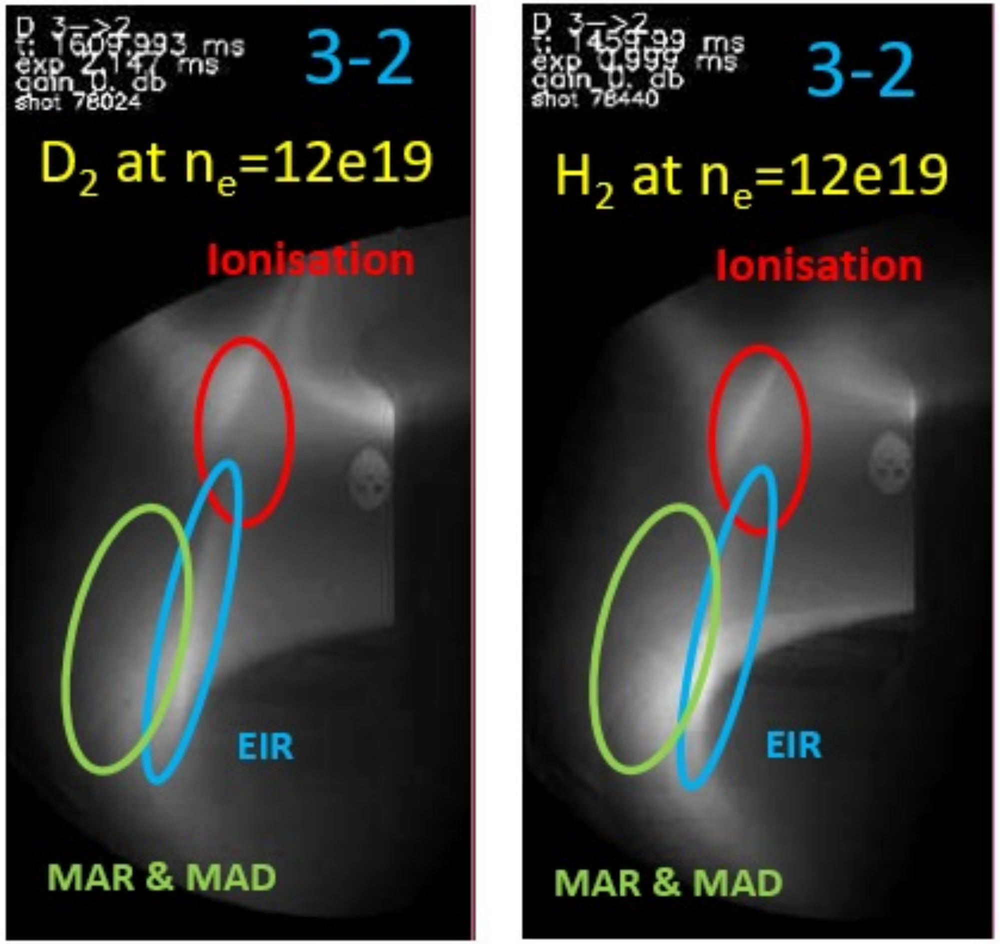
TCV Da emission: **impact isotope MAR & MAD**

Preliminary conclusion: MAR & MAD similar between H & D



Other devices (potentially (?) - to be determined/published)

- EuroFusion WPTE experiments plasma-neutral interactions
- **TCV** experiments - flexible divertor & baffles, advanced imaging **hydrogen & deuterium**

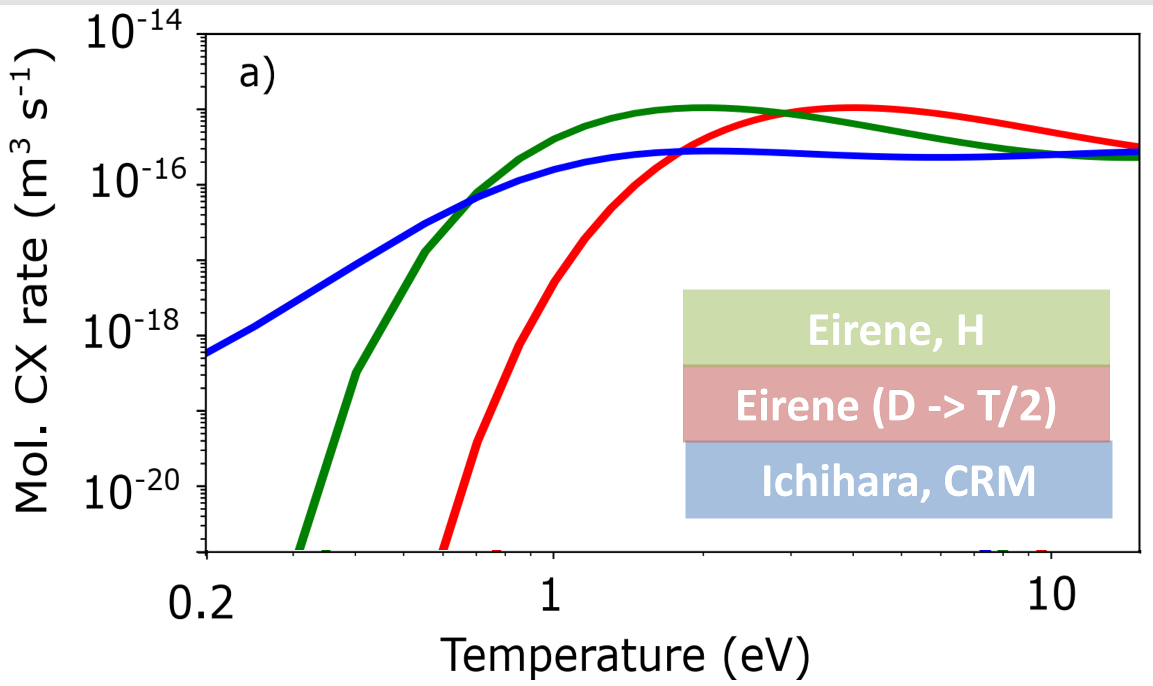
2. Evaluation of effective rates & plasma-edge modelling

Explorative studies using CRMs

- Initial scoping study: large discrepancies $D_2 + D^+ \rightarrow D_2^+ + D$ -> large uncertainties MAR & MAD

Interpretive exhaust simulations (D. Moulton)

- Investigate impact rates on exhaust simulation



UKAEA New Exhaust Code (NEC) in development (long term):

- Requires Collisional-Radiative Modelling capabilities -> effort on CRM development
- Can contribute to exhaust code validation studies

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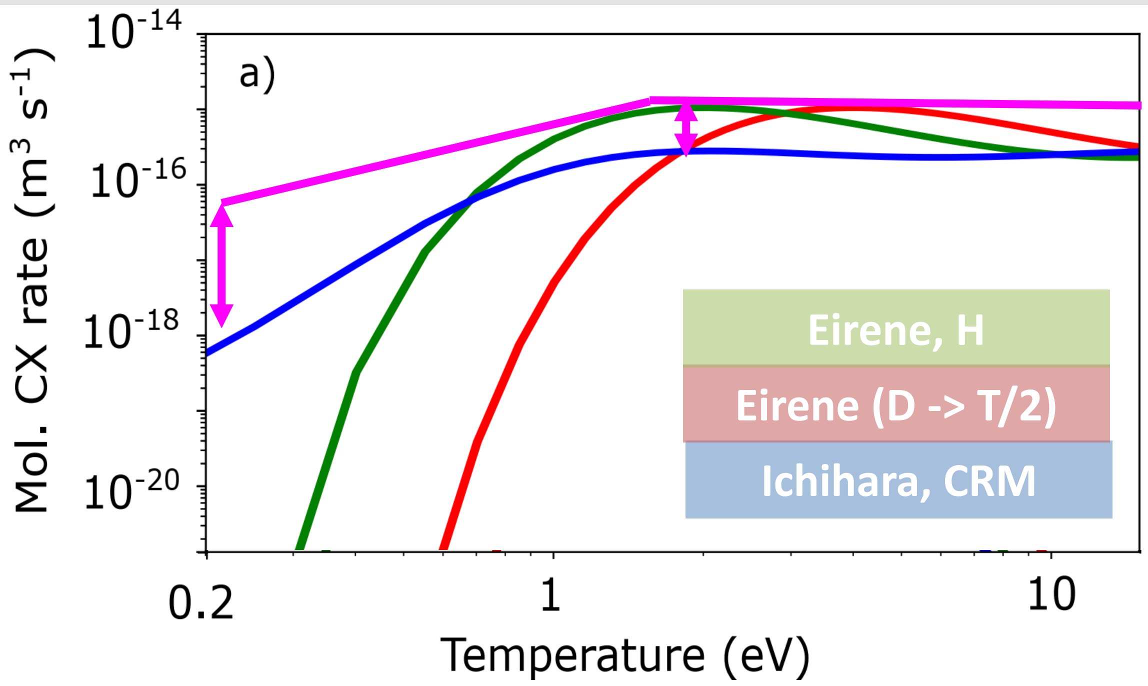

Significant uncertainties Mol. CX:

- **Uncertainties cross-sections $D_2(v) + D^+ \rightarrow D_2^+ + D$**
  Requires **fundamental data calculations**
- **Uncertainties vibrational distribution D2**
  Requires CRM studies

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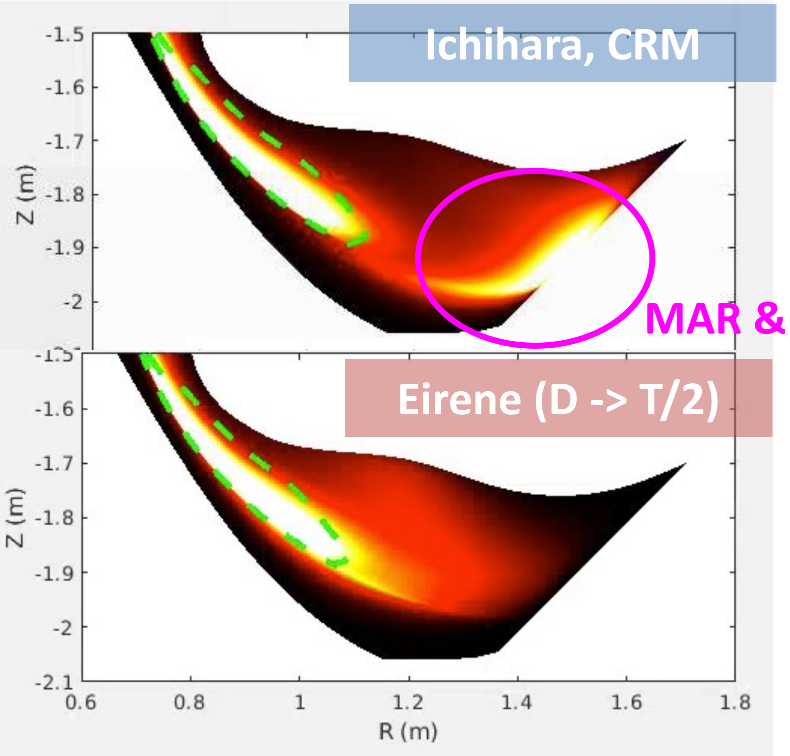
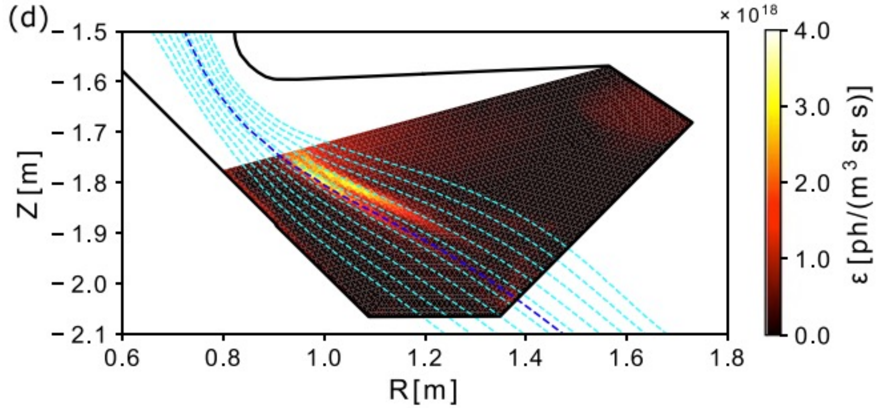
D2 Fulcher contour



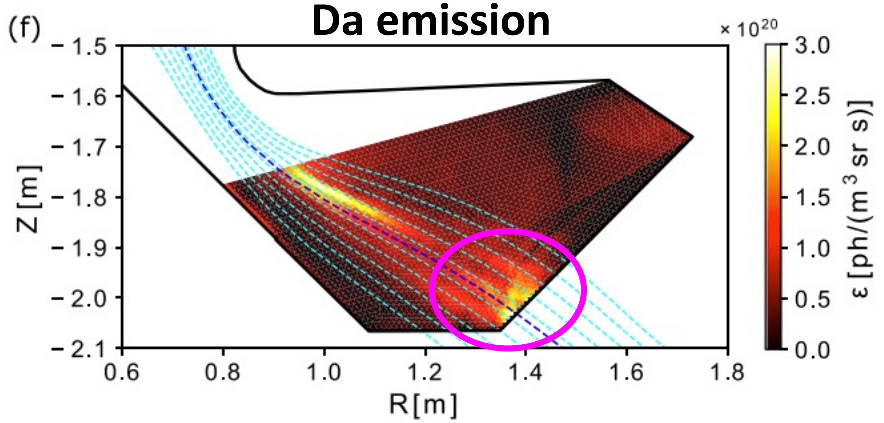
Preliminary: Da emission below D_2 Fulcher emission with new rate

Qualitative agreement with experiment!

D2 Fulcher emission



Da emission



Experiment: Da emission below D2 Fulcher emission region -> MAR & MAD **[Wijkamp, et al. 2023, Nucl. Fusion]**

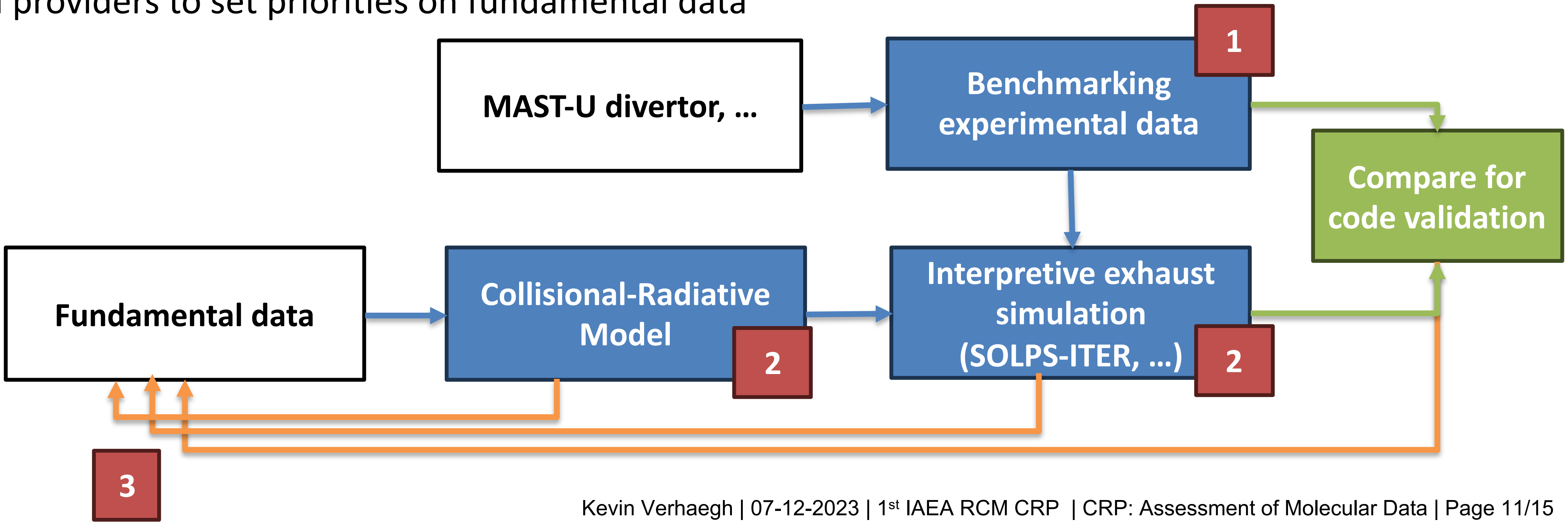
3. Assessment of Molecular Hydrogen Data

Recommendations on fundamental data needs

- CRM scoping studies & interpretive modelling -> sensitivity to fundamental data 2
- Compare interpretive simulations against experiments 1 for benchmarking codes -> **inform requirements fundamental data** 3

Inaccuracies rates -> real impact reactor design

- Practical approach: short-term & longer-term recommendations
- Work with data providers to set priorities on fundamental data



Workplan

Year 1

- Start compilation **cases for benchmarking** (from published works)
- **Assess rates** used **current exhaust codes** (SOLPS-ITER)
- List of processes & data sources & circulate

➢ Provide short and long-term recommendations for improved data sources

➢ Compute **effective rates** using improved data sources

Year 2

- **Continue evaluation effective rates** using improved data sources provided by CRP partners
- **Implement improved rates** in exhaust codes (SOLPS-ITER)
- Start **code validation efforts** of the CRMs

Year 3

- First attempt **sensitivity studies** & **uncertainty quantification** effective rates

➢ If possible, propagate **sensitivity study** to impact SOLPS-ITER

- **Code validation** efforts of **exhaust simulation codes** using compiled benchmark cases

CRP – expected outputs

1. **Test cases** (deeply detached divertors) for **benchmarking interpretive codes**

2. Contribute to **curated list** of r**elevant reactions & processes** in deeply detached divertors
   -> **recommendations for data improvements** (short term & longer term)

3. **Compile improved effective rates** with provenance from fundamental data to CRM using list (2)

4. Contribute to **code comparison studies** using **benchmark cases** (1) with improved effective rates (3)

Discussion points

1. **Revision molecular rate setup required for exhaust simulations**
    - Self-consistent vibrationally & electronically resolved setups
    - Coupling of vibrational & electronic states
    - Analytic scalings introduce large uncertainties -> use ab initio cross-sections instead
    - Improved provenance – initialise effective rates at the start of a simulation through CRM
    - Isotope resolved rates – where possible

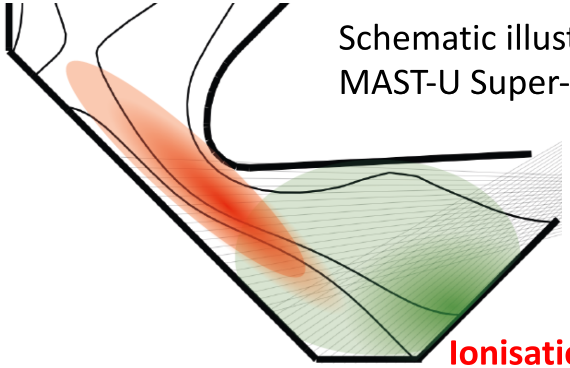
2. **Are additional processes & species required ?**
    - D_2^+ recombination ? [Wunderlich, et al.]
    - Should D^- be considered ?
    - Other interactions important (neutral collisions with D_2 (v), …. ?)

3. **Is a 0D CR approach with effective rates (ne, Te) appropriate for exhaust simulations ?**
    - Transport of D2 (v) & plasma-surface interactions -> deviates from 0D transport-less model

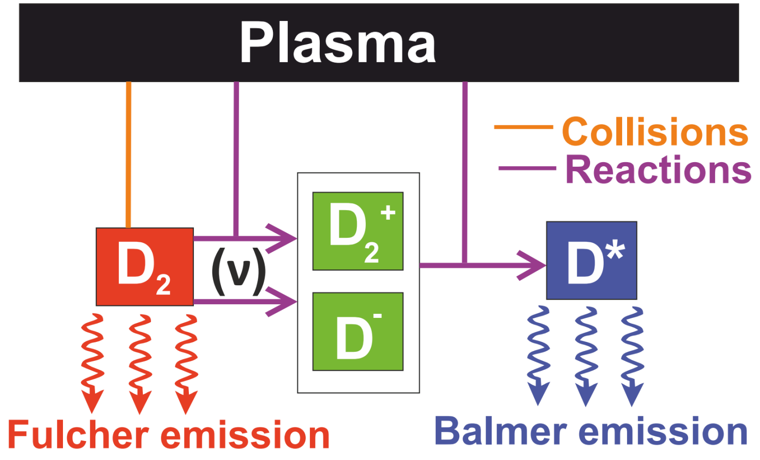
Conclusion

Plasma-molecular interactions can be important during detachment, even on the reactor scale, and are not well reproduced by exhaust codes

1. **Boosts D* emission ->** complications **diagnostic interpretation** & **control sensing capabilities**
2. **Drives dissociation (MAD) ->** increases **volumetric atom generation** & associated **power loss (20% of P_{SOL})**
3. **Ion sinks (MAR) -> induces particle flux reduction** at higher Te than EIR



Particularly relevant for strongly baffled & long-legged divertors - > can extend to reactor scale



Plasma-molecular chemistry, not well reproduced in simulations -> improved rates required, particularly molecular charge exchange

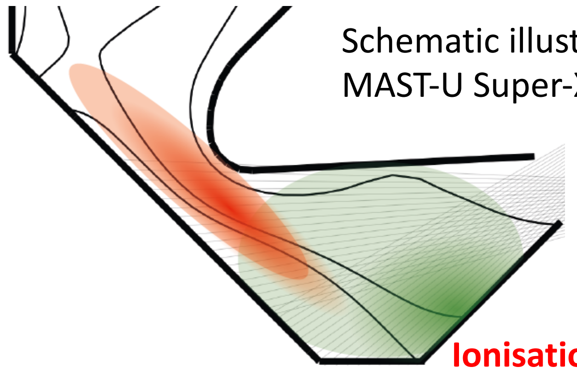
Impact of different rates can be far-reaching:

1. **Power exhaust physics:** D/D_2 balance; changes detachment window; fuelling efficiency; …..
2. **Diagnostic analysis & design –** including **detachment control sensor** strategies

We are looking forward to solving these challenges with you in this CRP !

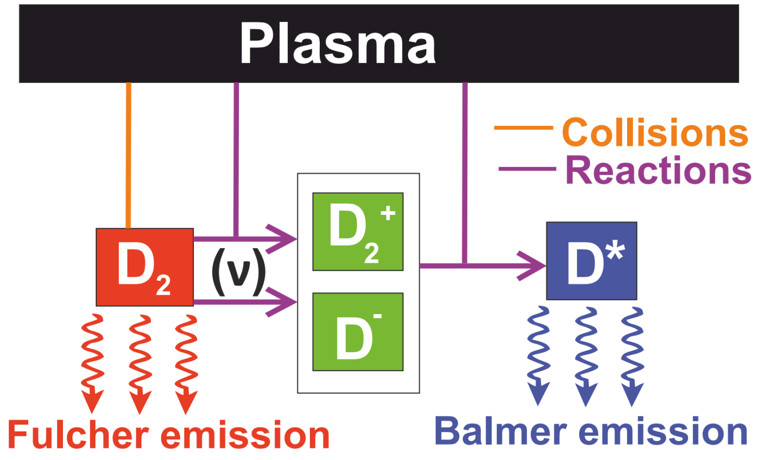
Plasma-molecular interactions can be important during detachment, even on the reactor scale, and are not well reproduced by exhaust codes

1. **Boosts D* emission ->** complications **diagnostic interpretation** & **control sensing capabilities**
2. **Drives dissociation (MAD) ->** increases **volumetric atom generation** & associated **power loss (20% of P_{SOL})**
3. **Ion sinks (MAR) -> induces particle flux reduction** at higher Te than EIR



Schematic illustration example
MAST-U Super-X divertor

Particularly relevant for strongly baffled & long-legged divertors - > can extend to reactor scale



Plasma-molecular chemistry, not well reproduced in simulations -> improved rates required, particularly <u>molecular charge exchange</u>

Impact of different rates can be far-reaching:

1. **Power exhaust physics:** D/D_2 balance; changes detachment window; fuelling efficiency; …..
2. **Diagnostic analysis & design –** including **detachment control sensor** strategies