The importance of plasma-chemistry in detached plasmas and the need for updated rates through CRM

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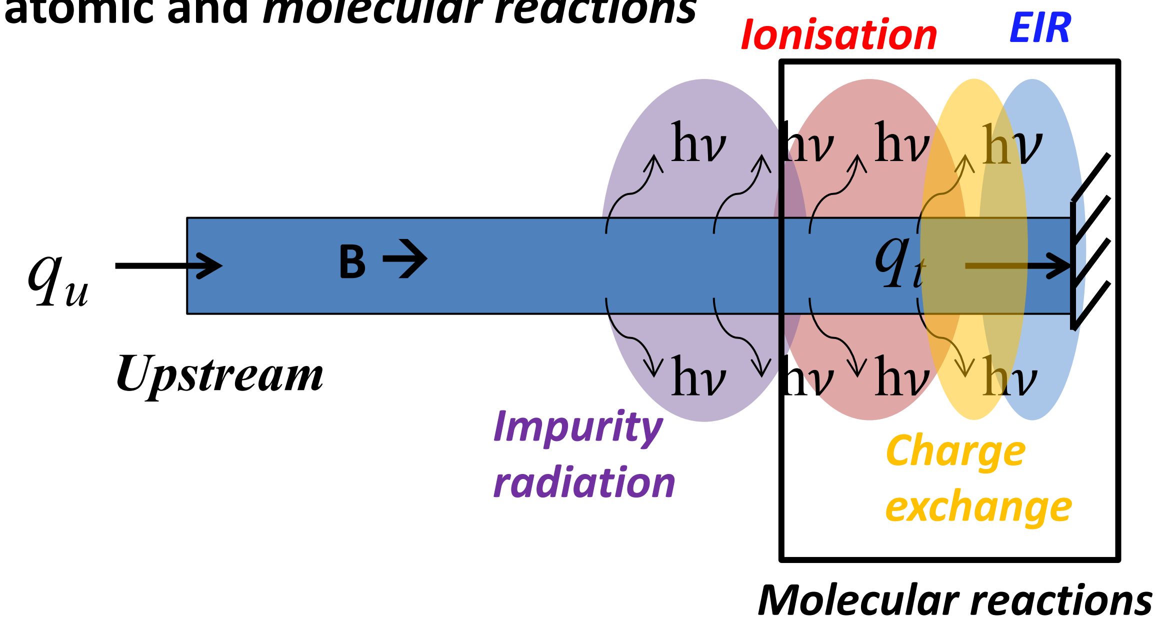
Detachment physics & plasma-molecular interactions

Detachment requires:

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

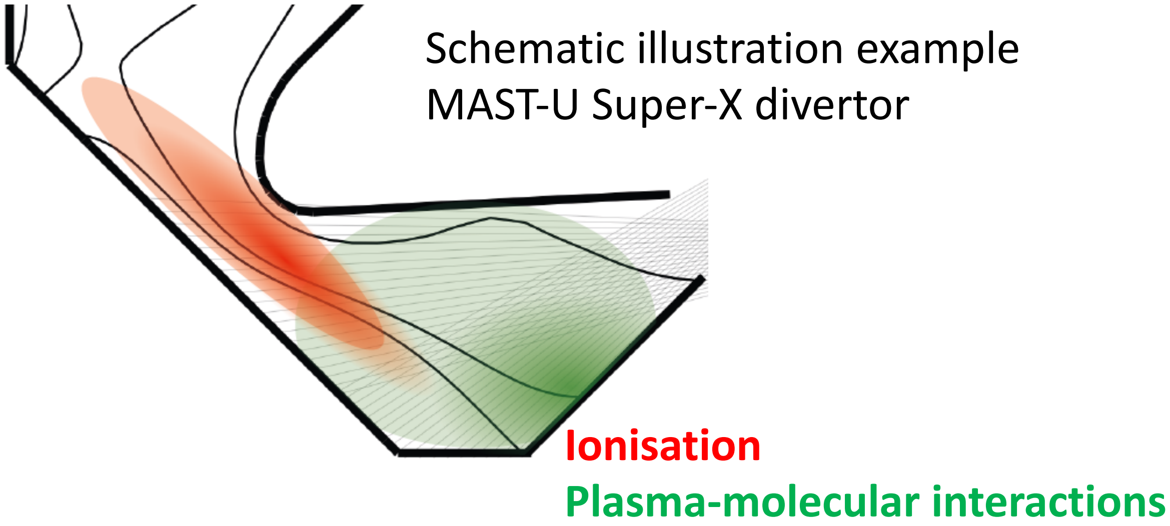
Detachment (< ~ 5 eV) induced by chain of **atomic and *molecular reactions***



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

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



Schematic illustration example MAST-U Super-X divertor

Detachment physics & plasma-molecular interactions

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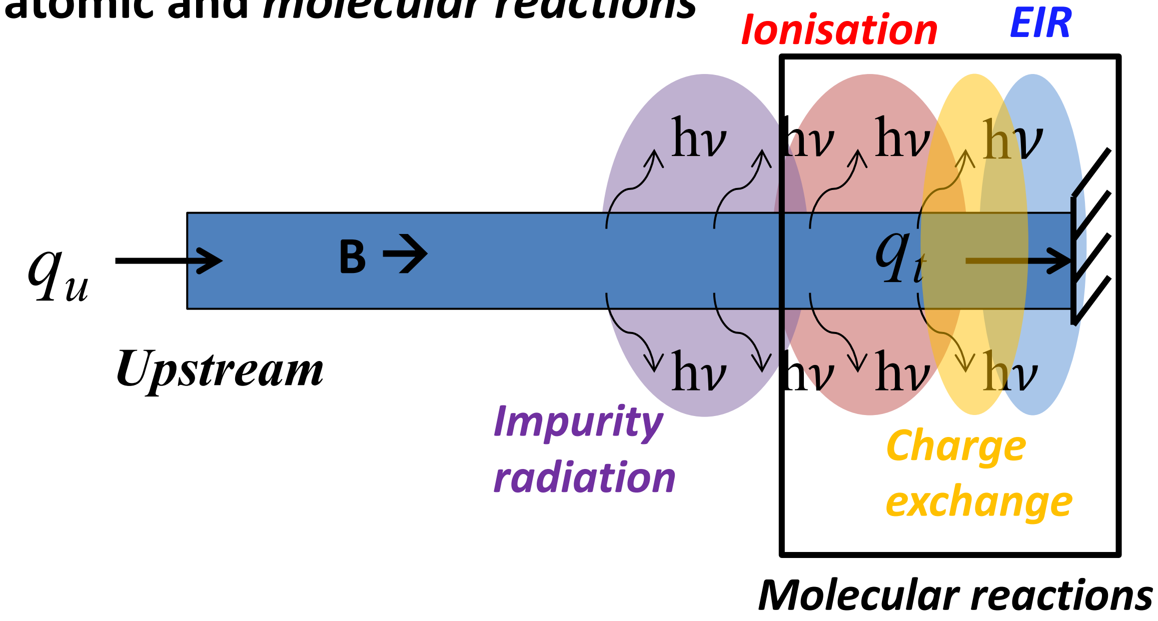
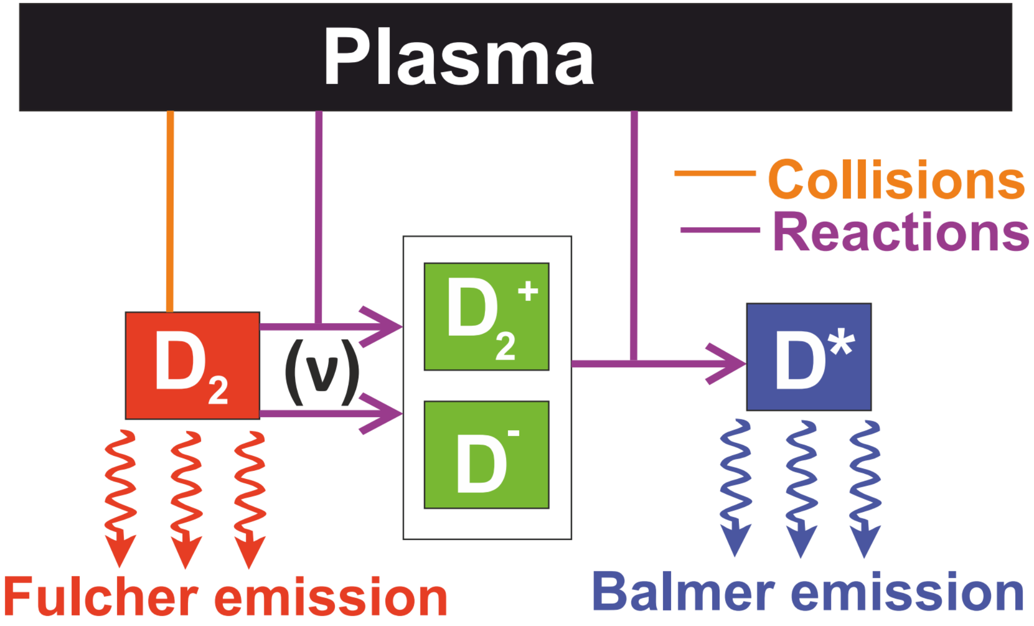


Plasma-molecular interactions impact power, particle and momentum balance:

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



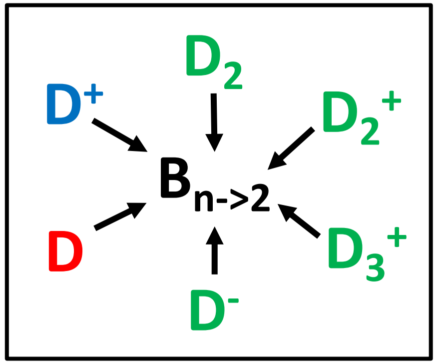
Detachment is driven by atomic/molecular reactions through dependencies between power, particle and momentum balances

Plasma-molecular chemistry with molecular ions

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

$D_2 + D^+$ -> D_2^+ + **D**;	$D_2^+ + e^-$ -> **D** + **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), requiring new ADAS EIR PECs [see presentation M. O'Mullane]
- **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!

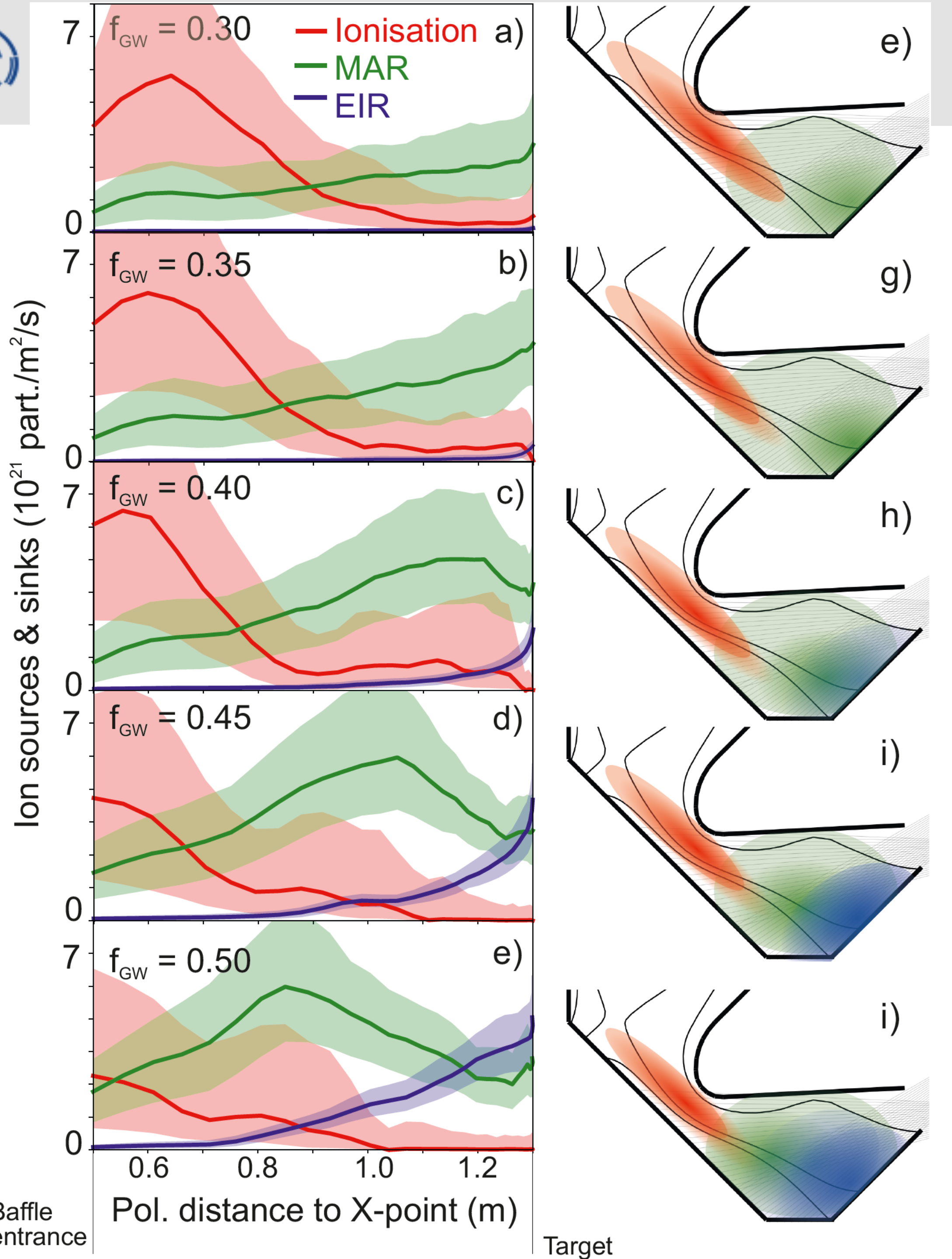
-> Can lead to significant divertor power dissipation (10-20% of power into divertor)

Ionisation

Electron-Ion Recombination (EIR)

Molecular Activated Recombination (MAR)

67% increase in density



Example – MAR/D on MAST-U

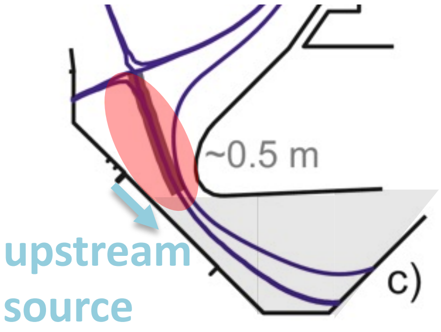
Integrate divertor ion sources & sinks for total divertor particle balance

[Verhaegh, 2023, ArXiV, 2311.08580]

- **Strong MAR ion sinks**, such that ion sources & sinks balance in divertor chamber throughout

- **EIR** at high n_{GW}, **but MAR remains dominant**

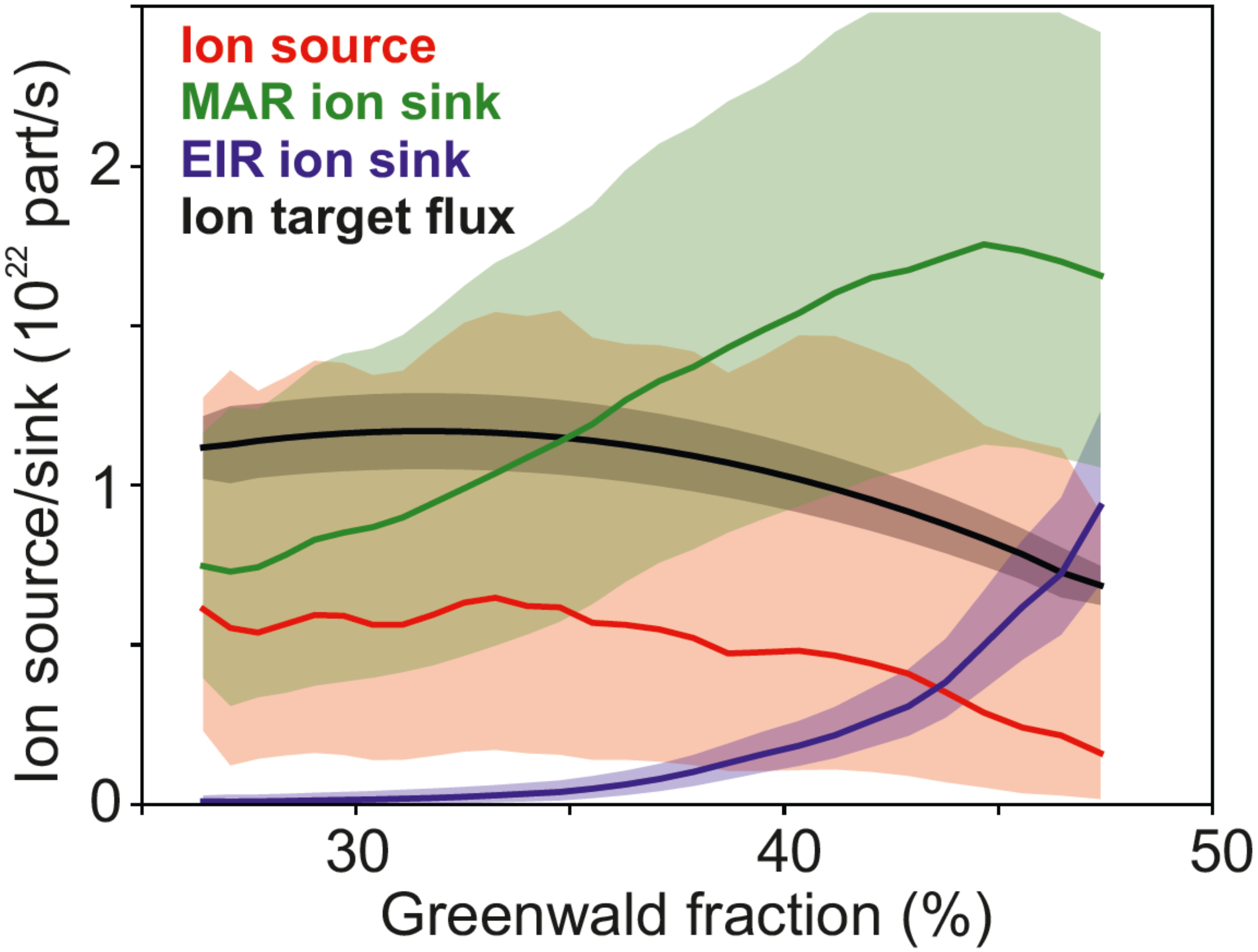
- **Dominance of MAR also observed in less strongly shaped divertor scenarios**



Particle balance

Target flux = tot. source – MAR – EIR

tot. source = div. + upstream source



MAR ion sinks dominant detachment mechanism in MAST Upgrade divertor

Intermezzo: D_2 Fulcher band spectroscopy

- **Balmer lines D* ->** information during **detached conditions**, however no ***direct information*** about D2

➢**D2 Fulcher emission** can provide direct information about D2, however little electronic excitation during detached conditions -> **strong MAR & MAD hard to diagnose with D2 Fulcher emission**

➢**<u>However, lack of D2 Fulcher emission can be used as a diagnostic</u>** <u>!</u>

Example – density ramp discharge

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

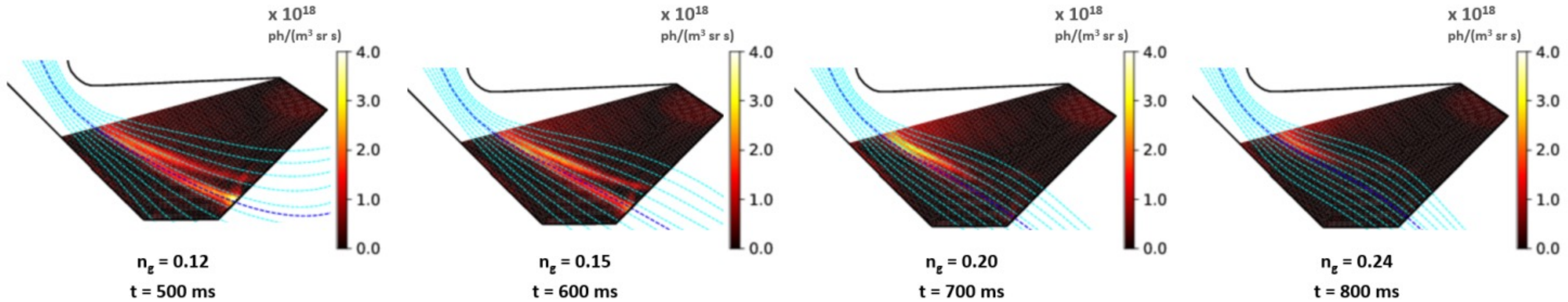
Multi-wavelength imaging diagnostic [T. Wijkamp, et al. 2023, Nucl. Fusion]

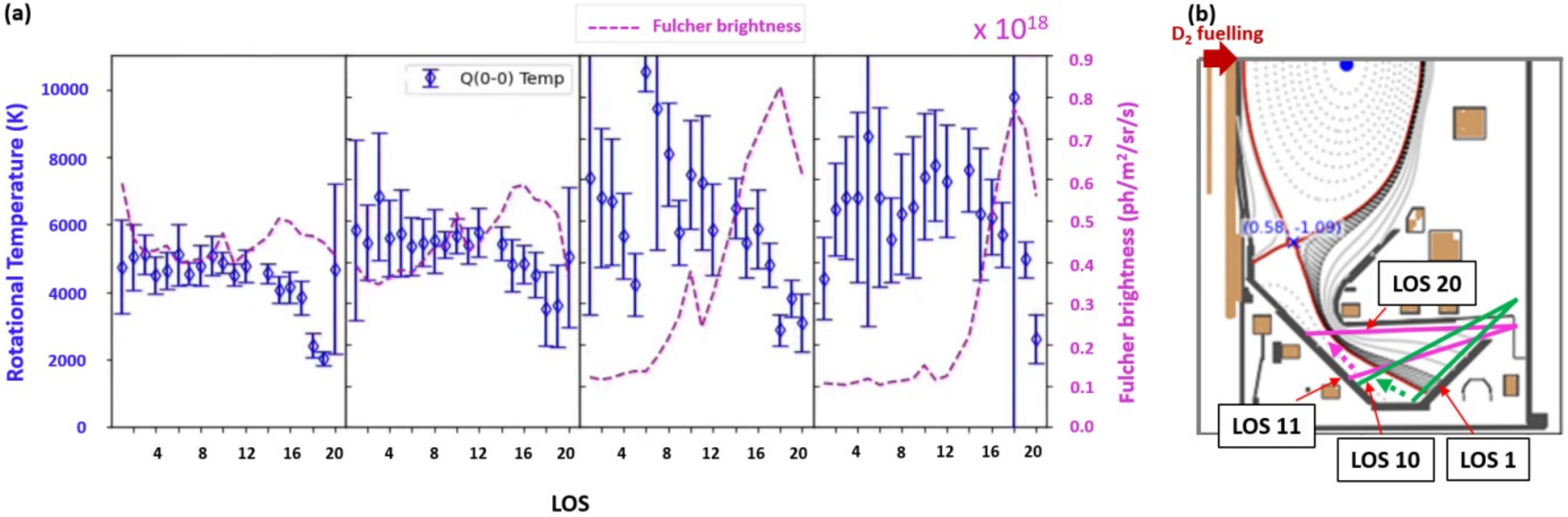
- **D_2 Fulcher emission intensity correlated with ionisation region** (energies required for electron-impact excitation of D and D_2 similar) [K. Verhaegh, et al. 2023, Nucl. Fusion 63 016014]
- 50% below Fulcher peak -> **use as proxy for the ionisation front** -> detachment analysis & real-time control

Intermezzo: D_2 Fulcher band spectroscopy

D2 Fulcher band study (N. Osborne):

- Rotational distribution consistent with Boltzmann. MAST-U: **high T_{rot} (4000-8000 K) at low n_e (2.10^{19} m^{-3})**
  - **Rotational temperature increases during deeper detachment** and decreases at deepest detachment
  - Molecules can survive longer in a detached plasma, which may explain T_{rot}





[N. Osborne, et al. 2023, arxiv]

Intermezzo: D_2 Fulcher band spectroscopy

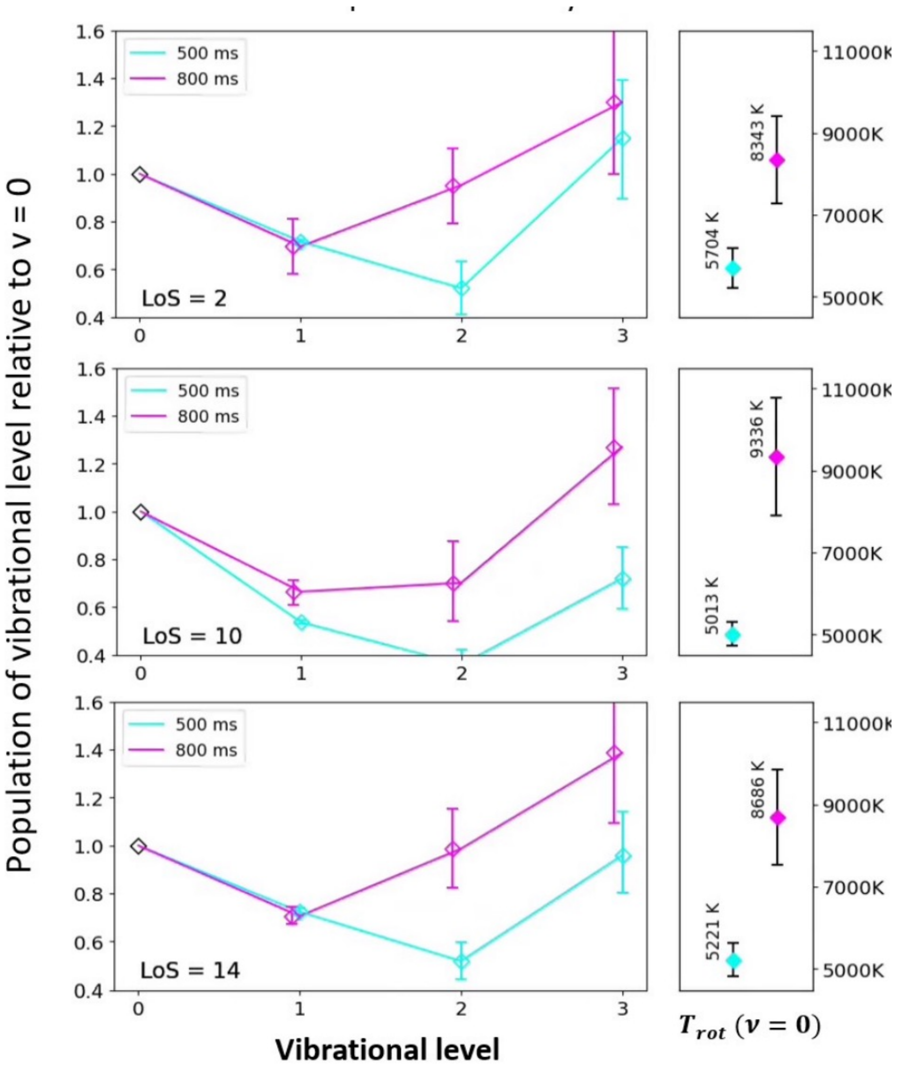
D2 Fulcher band study (N. Osborne):

- Rotational distribution consistent with Boltzmann distribution
  - **Rotational temperature increases during deeper detachment**
  - Molecules can survive longer in a detached plasma -> high T_{rot} ?
  - Comparison MAST-U & TCV **at different shapes/fueling/baffling ongoing –> suggest T_{rot} mostly depends on detached state**

- Vibrational distribution **inconsistent with Boltzmann distribution**
  - **Overpopulation v=3 increases during deeper detachment**
  - **Inconsistent with most CR models ?**

- D_2 Fulcher spectra MAST-U qualitatively similar to JET (E. Pawalec)

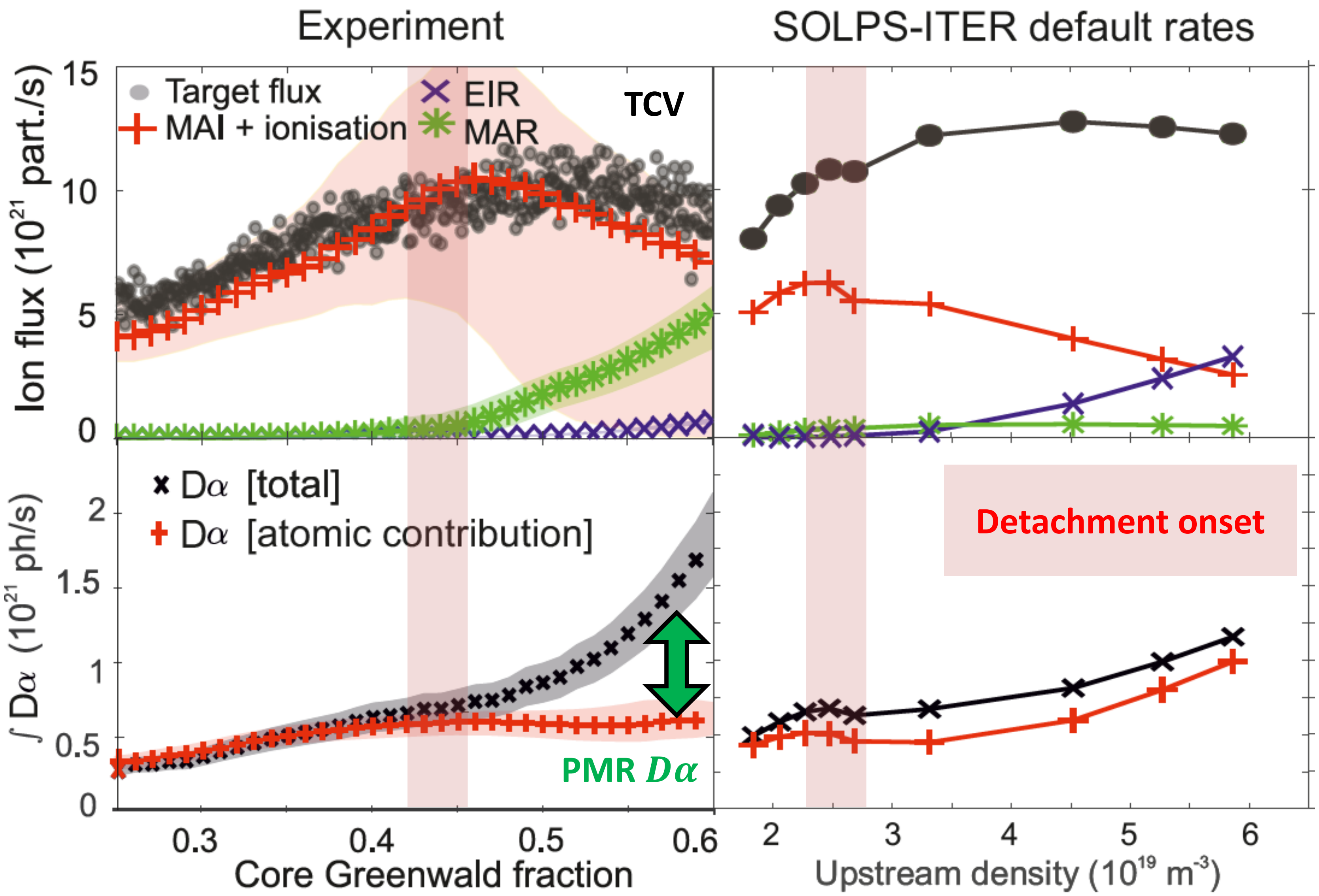
[N. Osborne, et al. 2023, arxiv]



Example – no MAR in interpretive simulations (TCV)

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

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 ?

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

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

Plasma-molecular interactions in exhaust simulations

Plasma-molecular interactions in Eirene

Effective rates – use 0D CRM to compute **hydrogen** rates (n_e and T_e), stored as tabled fits (AMJUEL)

$$< \sigma v >_{eff} (n_e, T_e) = \Sigma_\nu \, f_\nu(T) < \sigma v >_\nu \; (T, n_e)$$

- Vibrational ($f_\nu(T)$) and electronic resolved model decoupled: **electronic excitation not considered for $f_\nu(T)$**

Vibrational model ($f_\nu(T)$) – ‘H2VIBR’:

❖ Vibrational excitation through electron impact:	v=0 (Bardsley Wahedra 1979) rescaled to higher v
❖ Ion conversion*	v=0 (Holiday, 1971) rescaled to higher v
❖ Electron-impact dissociation	v=0 through b3S (Janev, 1987) rescaled to higher v
• Electron attachment	v=0 (Bardsley, Wahedra, 1979) rescaled to higher v
• Molecular ionisation	Gryzinski method

❖= Rescaled by scalar A_ν : $< \sigma v >_\nu \; (T) = A_\nu < \sigma v >_{\nu=0} (T)$ – difference in threshold energy neglected

* Depends on **ion velocity,** but Eirene cannot account for this and assumes **Ti = Te**, leading to erroneous mass rescaling:

Vibrational model heavily outdated and not self-consistent with effective rates

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$$< \sigma v >_{eff} (n_e, T_e) = \Sigma_\nu \, f_\nu(T) < \sigma v >_\nu \; (T, n_e)$$

- Vibrational ($f_\nu(T)$) and electronic resolved model decoupled:

Effective rates (vibr. resolved) **-** use a collisional-radiative model to compute **hydrogen** rates as function of n_e and T_e

• Electron-impact dissociation	$e^- + H_2 \rightarrow e^- + H + H$	Sawada
• Molecular Activated Ionisation	$e^- + H_2 \rightarrow 2e^- + H^+ + H$	Sawada
• Molecular ionisation	$e^- + H_2 \rightarrow 2e^- + H_2^+$	Sawada
• Ion conversion	$H^+ + H_2 \rightarrow H_2^+ + H$	Same as vibr. resolved setup
• Dissociative recombination/excitation/ionisation of H_2^+	$e^- + H_2^+ \rightarrow …$	Sawada

Sawada: only **electronically resolved** for **vibrational ground**. Analytic rescaling used:

$$< \sigma v >_{\nu}^{Elec,eff} \; (n_e, T_e) = A_\nu < \sigma v >_{\nu=0}^{Elec,eff} \; (T, n_e)$$

➢ **v dependence of dissociation energy threshold ignored (!)**

Discussion: disconnection AMOL & fusion community? How to improve?

Note: H- not included by default

Decoupling vibrational and electronic resolved model may lead to uncertainties in dissociation rates

Discussion points – molecular treatment in exhaust codes

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

2. **<u>Are additional processes & species required ?</u>**
    - D2+ recombination ? [Wunderlich, et al.]
    - Should D- be considered ?

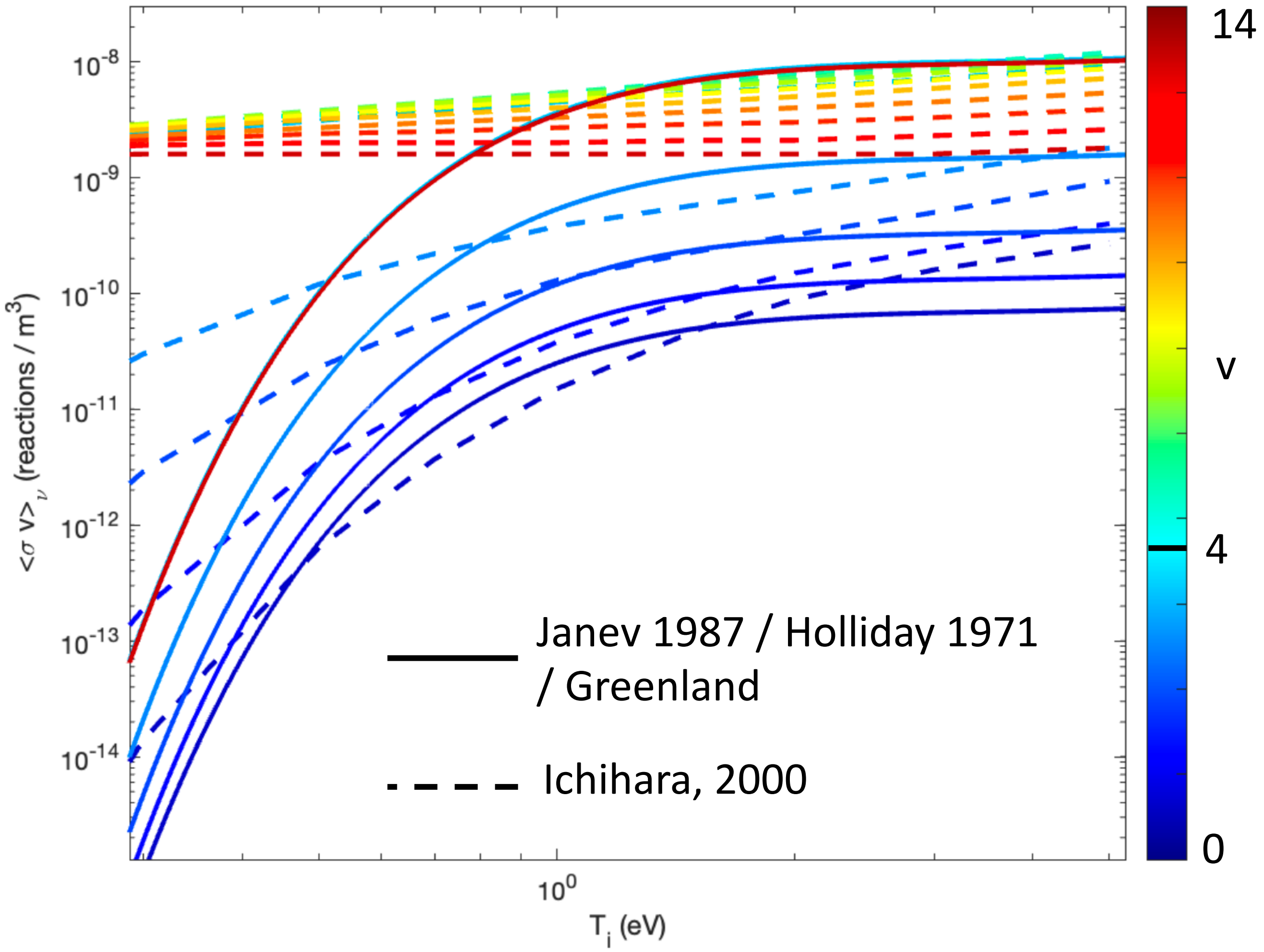
3. **<u>Is a 0D CR approach with effective rates (ne, Te) appropriate for exhaust simulations ?</u>**
    - Transport of D2 (v) -> deviates from 0D transport-less model
    - Plasma-surface interactions -> changes D2 (v) and requires tracking D2 (v)
    - Use robust mathematics approach (Greenland, et al.) to compute which states need to be tracked ?

Scoping study : investigate impact of **improved data** (1.)
& **additional processes** (D-) (2.)

- **Inaccuracy molecular charge exchange biggest impact !**
  - re-derivation of the molecular charge exchange rate
- **D-** may contribute to **MAR & MAD** (but data inconclusive)

Uncertainties in the molecular CX rate

Eirene vibrationally resolved cross-sections are underestimated at low T



Eirene – default molecular CX cross-sections

- Based on measurements for **vibrational ground state** (Janev 1987, Holliday 1971)
- **Analytic** Greenland 2001 **scaling** from ground -> higher vibrational levels ($A_\nu(\nu)$)

$$< \sigma v >_\nu^{H_2\,CX} (T_i, \dots) = A_\nu(\nu) < \sigma v >_{\nu=0} (T_i, \dots)$$

- Cross-sections in vibrational ground drop dramatically at Ti < 1.5 eV
- **Therefore, all vibrationally resolved cross-sections drop dramatically at Ti < 1.5 eV** (default Eirene rates)

Disagrees with vibrationally resolved cross-section calculations [Ichihara, 2000], which show Ti insensitivity at high v (which drive most mol. CX)

Rate scoping study

Use CRUMPET [A. Holm, et al.] (open source, easy to use Python package, provenance) to:
1) rebuild vibr. Resolved CRM used by Eirene
2) check impact of different reactions (including coupling electronic & vibrational states)

Vibrational excitation through electron impact	Laporta (ab. Initio)	D
Ion conversion	Ichihara (ab initio), 2002	H
Electron-impact dissociation	MCCDB (ab initio), Scarlett	D
Electron attachment	Laporta (ab initio)	D
Molecular ionisation	MCCDB (ab initio), Scarlett	D
Electronic excitation	MCCDB (ab initio), Scarlett	D
Radiative decay of electronic states	Fantz	D
Interactions with H2+ & H-	Keep same as Eirene	H

No coupling between D2 and D model, may impact separation D2 ionization & dissociation [Sawada]

See talks Scarlett, Laporta

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

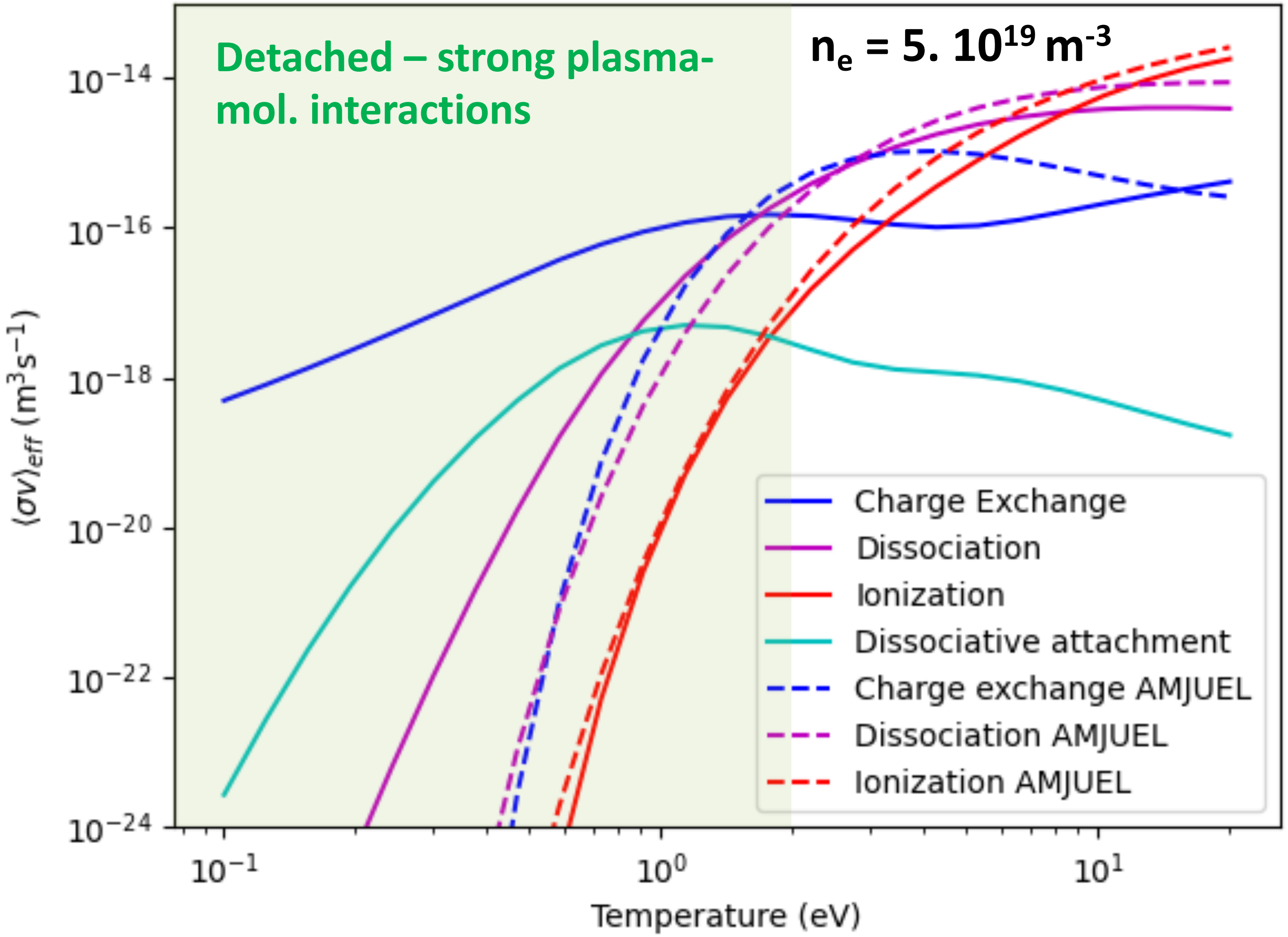
Rate scoping study

Use CRUMPET [A. Holm, et al.]
1) rebuild vibr. Resolved CRM used by Eirene
2) check impact of different reactions

- Vibrational excitation through electron impact
- **Ion conversion**
- **Electron-impact dissociation**
- **Electron attachment**
- Molecular ionisation
- Electronic excitation
- Radiative decay of electronic states
- Interactions with H2+ & H-

No coupling between D2 and D model, which can be important [Sawada]

See talks Scarlett, Laporta



- **Different ion conversion rate has the biggest impact**
- **Electron-impact dissociation increased in low Te region**
- **D- can play lead to MAR & MAD (20% of D2+ driven MAR/MAD)**
- **Consistent with experimental data MAST-U & TCV [Verhaegh, et al. NF, 2021; Verhaegh, et al. ArXiV 2311.08580], but inconclusive**

Rate scoping study

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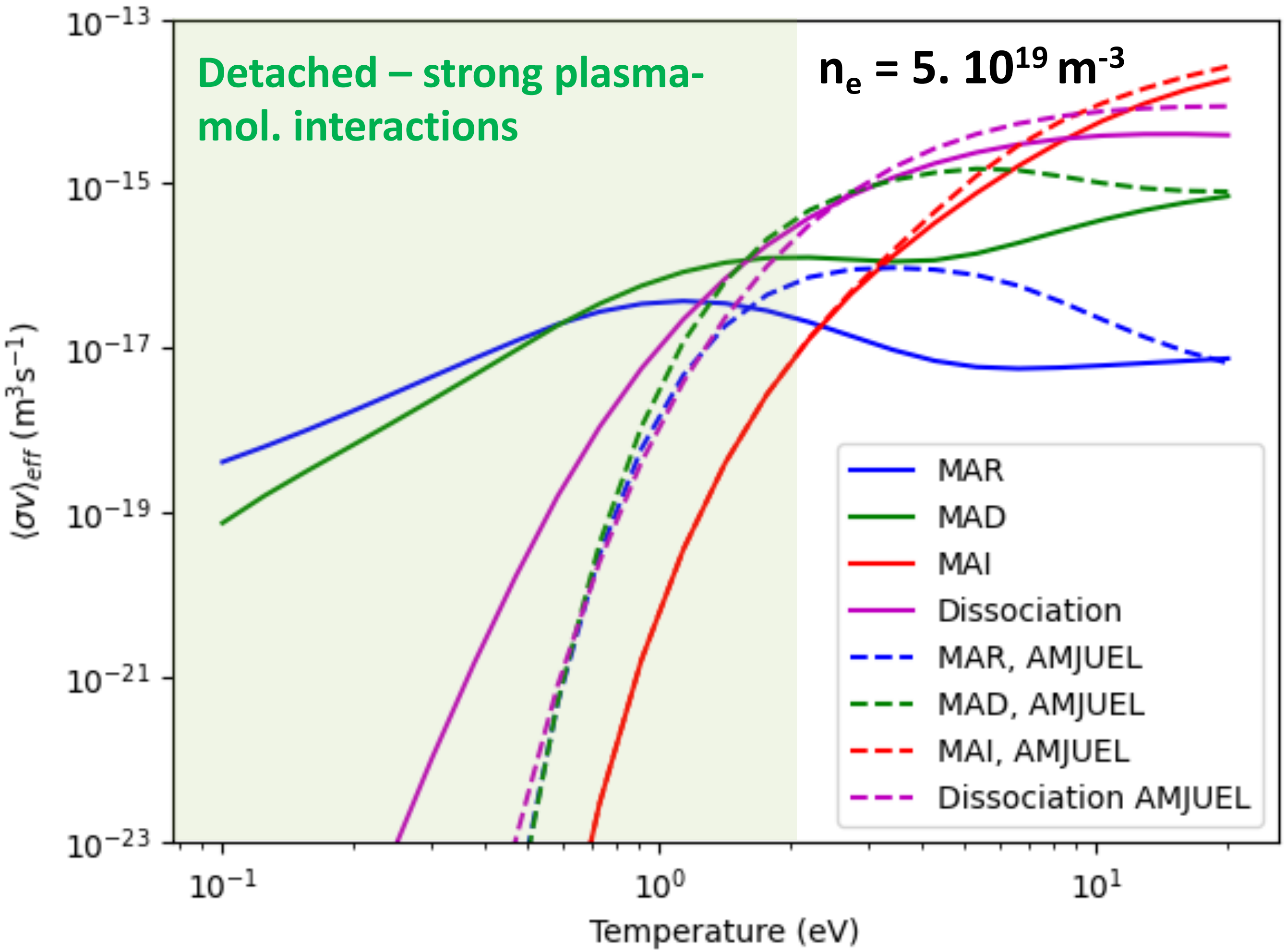
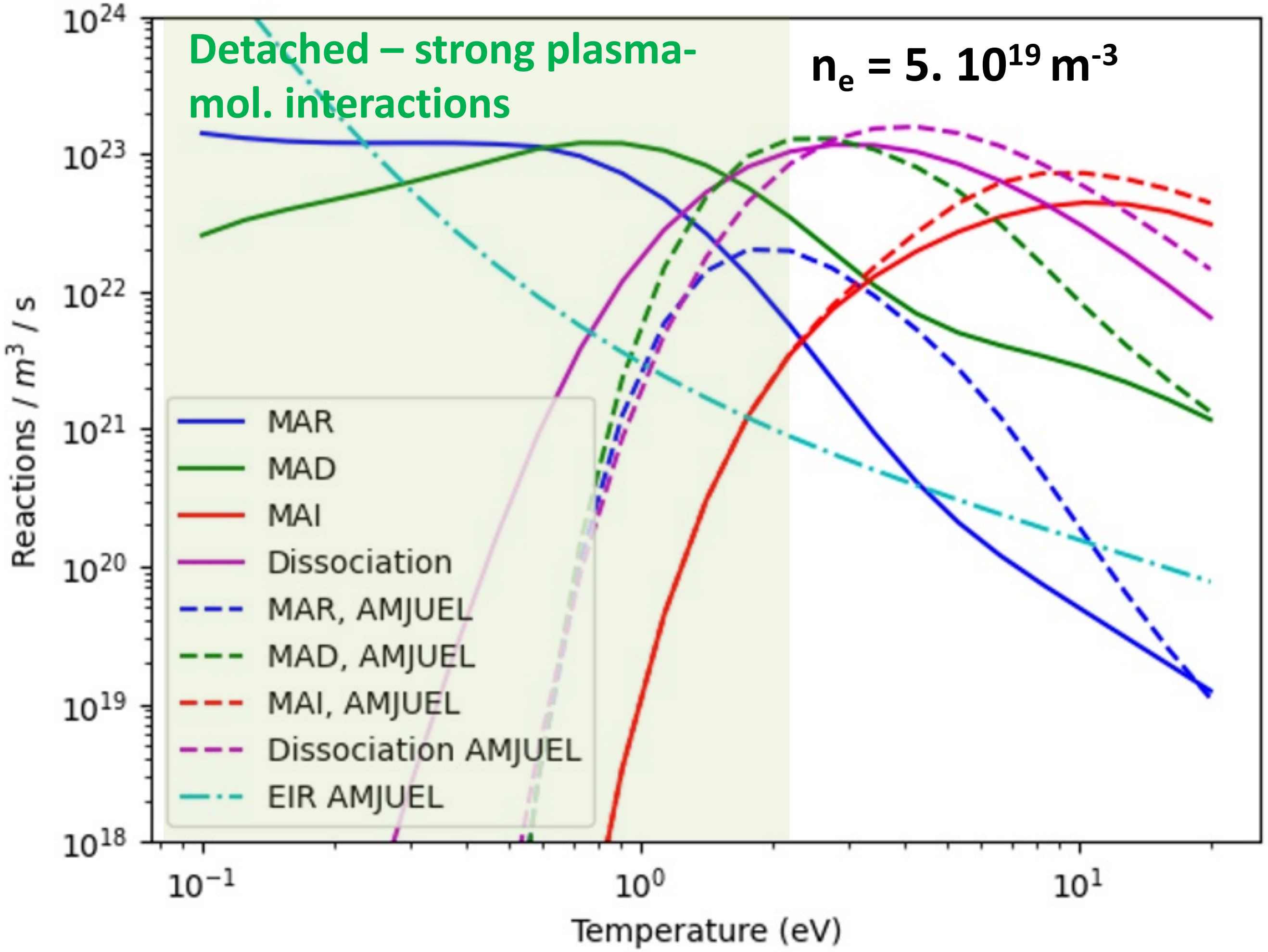


- **MAR & MAD enhanced by orders of magnitude in low Te region**
- **Electron-impact dissociation increased in low Te region**

Rate scoping study

Toy model: Use scalings for increase D2 density as function of Te (SOLPS – MAST-U)

- Molecular density increase at low Te exacerbates discrepancies
- Simplified toy model: **MAR > EIR up to Te=0.25 eV** (MAST-U conditions, $n_e = 5 . 10^{19}$ m^{-3})
- Extrapolating to higher n_e (10^{21} m^{-3})
  -> **MAR & MAD still important up to 0.5 eV**
- **MAR important at low Te with new rates in agreement with experiment**



Detached plasma -> molecular density increases at low Te

- **MAR & MAD enhanced by orders of magnitude in low Te region**
- **Electron-impact dissociation increased in low Te region**
- **Increase of molecular density at low Te boosts MAR & MAD**
- **Improved rates in better agreement with MAST-U behaviour**

Can molecular charge exchange rate inaccuracies impact exhaust simulations ?

1. **Rate modifications** can **impact simulations** & **improve agreement experiment**
2. **Rate modifications can matter on the reactor scale** for tightly baffled divertors with alternative divertor configurations

- **Rate improvements required for reducing uncertainties in extrapolating current knowledge to reactors**

Molecular rate modifications & exhaust modelling

Eirene $D^+ + D_2$ -> $D_2^+ + D$ 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**

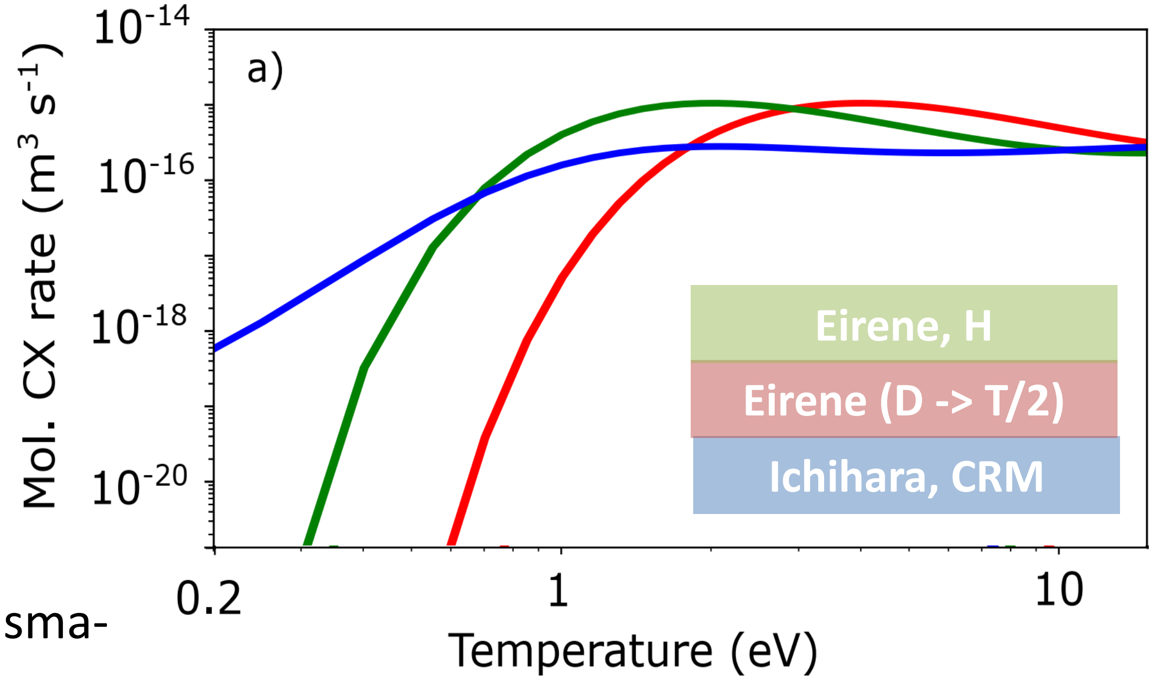
Eirene, H

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



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

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

Molecular rate modifications & exhaust modelling

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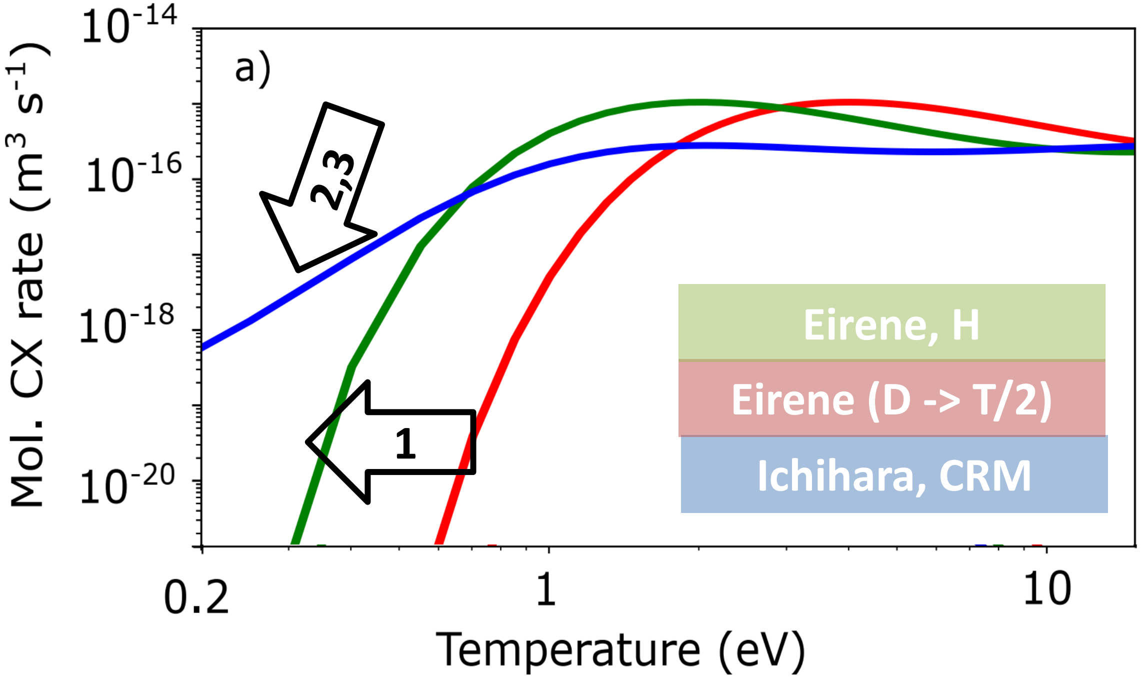
Collisional-radiative modelling

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

1. **Sensitivity study TCV tokamak: disable mass rescaling** [K. Verhaegh, 2023, NF, 076015] **Eirene, H**
2. **Post-process** converged **reactor-scale simulations with** **Ichihara, CRM**
3. **Self-consistent simulations with** **Ichihara, CRM** on MAST-U in progress

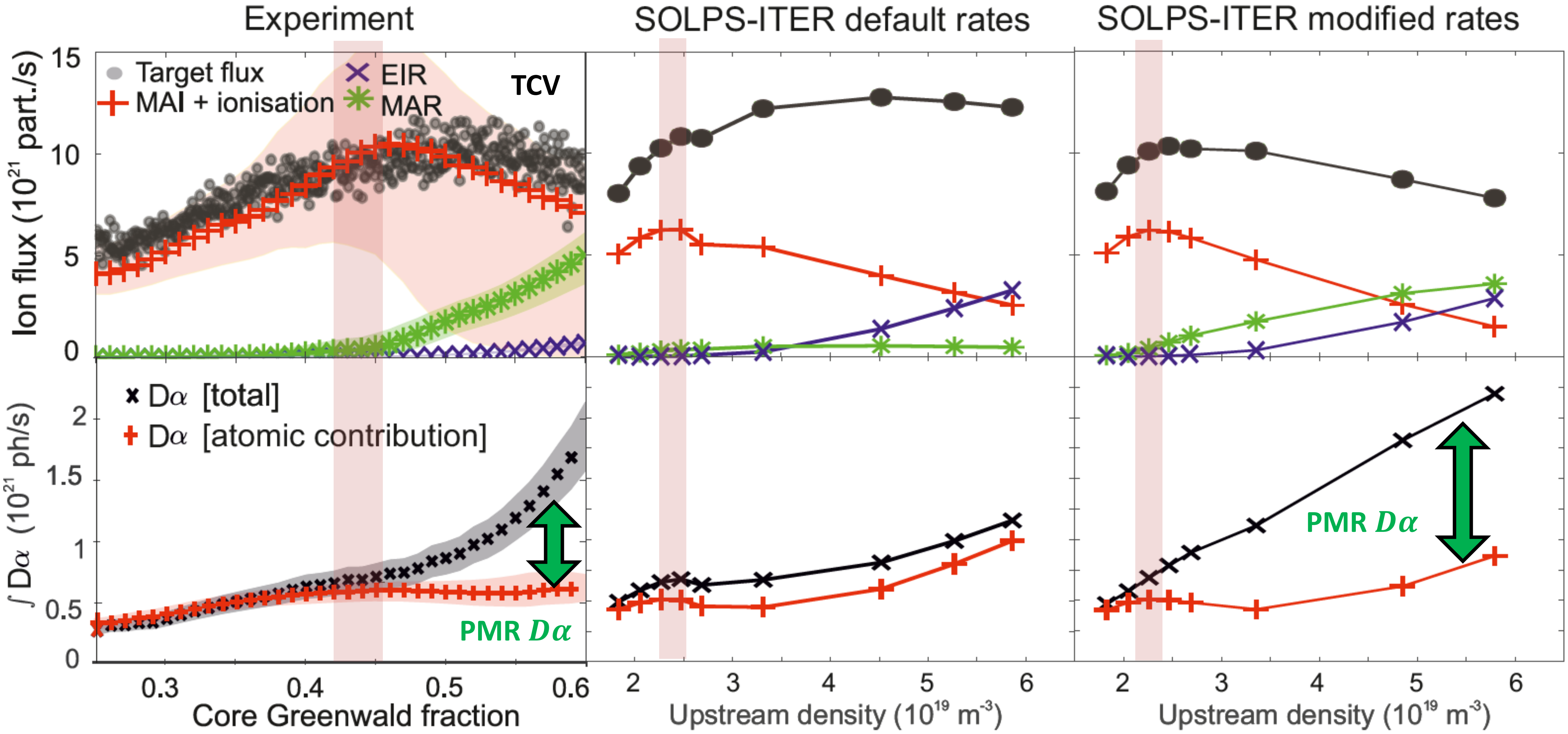


Underestimation of molecular CX expected at Te < 2 eV -> MAR underestimated in detachment

Disable ion mass rescaling **TCV**

[K. Verhaegh, 2023, NF, 076015]

TCV tokamak - #56567 – single null conventional non-baffled, 2016-2018



Experiment

SOLPS-ITER default rates

SOLPS-ITER modified rates

PMR $D\alpha$

PMR $D\alpha$

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

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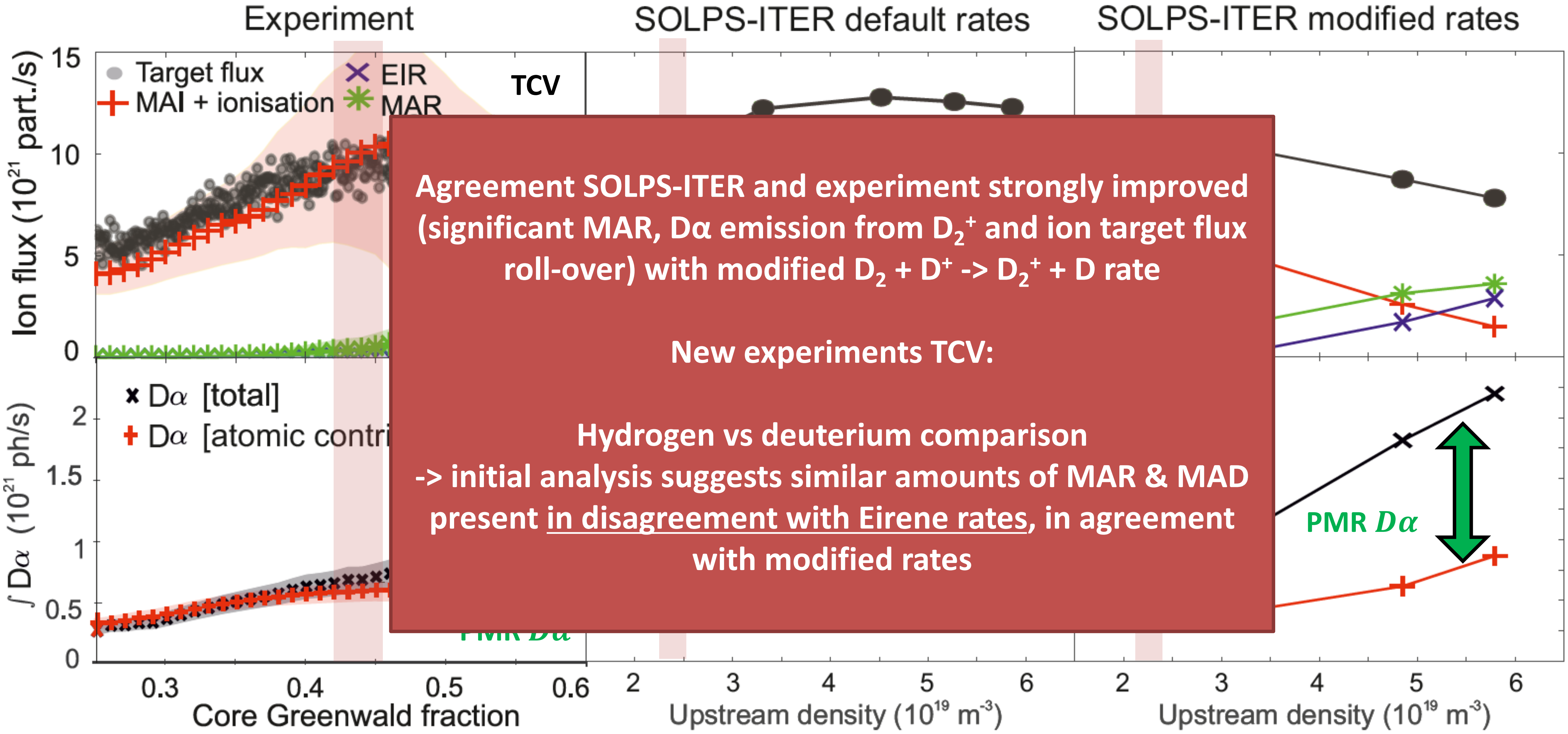


Agreement SOLPS-ITER and experiment strongly improved (significant MAR, Dα emission from D_2^+ and ion target flux roll-over) with modified $D_2 + D^+ \rightarrow D_2^+ + D$ rate

New experiments TCV:

Hydrogen vs deuterium comparison
-> initial analysis suggests similar amounts of MAR & MAD present in disagreement with Eirene rates, in agreement with modified rates

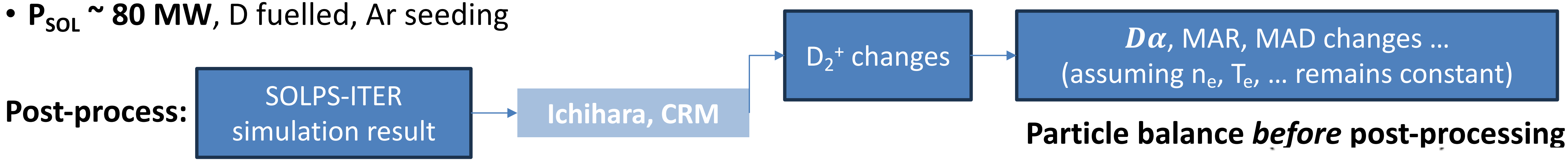
MAR: $D_2 + D^+ \rightarrow D_2^+ + D$; $D_2^+ + e^- \rightarrow D^* + D$

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])

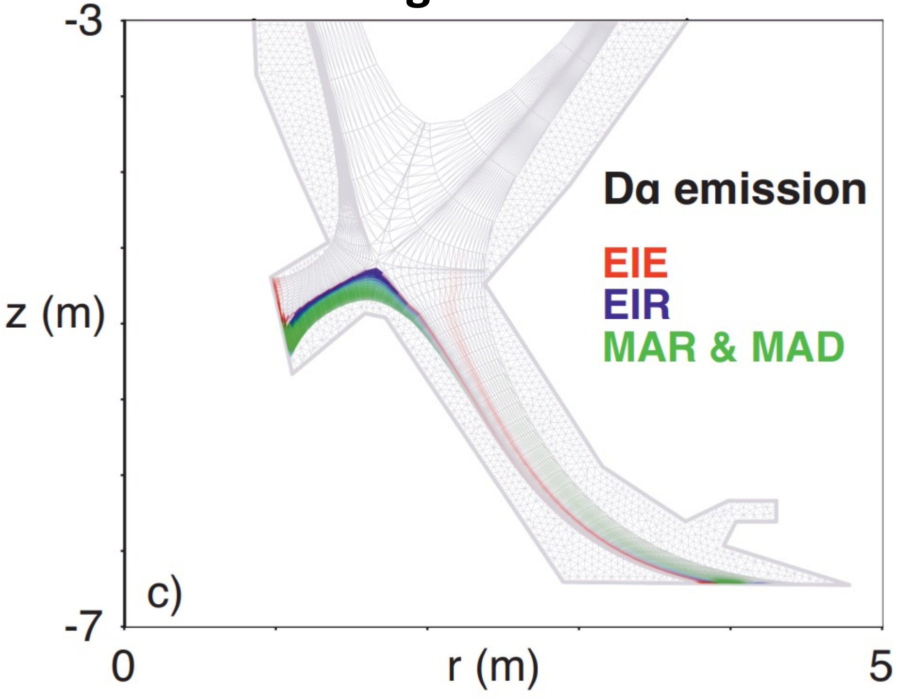
- **Tightly baffled** double null **Alternative Divertor** (Elongated / X-Divertor - outer / inner target)
- **P_{SOL} ~ 80 MW**, D fuelled, Ar seeding



Post-process:

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

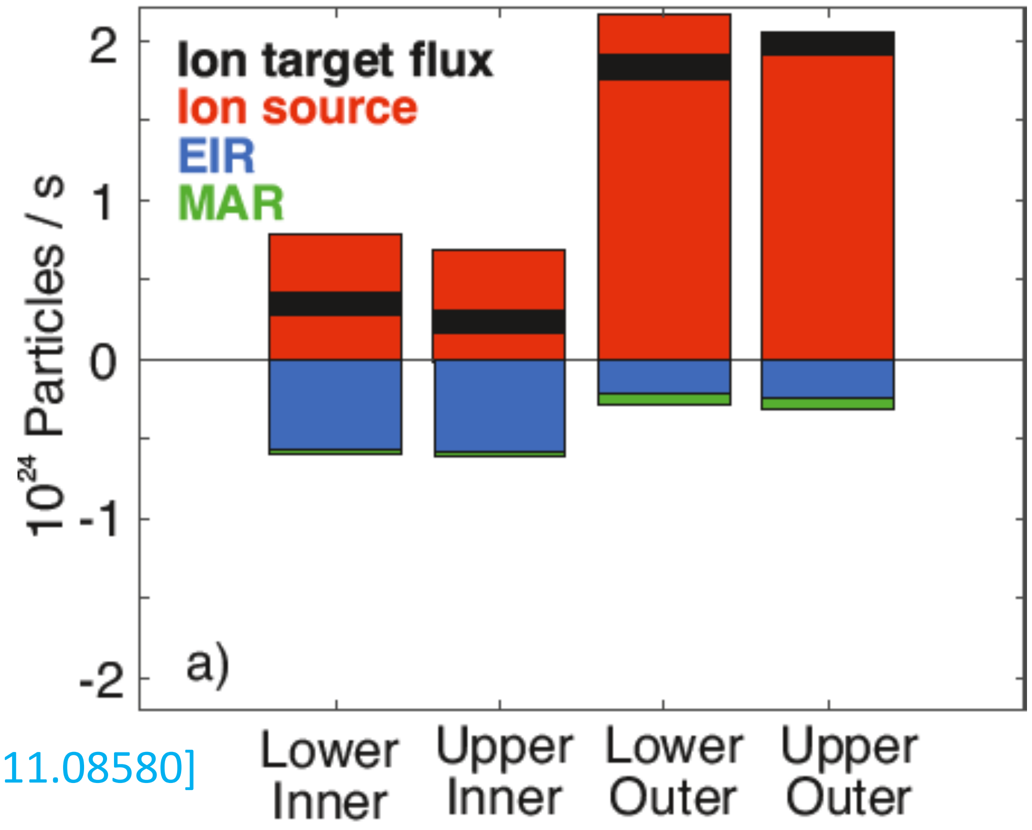
Simulation grid with $D\alpha$ emission (post-processed)



Simulation near detachment onset (ionisation near target)

[K. Verhaegh, 2023, ArXiV:2311.08580]

Particle balance *before* post-processing



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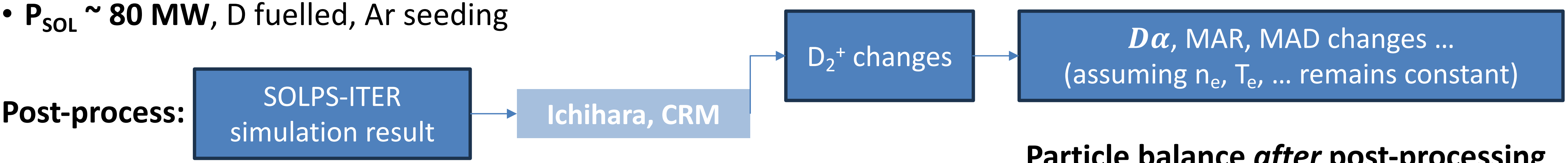


Post-process:

SOLPS-ITER simulation result

Ichihara, CRM

D_2^+ changes

$D\alpha$, MAR, MAD changes …
(assuming n_e, T_e, … remains constant)

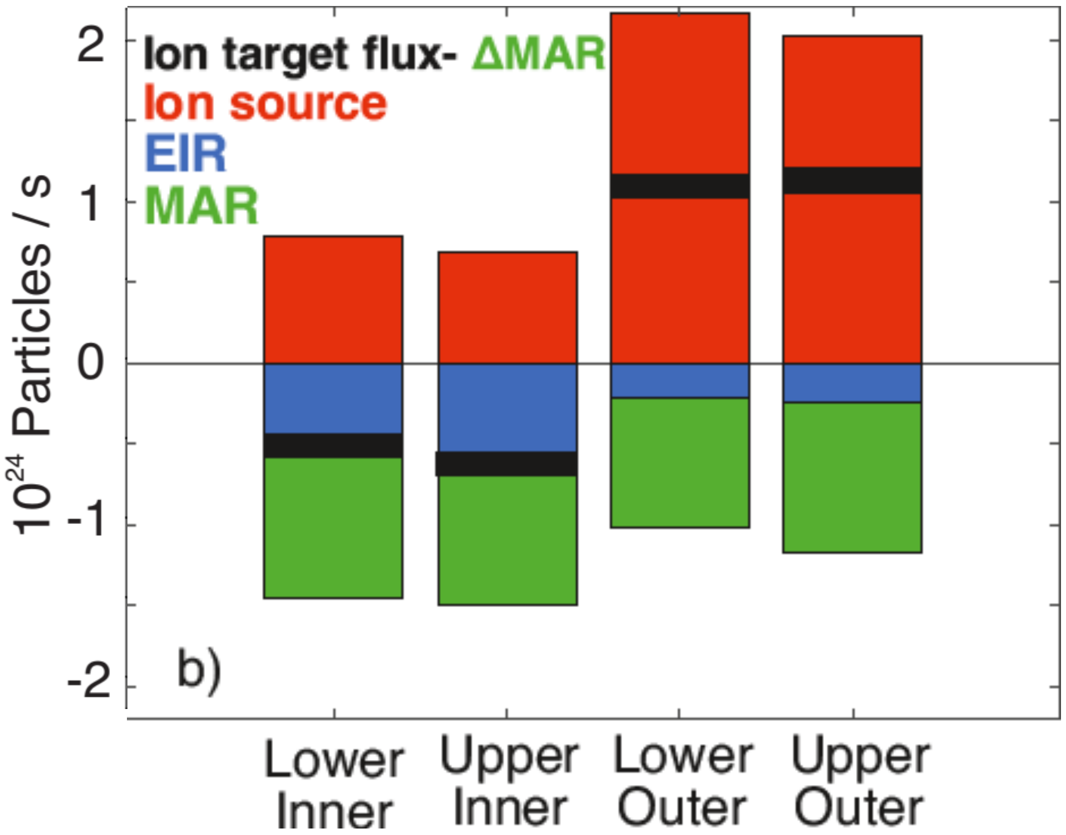
- **MAR > EIR ion sinks** (despite n_e ~ 10^{21} m^{-3})
- **MAR > inner target ion flux**

- **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



3. Is a 0D CR approach with effective rates (ne, Te) appropriate for exhaust simulations ?

- **Potential impact of transport of D2 (v) on MAR/MAD ?**
- **Potential impact of plasma-surface interactions on MAR/MAD ?**

Potential impact of transport of D2 (v)

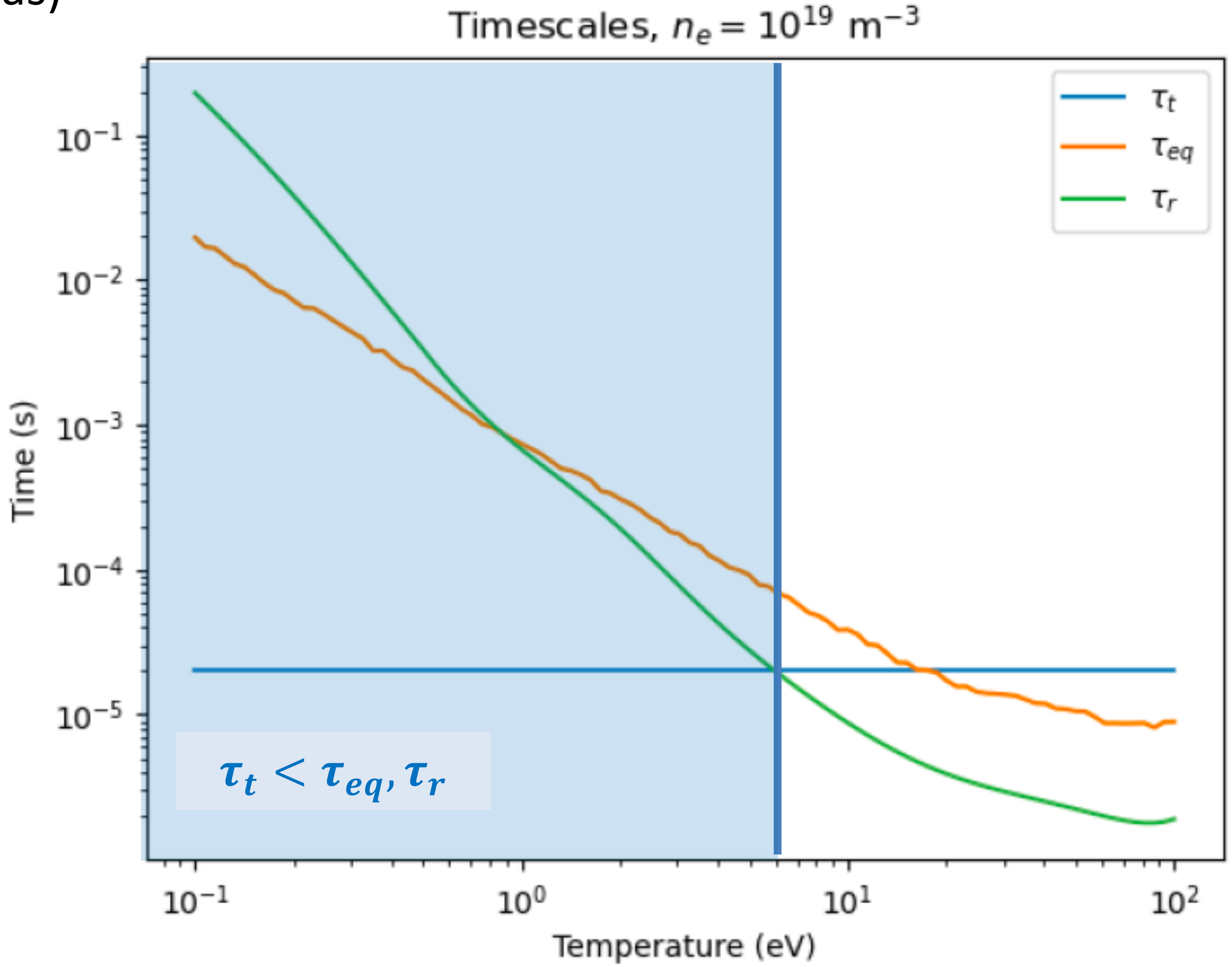
Timescales of D2 (v)

- Equilibration time τ_{eq} (increases for detached plasmas)
- Transport τ_t (constant – for constant D2 temperature – assume 0.5 eV & 10 cm)
- Lifetime τ_r (increases for detached plasmas)

Transport of D2 (v) is likely if the transport timescale is the shortest: $\boldsymbol{\tau_t < \tau_{eq}, \tau_r}$

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

D(v) transport can be significant on MAST-U and may be non-negligible in reactors at detachment-relevant conditions



Potential impact of transport of D2 (v) on MAR & MAD

Timescales of D2 (v)

- Equilibration time τ_{eq}
- Transport τ_t
- Lifetime τ_r

Transport of D2 (v) is likely if the transport timescale is the shortest: $\tau_t < \tau_{eq}, \tau_r$

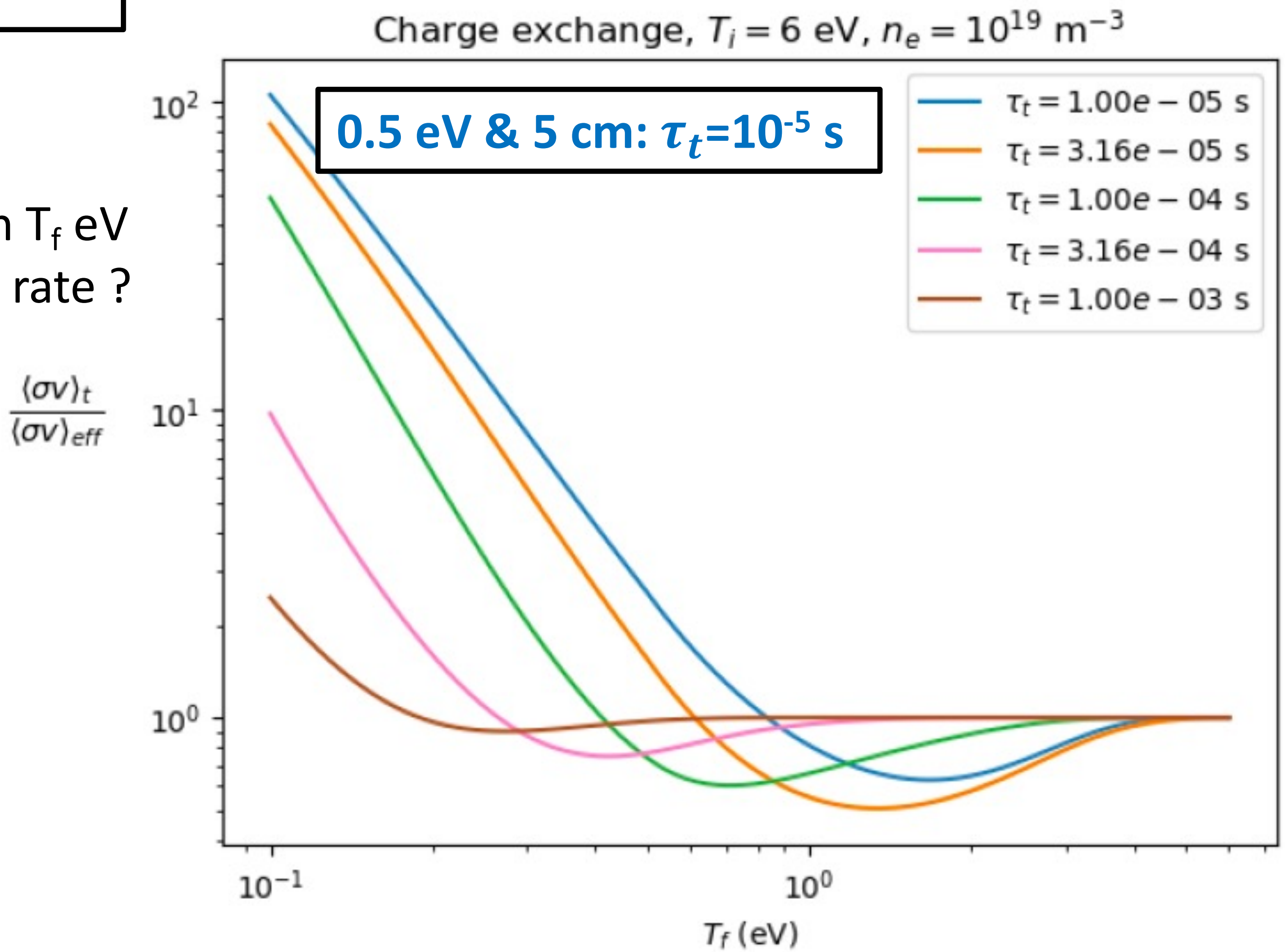
Toy model to for impact on MAR & MAD

- Molecule equilibrated @ 6 eV, travels τ_t through an T_f eV region, how much will this raise D2 + D+ -> D2+ + D rate ?

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

D(v) transport can be significant on MAST-U at detachment-relevant conditions

Can raise D2+ MAR & MAD by x100
Can raise D- MAR & MAD by x10000



0.5 eV & 5 cm: τ_t=10^{-5} s

Potential impact of transport of D2 (v) on MAR & MAD

Timescales of D2 (v)

- Equilibration time τ_{eq}
- Transport τ_t
- Lifetime τ_r

Transport of D2 (v) is likely if the transport timescale is the shortest: $\boldsymbol{\tau_t < \tau_{eq}, \tau_r}$

Te (eV)	Ne (m^{-3})
6	10^{19}
1.5	10^{20}
0.5	10^{21}

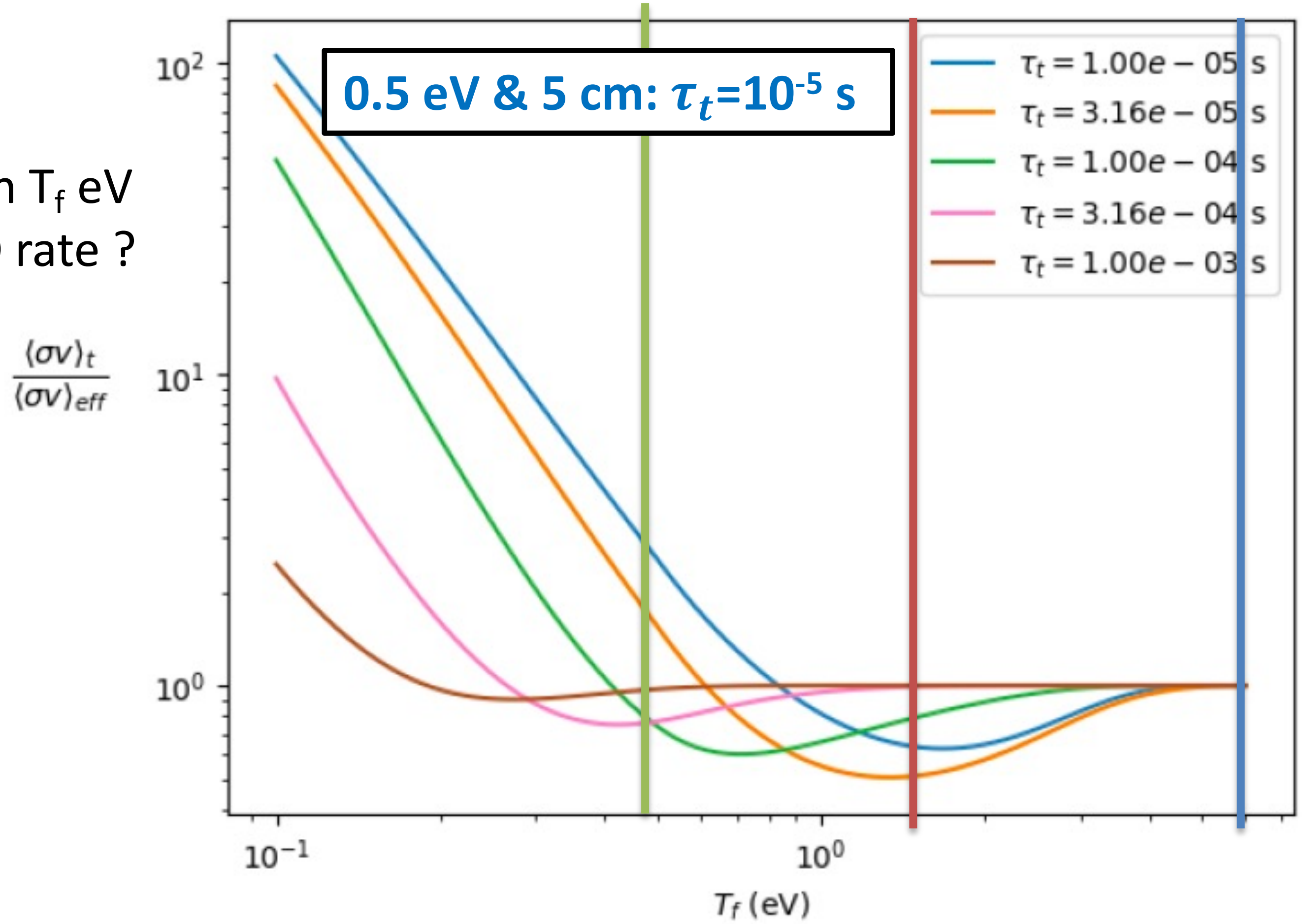
Toy model to for impact on MAR & MAD

- Molecule equilibrated @ 6 eV, travels τ_t through an T_f eV region, how much will this raise $D2 + D+ \rightarrow D2+ + D$ rate ?

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

D(v) transport can be significant on MAST-U at detachment-relevant conditions, which may also occur at reactor-relevant n_e

Can raise D2+ MAR & MAD by x100
Can raise D- MAR & MAD by x10000



0.5 eV & 5 cm: τ_t=10^{-5} s

Potential impact of surface interactions on MAR/D

Probability functions for **D2(v) released from the wall**, -> toy model potential impact plasma-surface interactions

- Plasma surface interactions -> source of high vibrational D2(v)
- Introduce additional source into CRM

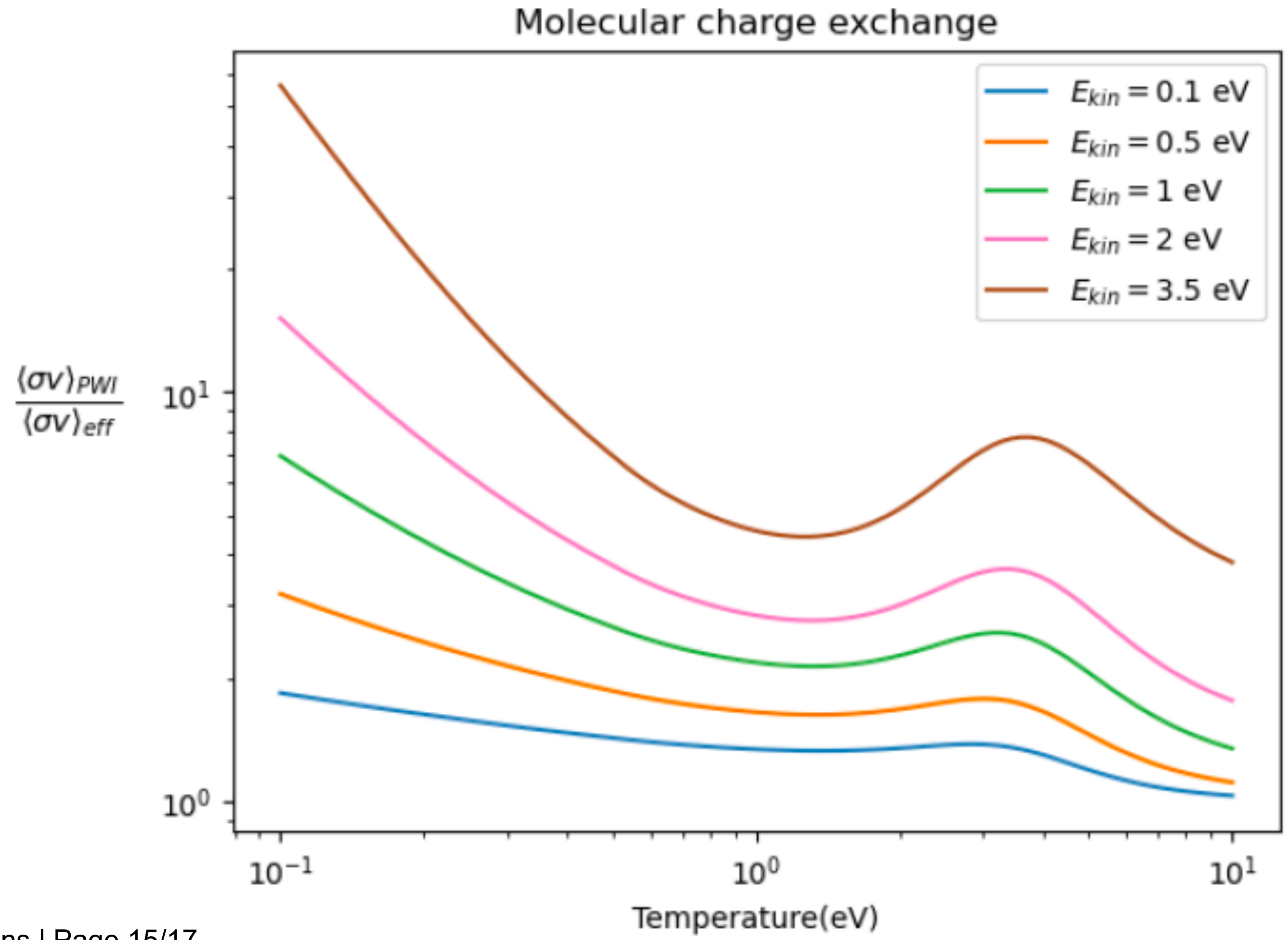
➢**Raises vibrational levels D2(v)** overall
-> can increase molecular charge exchange -> **MAR**

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

D2 (v) from Rugliano, et al. 2011
Assumes D2 influx from re-association on the wall on Tungsten through Elay-Rideal process

Similar results found by **Saito, et al.** based on **molecular dynamics modelling**

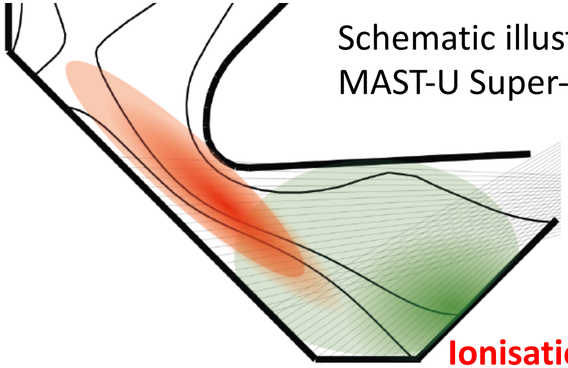
Plasma surface interactions could further raise MAR near target in the detached region



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

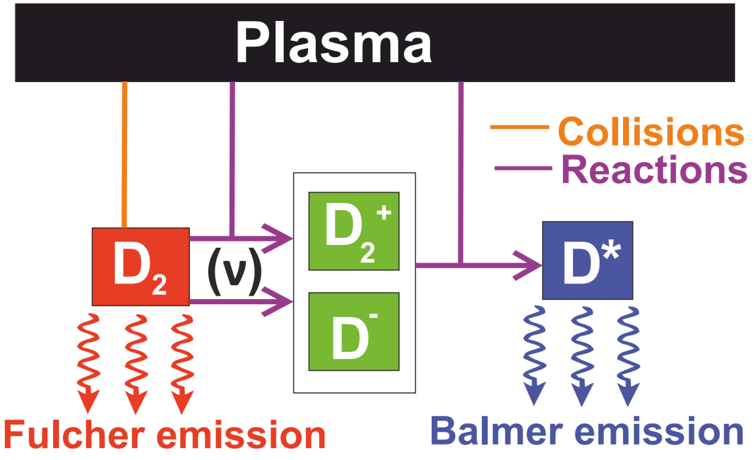


Schematic illustration example MAST-U Super-X divertor

Ionisation

Plasma-molecular interactions

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/D2 balance; changes detachment window; fuelling efficiency; …..
2. **Diagnostic analysis & design –** including **detachment control sensor** strategies

Discussion points – molecular treatment in exhaust codes

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

2. **Are additional processes & species required ?**
    - D2+ recombination ? [Wunderlich, et al.]
    - Should D- be considered ?

3. **Is a 0D CR approach with effective rates (ne, Te) appropriate for exhaust simulations ?**
    - Transport of D2 (v) -> deviates from 0D transport-less model
    - Plasma-surface interactions -> changes D2 (v) and requires tracking D2 (v)
    - Use robust mathematics approach (Greenland, et al.) to compute which states need to be tracked ?