UK Atomic Energy Authority

Neutral processes in SOLPS-ITER

D Moulton

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CULHAM CENTRE FOR FUSION ENERGY

Overview

- Introduction
- Consider reactions / collisions involving:
  - Atoms and plasma
  - Atomic ion and electron recombination
  - Molecules and plasma
  - Molecular ions and plasma
  - Neutral-neutral collisions
- Surface processes
- Concluding remarks / other issues

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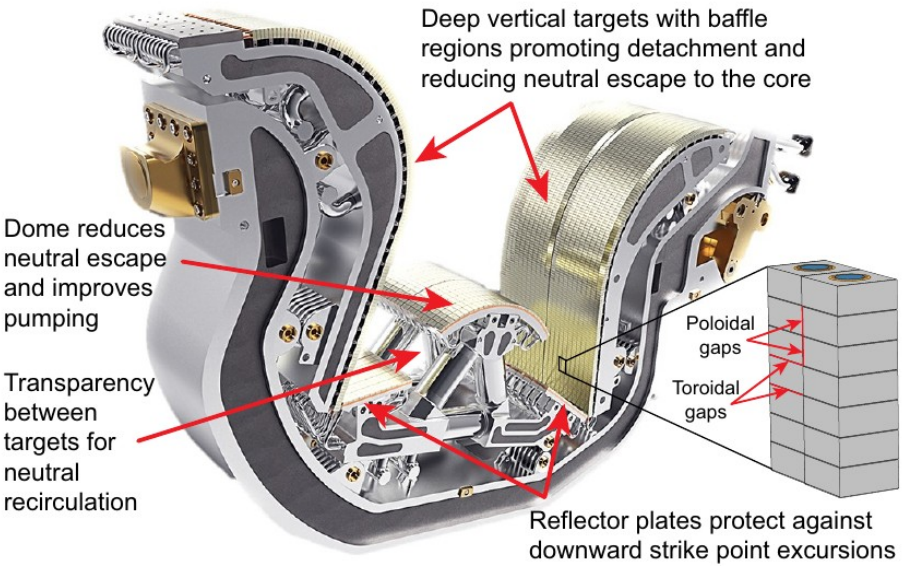

[Pitts et al. NME (2019) **20** 100696]

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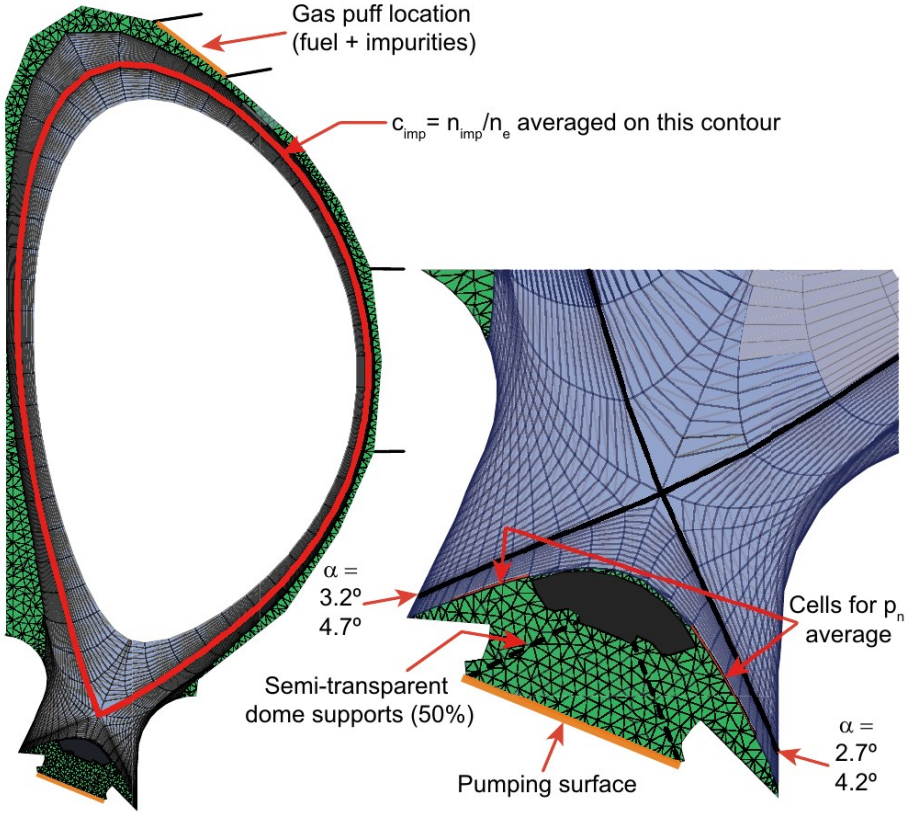

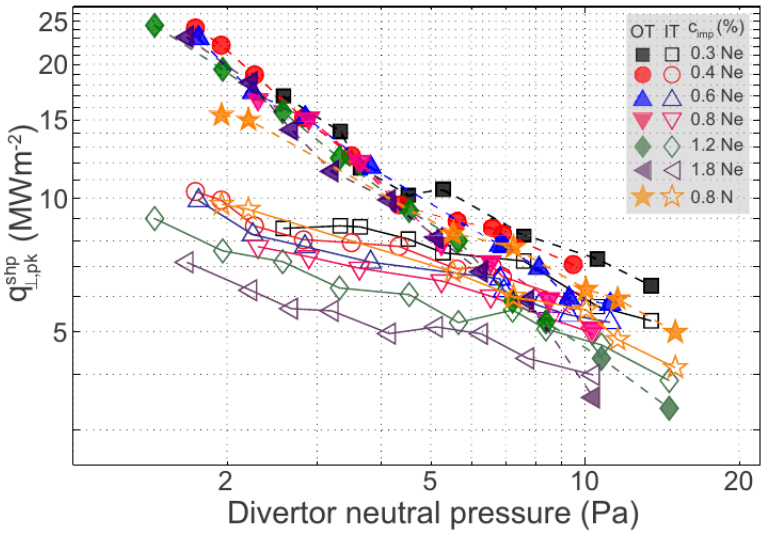

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Introduction

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- SOLPS-ITER consists of a coupling between a multifluid (D, He, Ne…) plasma fluid code (“B2.5”) and a kinetic Monte-Carlo neutral code (“EIRENE” [www.eirene.de, V Kotov PhD Thesis (2007) “Numerical study of the ITER divertor plasma with the B2-EIRENE code package”])
- Neutrals are likely to be an important mechanism for reducing target loads in a reactor; getting neutral processes correct is essential
- Neutral processes also influence
  - neutral penetration to the core plasma (affects confinement)
  - helium pumping
  - impurity enrichment in the divertor
- I won’t talk about the code itself here but rather the ‘default’ neutral processes that it models

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Atoms and plasma

$H + e \rightarrow H^+ + 2e$	Ionisation	AMJUEL H.4,10 2.1.5
$H^+ + H \rightarrow H + H^+$	Charge exchange	HYDHEL H.1,3 3.1.8

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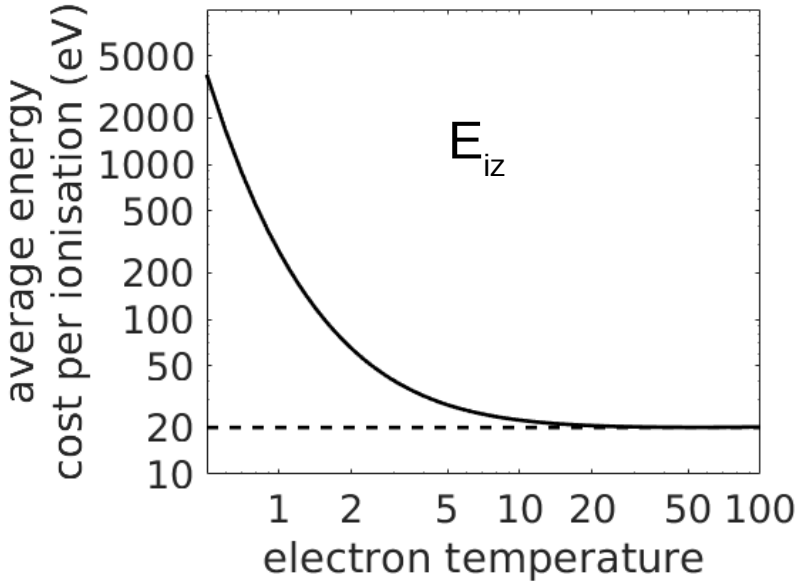

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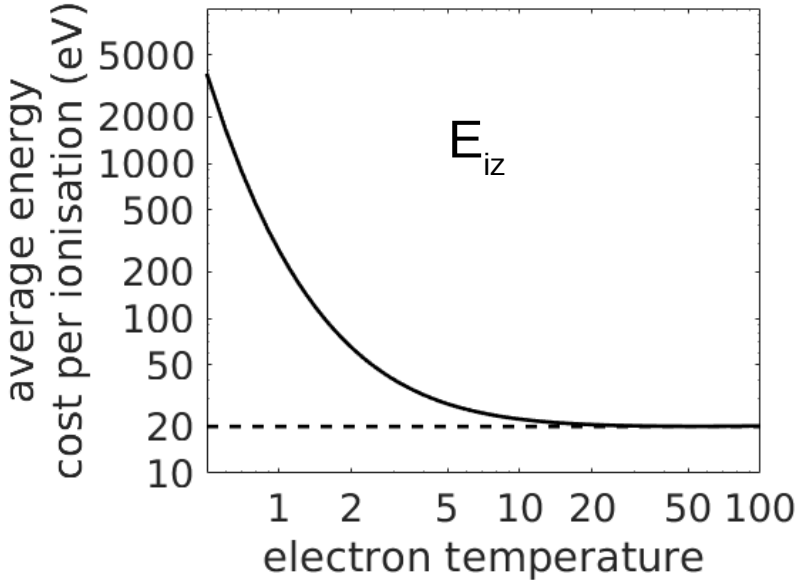
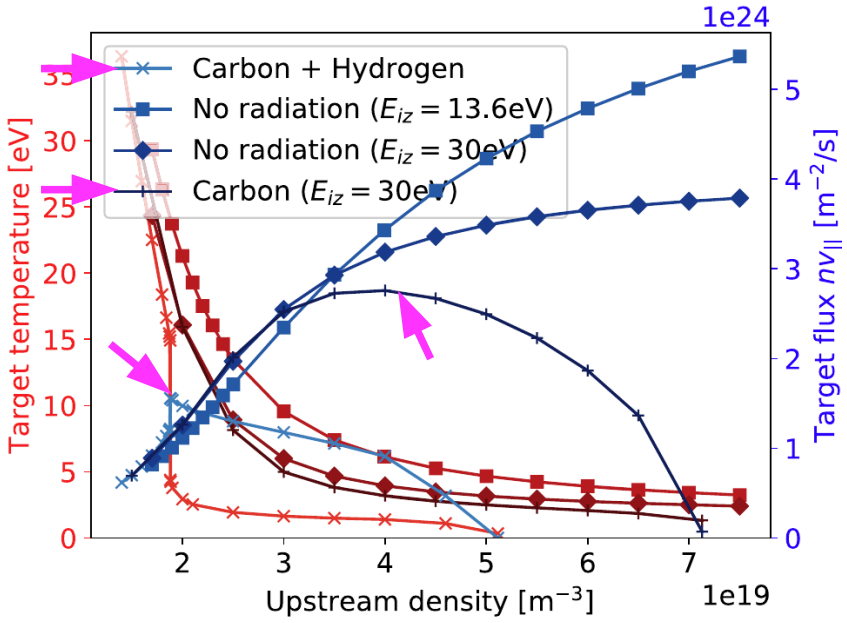
- In SD1D simulations, this behaviour significantly shifts the upstream density at which the target ion flux rolls over [Dudson et al. PPCF (2019) **61** 065008]





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- The atom ionisation particle and energy rates used are '**effective**' rates.
- '**Effective**' means that, although they are applied to ground state atoms, the rates assume a population distribution for the electronically excited states of the atoms.
- When calculating that population distribution, a collisional-radiative model is applied that assumes
  - Maxwellian background electrons
  - H atoms with excited energy state lifetimes << both their transport time scales and the characteristic time scale of heavy particle collisions
  - No molecules (when deciding whether to ionise an atom, we assume that recently-dissociated atoms do not contribute significantly to the excited atom population distribution)

Atoms and plasma

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- In the absence of molecules, charge exchange is the dominant plasma momentum sink in the volume.
- With molecules, elastic collisions between H_2 and H^+ tend to dominate the momentum sink (see later)
- However, charge exchange still plays a key role in setting the mean free path of the atoms, important in setting the atom distribution over the entire volume.

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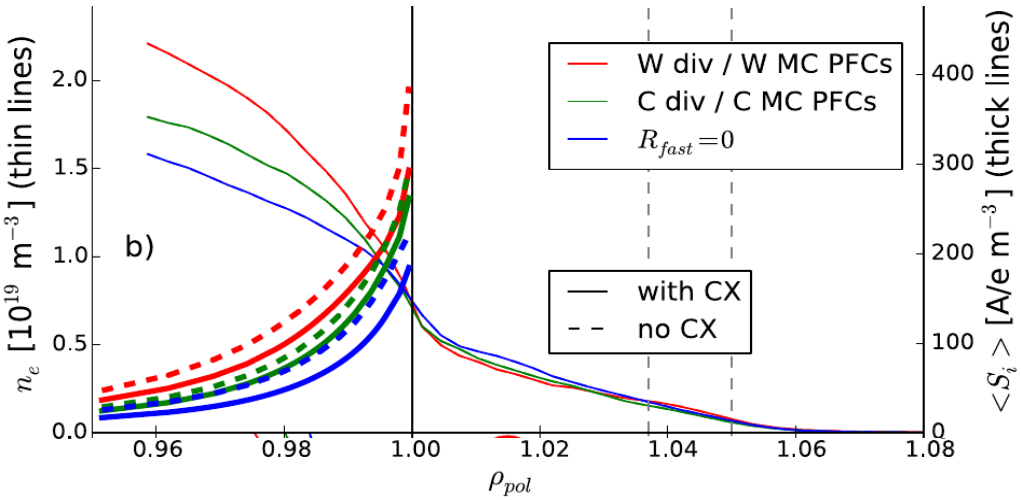
- CX is important in setting the flux of neutrals that cross the separatrix, which can itself influence the pedestal pressure.
- In EMC3-EIRENE simulations of ASDEX-Upgrade, CX was found to **decrease** the neutral flux across the separatrix [Lunt et al. PPCF (2017) **59** 055016]
- Isotropic scattering of neutrals that were otherwise moving towards the separatrix outweighs the gain in MFP due to higher atom energy after CX collision.



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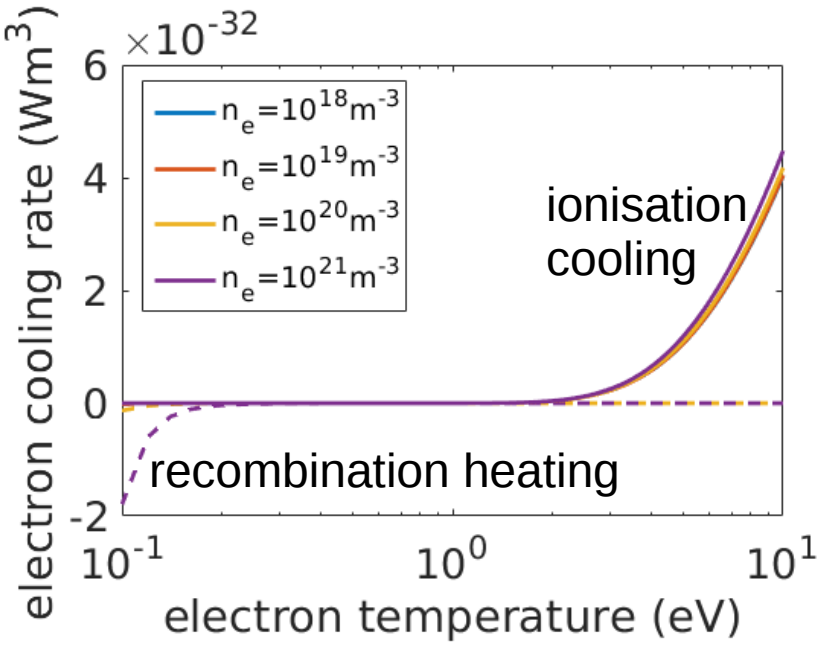
Atomic ion-electron recombination

$H^+ + e \rightarrow H + h\nu$	Radiative recombination	AMJUEL H.4,10 2.1.8
$H^+ + 2e \rightarrow H + e$	3-body recombination	

- The effective recombination rate accounts for radiative and 3-body recombination
- Rates become significant below ~1 eV
- Potentially important in reducing the D^+ flux to the target and associated surface recombination load (see later)
- At low n_e, radiative recombination dominates: the potential energy gain of recombination is lost to photons and electrons are neither heated nor cooled
- At high n_e, 3-body recombination dominates and the potential energy gain of recombination is carried away by the secondary electron, heating the electron population



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$H_2 + e \rightarrow H + H^+ + 2e$	Dissociative ionisation	AMJUEL H.4 2.2.10
$H_2 + H^+ \rightarrow H_2^+ + H$	Ion conversion	AMJUEL H.2 3.2.3
$H_2 + H^+ \rightarrow H_2 + H^+$	Elastic collision	AMJUEL H.0,1,3 0.3T

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- As for the effective atom ionisation, the effective molecular rates account for the distribution of (some) electronically-excited and vibrationally-excited states, calculated using a collisional-radiative model.

Molecules and plasma

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- When vibrational states are considered, the following assumptions are made:
  - Only vibrational excitation by electron impact is accounted for (no radiative decay of electronically excited states).
  - The transport time of vibrational states is assumed long compared to their lifetime (may not be a good assumption in the divertor – see later).
  - Rotational energy of molecules is not accounted for.
  - For ion conversion, a fixed KE for H_2 of 0.1 eV is assumed, and that $T_e = T_i$ → rate coefficient is a function of T_e only.

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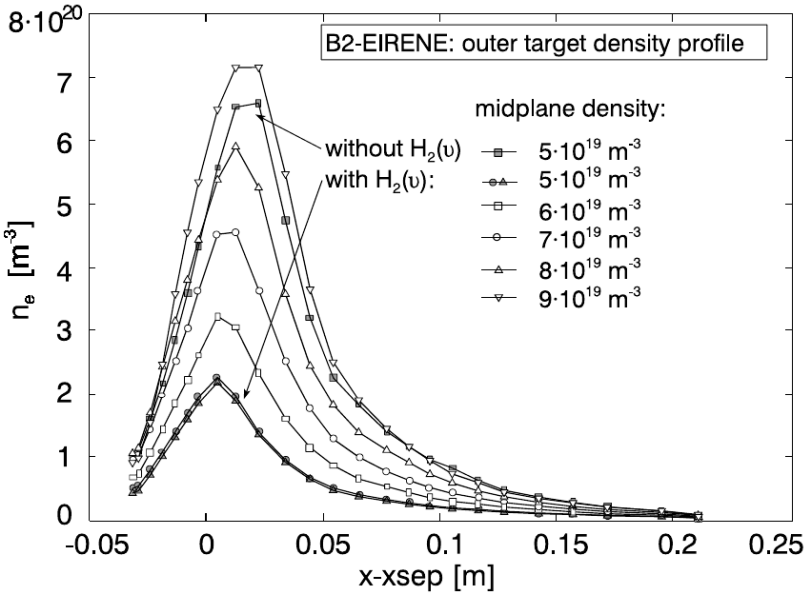
- [Fantz et al. JNM (2001) 290-293 367] looked at the effect of tracking the movement of vibrational states within EIRENE
- Found a significant effect on target density for the same upstream density on ASDEX-Upgrade



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- Energy balance is strongly simplified
- E.g. for dissociation: both resulting atoms have 3 eV kinetic energy (+4.5 eV potential energy of the molecule → 10.5 eV loss from electron channel)
- Similarly simple assumptions for all other electron-molecule and electron-molecular ion reactions
- There are electron energy loss rates available within AMJUEL for dissociation and non-dissociative ionisation (H.10 2.2.h2c), but not currently used by default? References looking into this effect?

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- Elastic collisions between atomic ions and molecules are treated classically [section 3.1 of Kotov's PhD thesis]
- They are typically the dominant momentum sink, and can be an important ion energy sink as well

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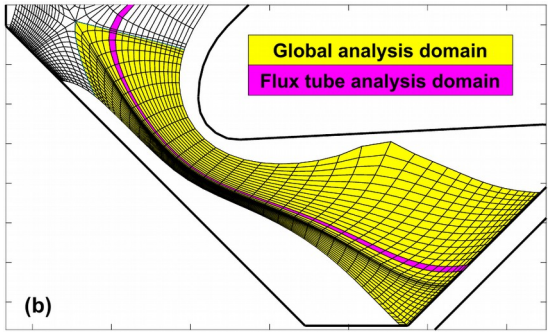
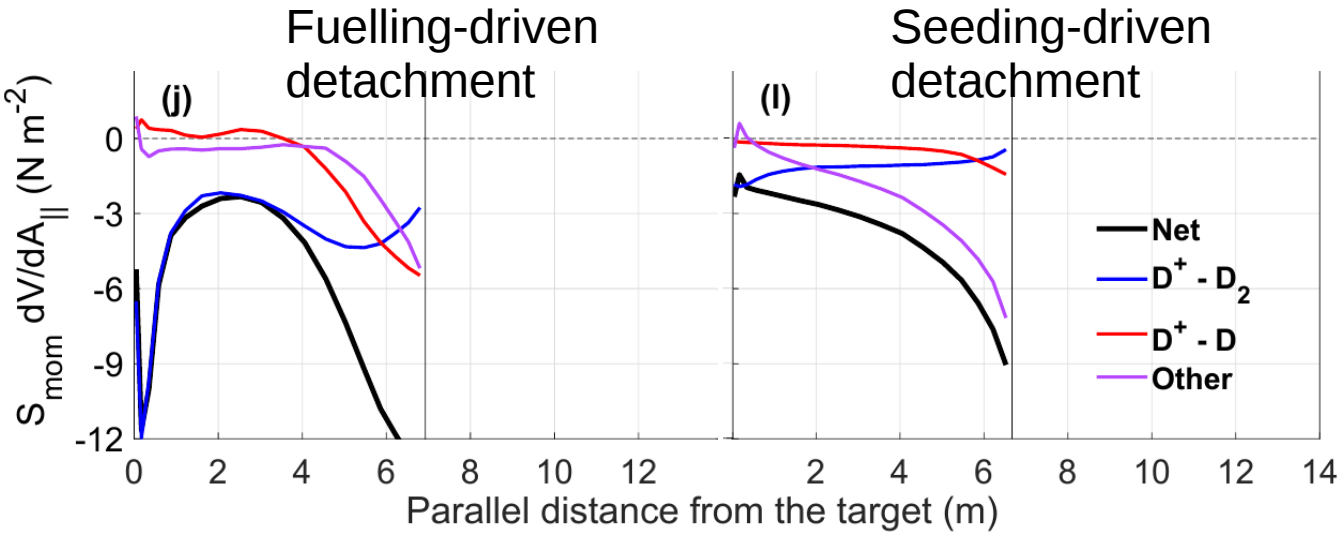
MAST-U predictive simulations [O Myatra et al., to be submitted]





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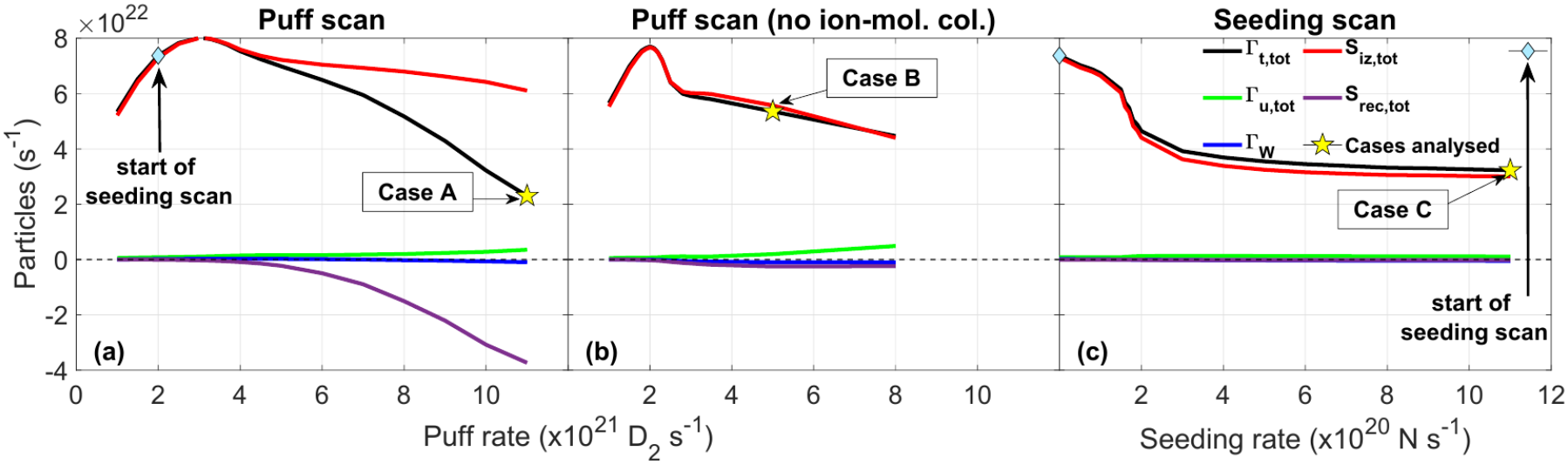

- D_2+D^+ elastic collisions are necessary for the fuelling-driven detachment simulations to have significant recombination, not seen in seeding-driven detachment

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Molecular ions and plasma

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$H_2^+ + e \rightarrow 2H^+ + 2e$	Dissociative ionisation	AMJUEL H.4 2.2.11
$H_2^+ + e \rightarrow 2H$	Diss. recombination	AMJUEL H.4,8 2.2.14

- Transport of H_2^+ molecular ions are not followed (marginal assumption if n_e<1E20m^{-3}).
- Recombination of molecular ions into molecules is not accounted for, neither are negative ions H^- or molecular ions H_3^+.
- Vibrational states of H_2^+ are not taken into account explicitly, but the rate coefficients are averaged over the vibrational distribution of the products of non-dissociative ionisation $H_2 \rightarrow H_2^+$.
- Simple energy loss models are used by default (e.g. both atoms after dissociative recombination given 0.5 eV).
- Exception is dissociative recombination where effective energy loss calculated by collisional radiative is used.

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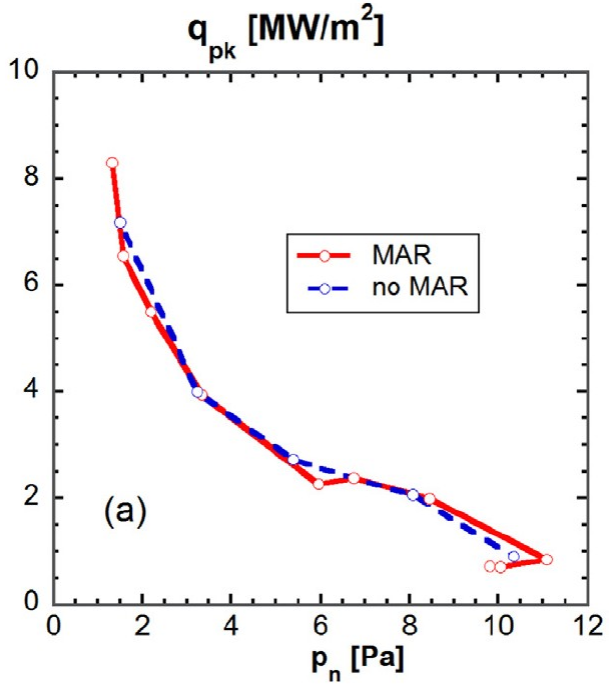
- Ion conversion ($H_2 + H^+ \rightarrow H_2^+ + H$) followed by dissociative recombination is termed “molecular assisted recombination” (MAR) and can act as a sink of atomic ion-electron pairs
  - potentially reduces the surface recombination heat load
- Inclusion of MAR in SOLPS modelling of ITER has so far not shown a strong influence on most important parameters [Kukushkin et al. NME (2017) **12** 984]



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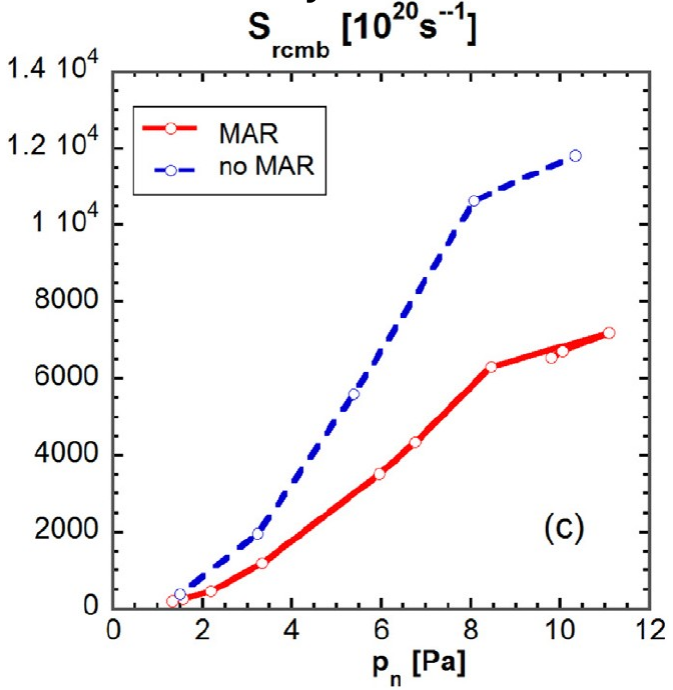
- Three-body recombination seen to compensate for MAR, possibly due to additional electron heating → more ionisation → higher density → more three body recombination.

three-body recombination



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Neutral-neutral collisions

- "BGK" collision rates calculated using empirical data on viscosity and diffusivity.
- Neutral-neutral collisions are not particularly important on most current machines (e.g. JET [Kotov et al PPCF (2008) **50** 105012], MAST-U).

No	Description
1	EIRENE 1996
2	Model 1 plus up-to-date chemistry of D_2 and MAR
3	Model 2 plus elastic collisions $D_2 + D^+$
4	Model 3 plus neutral–neutral collisions
5	Model 4 plus photon opacity

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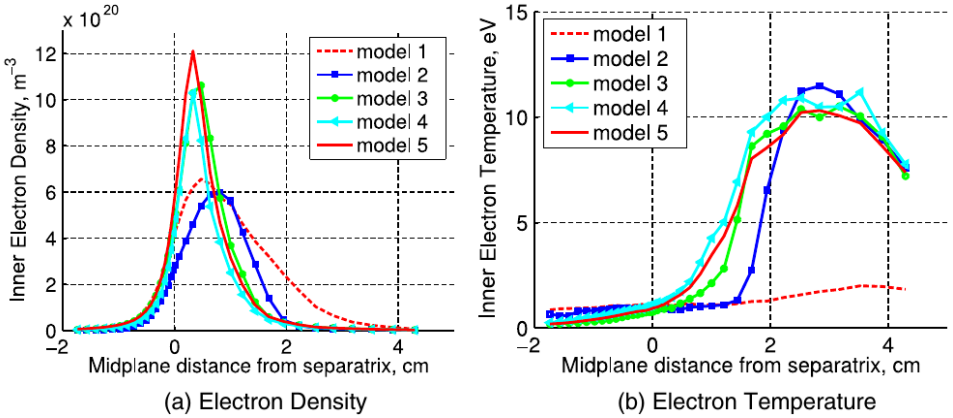

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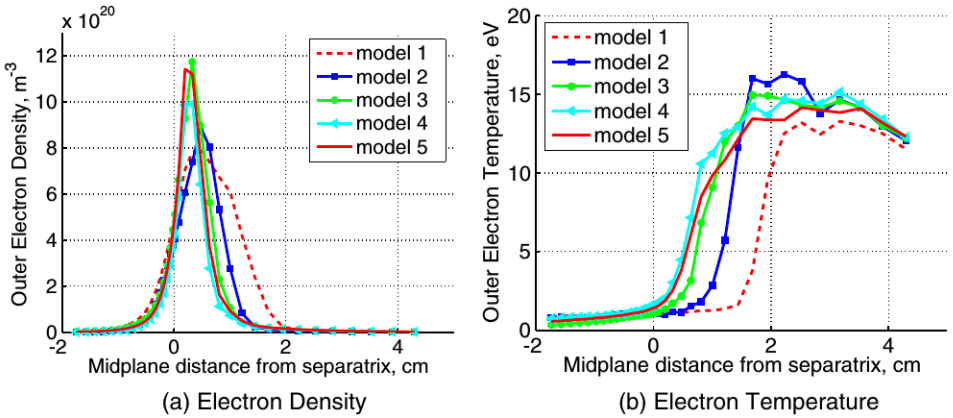

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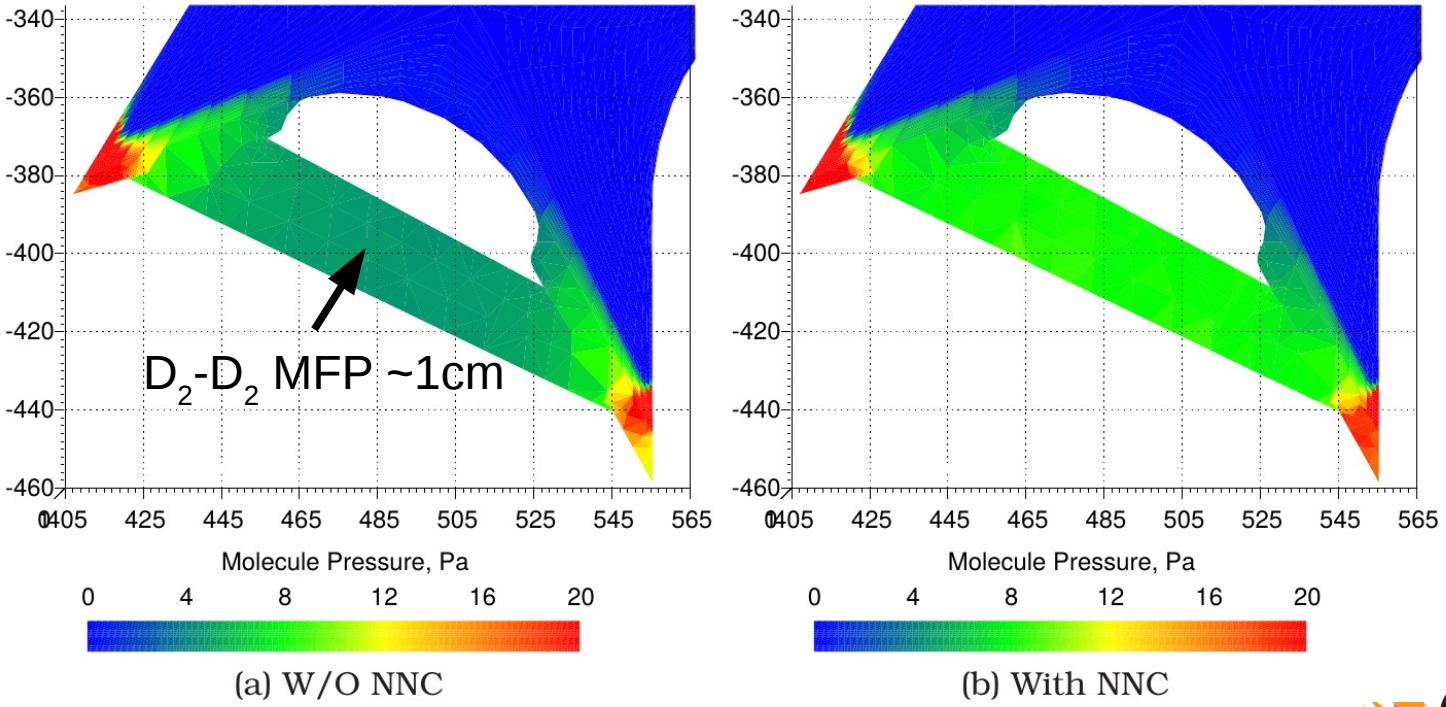
- Only important in very high (neutral) density machines (e.g. C-Mod, ITER).
- For ITER, neutral-neutral collisions are necessary for correct prediction of neutral conductance under the ITER dome, and for correct prediction of helium pumping [Kotov PhD thesis],



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  - Reflect as fast atoms, losing relatively little kinetic energy
    - Pre-computed tables are calculated from the TRIM code.
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    - Provide PDFs for the existence, energy and angle of the reflected atom, given the incoming energy and angle, and the wall material
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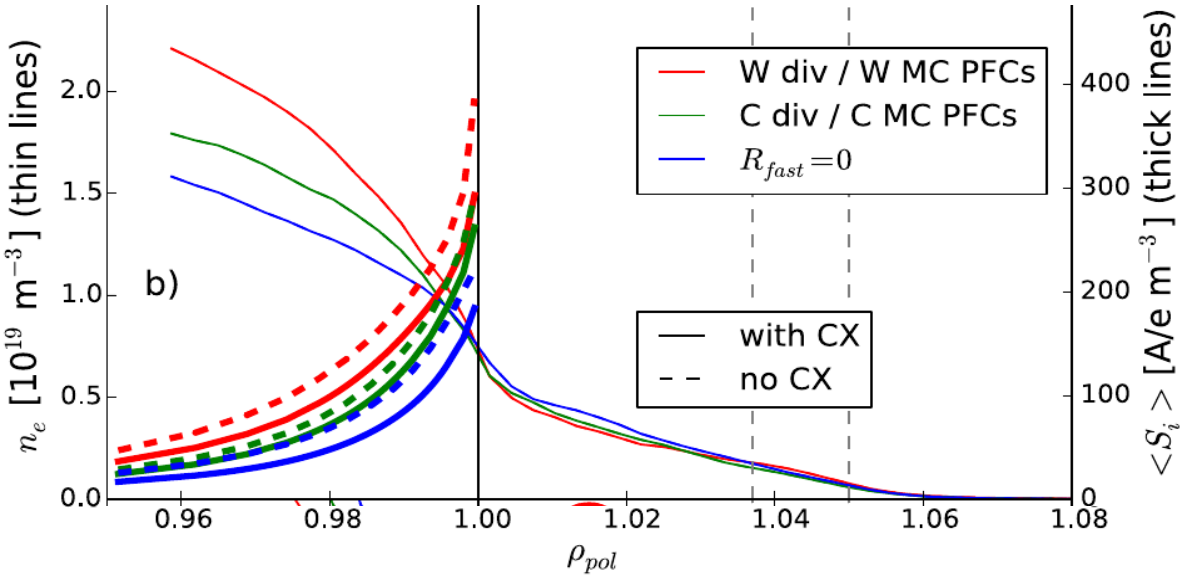
    - [Lunt et al. PPCF (2017) **59** 055016] showed significant effect of wall material on the neutral penetration in EMC3-EIRENE simulations.



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- Getting neutral processes right is of critical importance for edge plasma modelling in tokamaks
- Knowing what you're missing is not easy when
    - You're a model user rather than a neutral / molecular expert
    - There are many other uncertainties within the SOLPS-ITER model that might cause discrepancies with experiment, besides the rates used
    - Uncertainties in the rates used are not available
- Other 'rate' issues:
    - Ammonia formation when nitrogen is seeded to reduce target loading
    - Carbon sputtering in a carbon wall; following of hydrocarbons [M Wischmeier PhD Thesis (2004)]
    - Tungsten prompt redeposition
    - Mass rescaling
    - Isotope effects (driven by molecular structure rather than just mass)
    - Photon trapping
    - Effect of wall recycling on the distribution of vibrational states.
    - Elastic scattering between D_2 and impurity ions
    - Impurity ion rates (currently taken from ADAS)

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