

Adding Molecules to Hermes-3

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Context

- Molecules are expected to play an important role in detachment in tokamak divertors.
- This poster describes a new fluid implementation of molecular chemistry in Hermes-3, based on the Kotov (2008) mechanism [3].

Reactions Framework

The code parses input reaction strings and generates a **stoichiometric matrix**. The elements of the matrix are the species population changes:

```
[reactions]
type = (
  H + e -> H+ + 2e,    # R1
  H+ + e -> H,          # R2
  He + e -> He+ + 2e,   # R3
  He+ + e -> He,        # R4
)
```

	R1	R2	R3	R4
H	-1	1	0	0
H ⁺	1	-1	0	0
He	0	0	-1	1
He ⁺	0	0	1	-1
e	1	-1	1	-1

Hermes-3 reactions settings. Corresponding stoichiometric matrix.

Reaction rate (K) and density source term (S) are

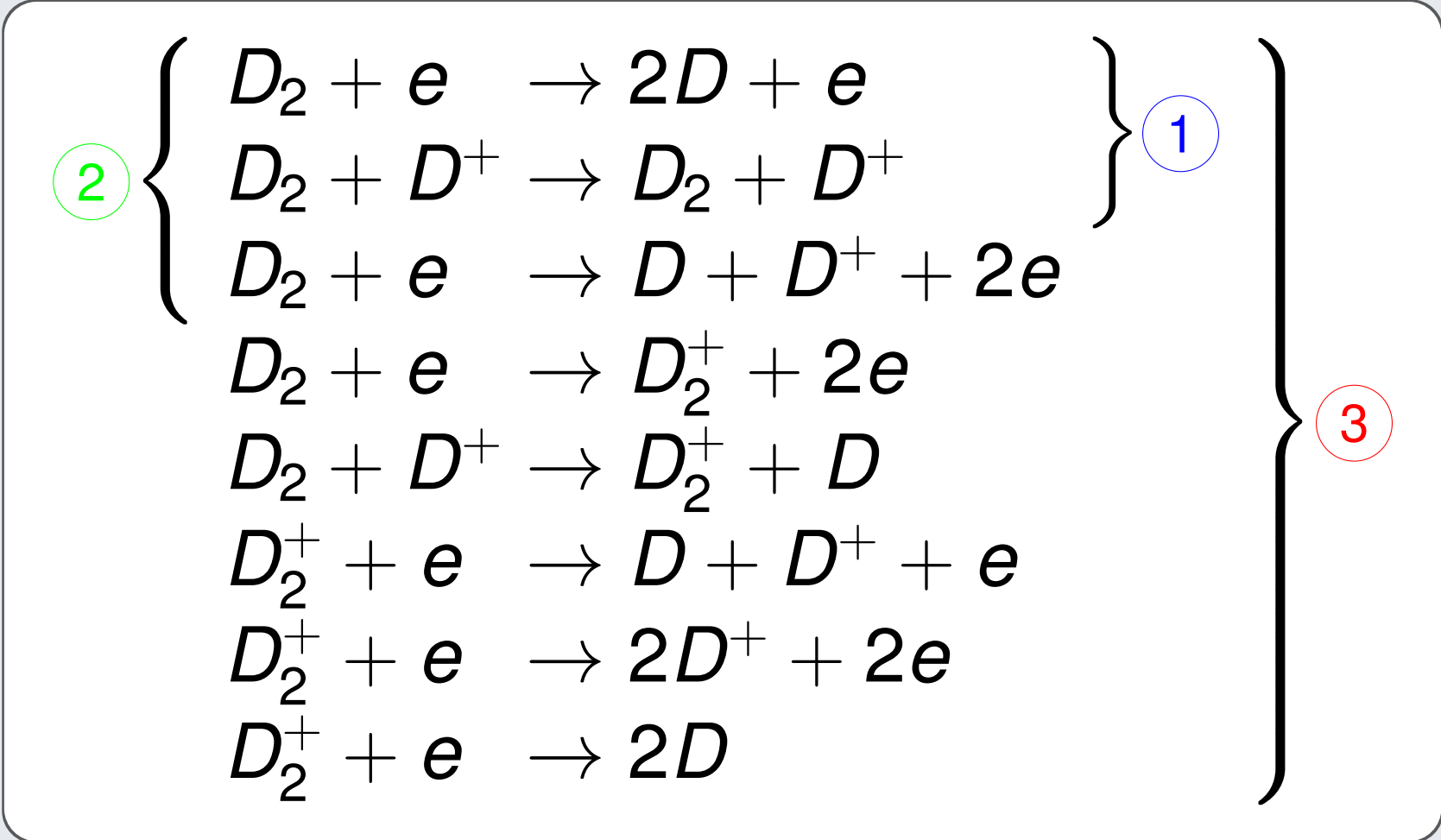
$$K = \prod_r n_r \langle \sigma v \rangle \quad C_s: \text{pop. change for species } s$$
$$S = C_s K \quad n_r: \text{density of reactant } r$$
$$\langle \sigma v \rangle: \text{reaction rate coefficient}$$

Momentum (F) and energy source terms depend on the sign of the stoichiometric coefficient. For momentum:

$$F = \begin{cases} C_s K (n v)_s & C_s < 0 \\ f_{nv,s} K \sum_{r'} -C_{r'} (n v)_{r'} & C_s > 0 \\ 0 & C_s = 0 \end{cases} \quad \begin{matrix} (n v)_s: \text{momentum of } s \\ f_{nv,s}: \text{momentum frac. transferred to } s \end{matrix}$$

The Kotov Mechanism

Atomic ionisation, recombination and charge exchange are included, together with the following molecular reactions:



- All rate coefficients are $\langle \sigma v \rangle(n, T)$ from AMJUEL [4]*.
- $D_2 + D^+ \rightarrow D_2 + D^+$ represents molecule-ion elastic collisions.

*N.B. The original Kotov (2008) mechanism uses atomic CX coefficients $\langle \sigma v \rangle(T)$ from HYDHEL [5].

Numerical Challenges

Runs with molecular chemistry initially proved problematic for solver numerics due to two related issues:

Issue	Excessively steep molecular density gradients near the target
Mitigation(s)	Neutral Parallel Diffusion included to soften density peaks. Low-density species boosted using pseudo-reactions. These add reaction-like sources that transfer particles from abundant species to depleted ones.
Issue	Highly supersonic neutral velocities
Mitigation(s)	Explicit neutral velocity limits applied based on the thermal speed.

Low-density sources conserve energy and momentum. Should they?

1D Test Setup

Initial tests with different combinations of species, reactions:

Label	D_2	D_2^+	Molecular reactions	Recycling
No molecules	N	N	None	$D^+ \rightarrow D$
Holm '22 "DEID" [1]	Y	N	1	$D^+, D \rightarrow D_2$
Kotov '08 (no D_2^+)	Y	N	2	$D^+ \rightarrow D_2$
Kotov '08 [3]	Y	Y	3	$D^+ \rightarrow D_2$

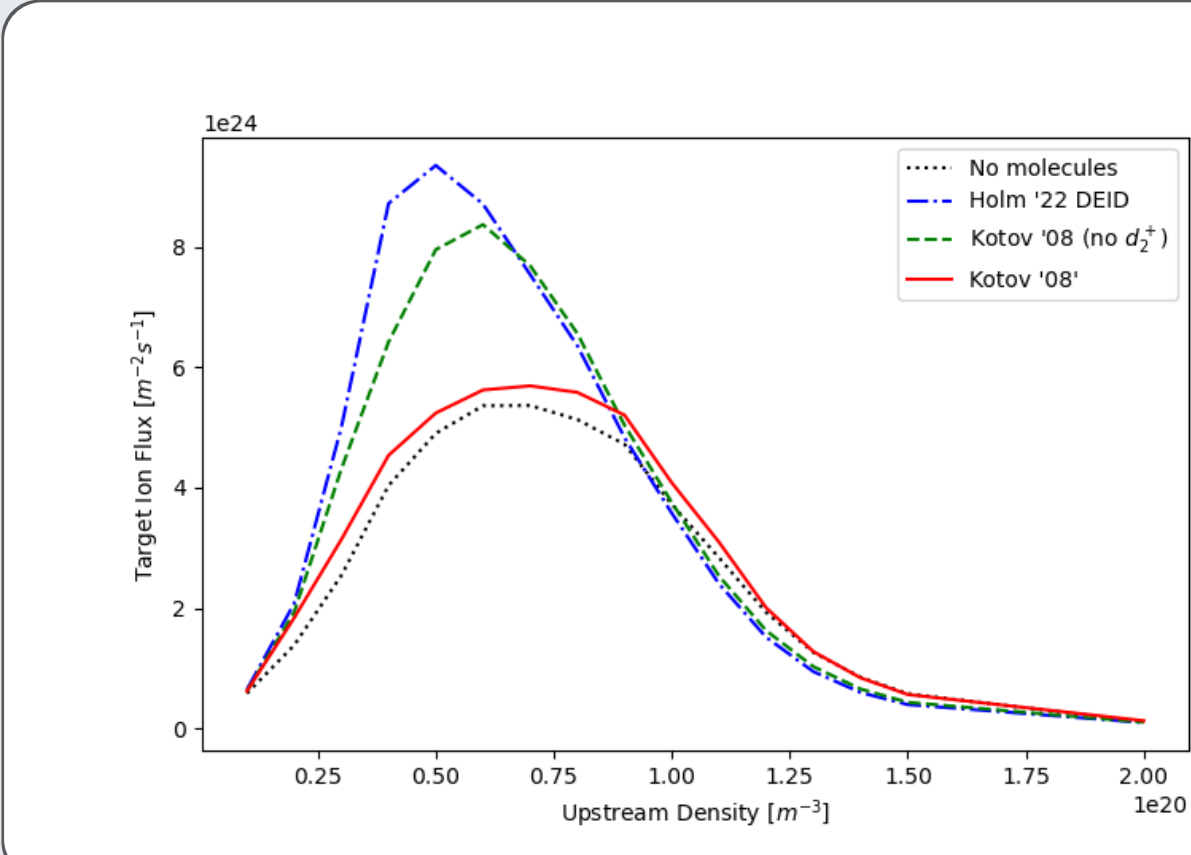
Common configuration:

- Evolve density, momentum, pressure for D^+ , D , D_2 , D_2^+ ; pressure for e .
- Midplane boundary conditions (BCs): reflective/no-flow.
- Target BCs: reflective for neutrals, molecules; sheath for ions.
- Electrons lose a (model-dependent) fixed energy per dissociative reaction.
- 100% recycling (one recycled D nucleus per incident nucleus).
- Low-n sources active below 10^{12} m^{-3} for D and 10^{11} m^{-3} for D_2 .

First 1D Results

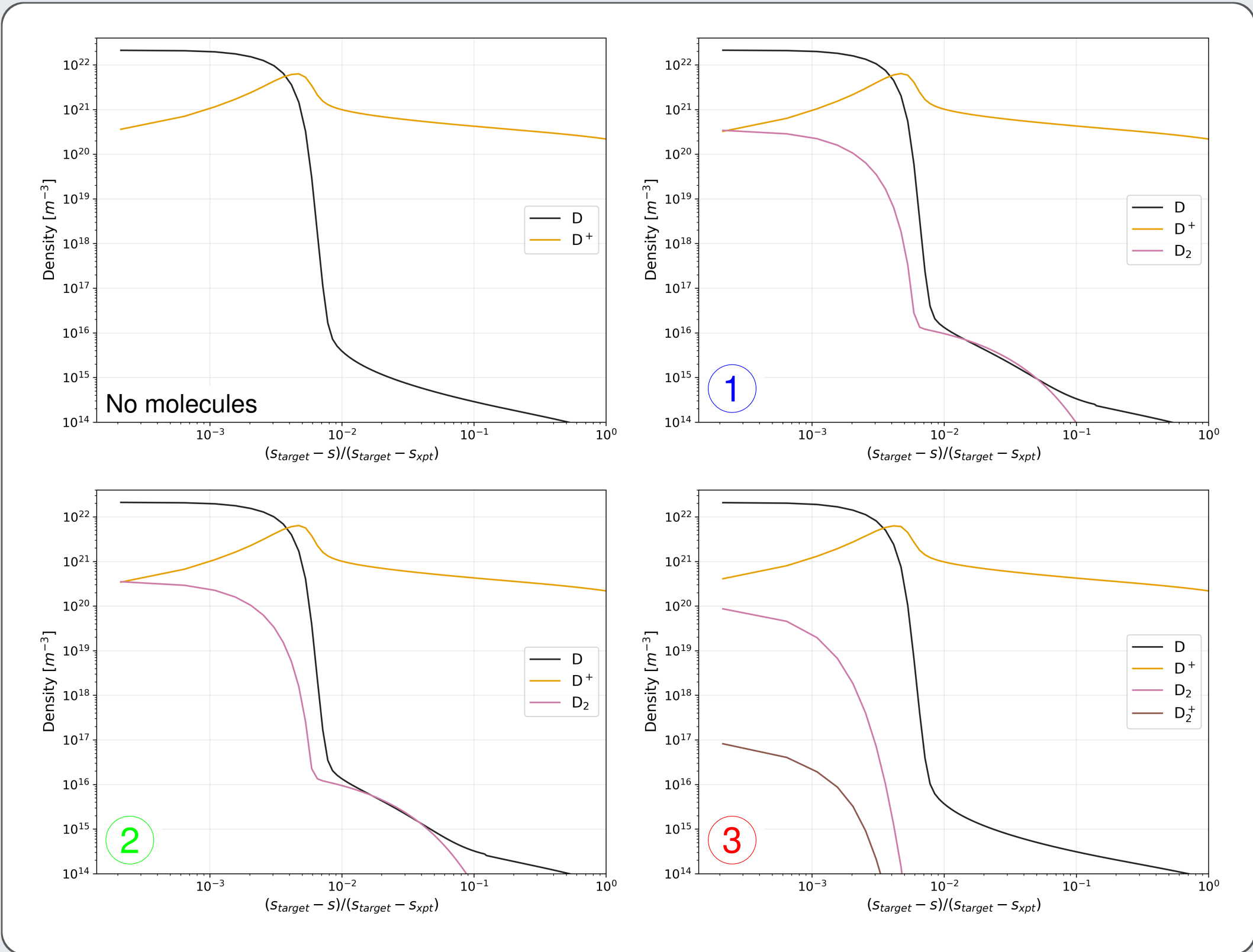
Rollover plots

- Look for detachment onset with rollover plots.
- Ion flux at the target turns over at a particular upstream ion density.
- Molecules are expected to affect the peak flux and rollover point.



Density profiles

- Steady state D^+ , D , D_2 , D_2^+ profiles at the highest upstream ion density:



- No model is molecule-dominated at the target, despite maximal recycling.

Next Steps

- Further testing and validation in 1D, 2D.
- Additional mechanisms, comparison to other molecular chemistry implementations, e.g. in SOLPS-ITER [3], SD1D [6], DIV1D [2].
- Comparison to MAST-U data.

[1] A Holm. *Thesis: Role of hydrogenic molecules in fusion-relevant divertor plasmas*. en. Aalto University, 2022. ISBN: 978-952-64-0890-3.

[2] S.P. Kobussen et al. "On the role of atomic momentum and molecules in self-consistent 1D scrape-off layer simulation of MAST-U, using DIV1D". In: *Nuclear Fusion* 65.8 (July 2025), p. 086027.

[3] V Kotov et al. "Numerical modelling of high density JET divertor plasma with the SOLPS4.2 (B2-EIRENE) code". In: *Plasma Physics and Controlled Fusion* 50.10 (Sept. 2008), p. 105012.

[4] Detlev Reiter et al. *AMJUEL: Additional atomic and molecular data for EIRENE*. 2026.

[5] Detlev Reiter and Ratko K. Janev. *The Data File HYDHEL: Atomic and Molecular Data for EIRENE*. Version: January 13, 2020. Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung. 2020.

[6] Y Zhou et al. "Investigation of the role of hydrogen molecules in 1D simulation of divertor detachment". en. In: *Plasma Physics and Controlled Fusion* 64.6 (May 2022), p. 065006. ISSN: 0741-3335.