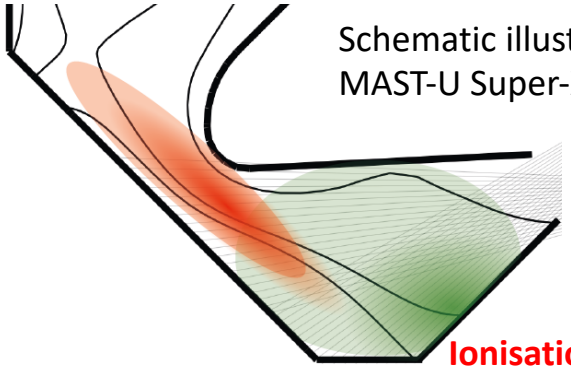
Conclusion

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

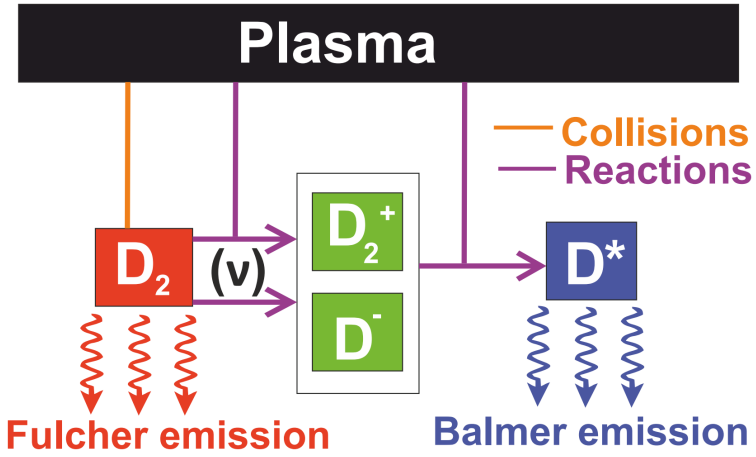
1. **Boosts D* emission ->** complications **diagnostic interpretation** & **control sensing capabilities**
2. **Drives dissociation (MAD) ->** increases **volumetric atom generation** & associated **power loss (20% of P_{SOL})**
3. **Ion sinks (MAR) -> induces particle flux reduction** at higher Te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