

Modelling of high density collisional sheath

D. Tskhakaya

Institute of Plasma Physics of the CAS, Prague, Czech Republic

Report for TSVV - 7

Proposed tasks (for 2022)

- The study of extremely high density DEMO (and ITER) relevant sheath, $\sim n_e > 5 \times 10^{21} \text{ m}^{-3}$
- Two sets of modelling: one with only D^+ , another with molecules included (D_2^{+i})

Completed tasks

- BIT1 updated; relevant for TSVV3, 4, 7 and WP-PWIE
- DEMO-relevant plasma sheath with only D^+

Ongoing tasks

- DEMO-relevant plasma sheath including molecules

Publications / Presentations

D. Tskhakaya, 12th International Conference on Atomic and Molecular Data and Their Applications (ICAMDATA), 25-29.09.2022, Mola di Bari, Italy.

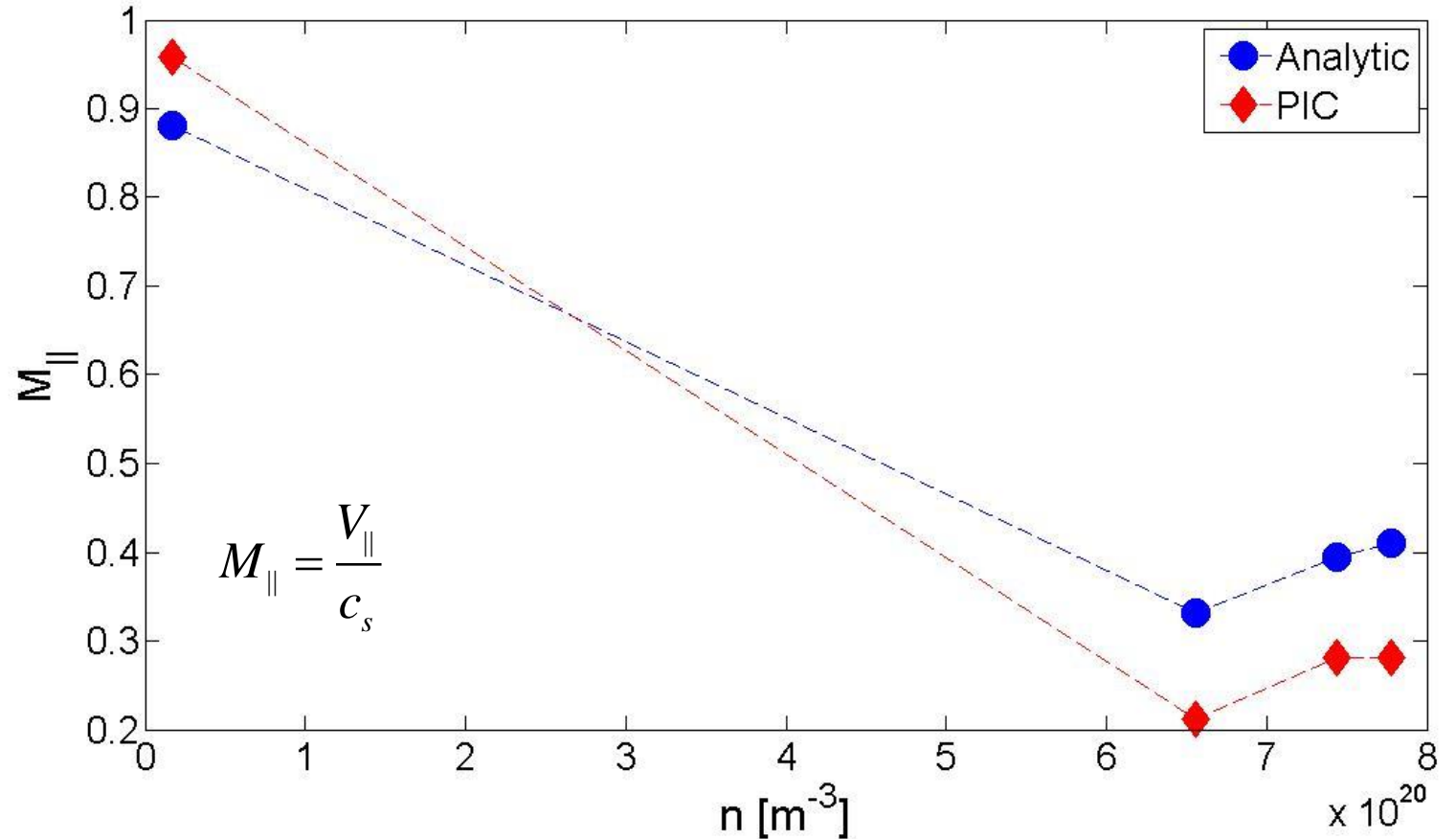
2 publications under preparation.

	Divertor sheath	
	n_{\max} [10^{20} m^{-3}]	T_{\min} [eV]
COMPASS	0.3	10
ASDEX-U	2	1
JET	5	1
ITER	50	0.3
EU DEMO	~100	0.2 (?)

Sheath edge:

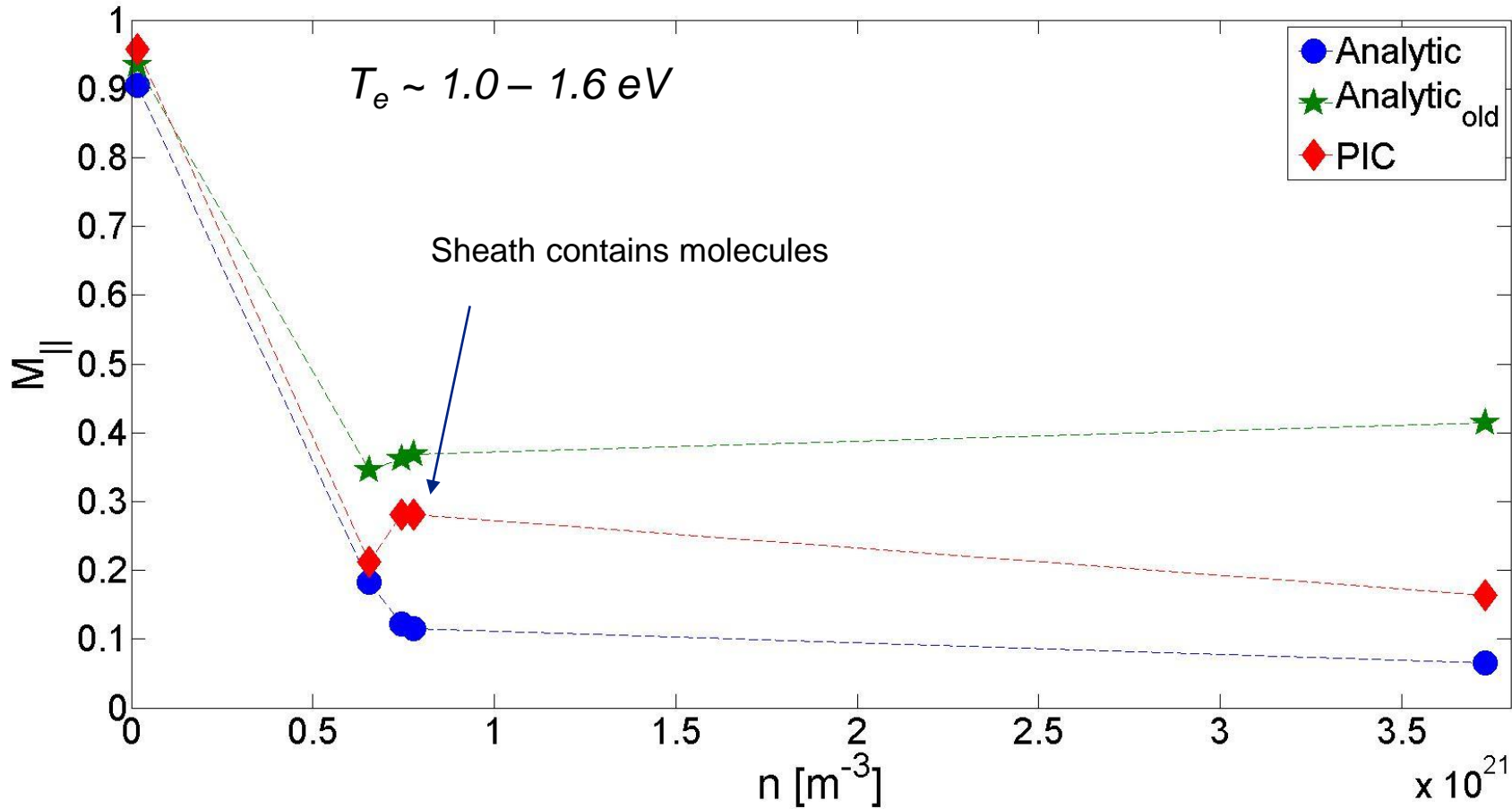
$$M_{\parallel} = 1 + \chi - \sqrt{\chi^2 + 2\chi} < 1$$

$$\chi = \frac{v_{mt}(1 - V_{\parallel}^n / V_{\parallel})}{2c_s \sin(\theta)} x_{wall}$$



From PIC modelling^[1] of the sheath

[1] Tskhakaya, 47th EPS 2021

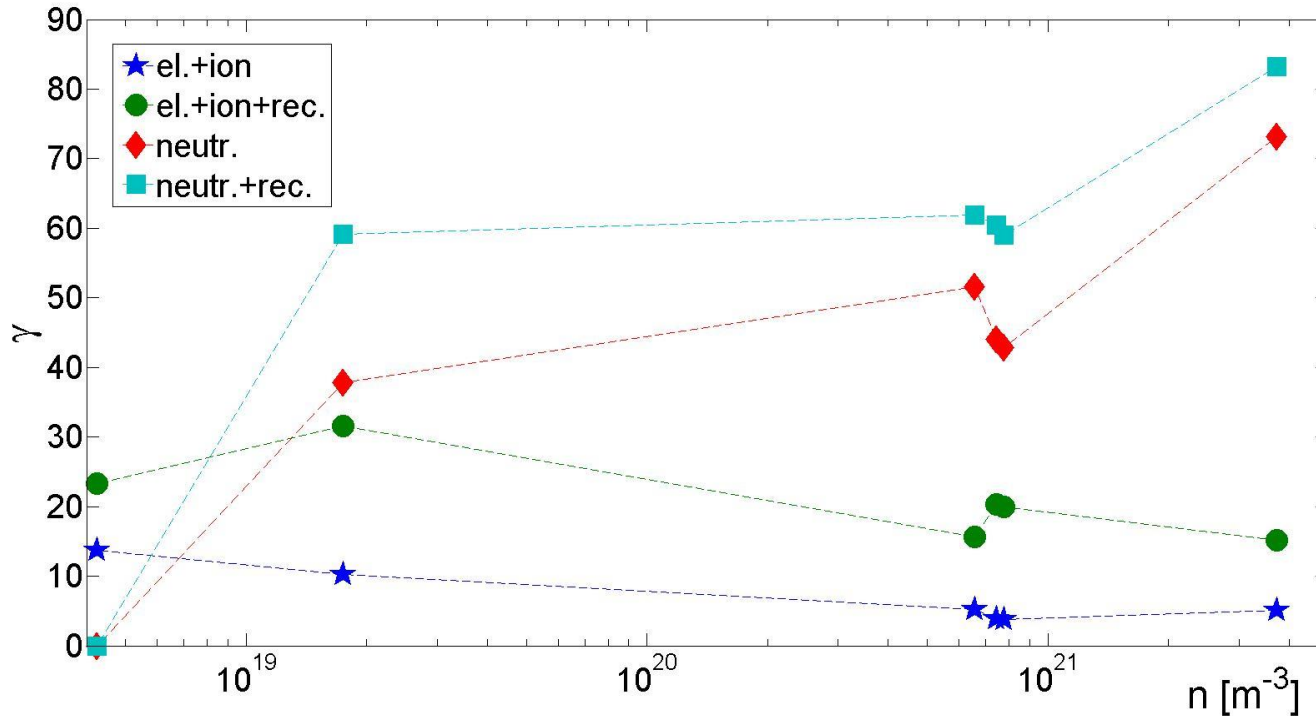


Sheath edge:

$$M_{\parallel} = 1 + \chi' - \sqrt{\chi'^2 + 2\chi'} < 1$$

$$\chi' = \frac{v_{mt}(1 - V_{\parallel}^n / V_{\parallel}) + v_{ei}}{2c_s \sin(\theta)} x_{wall}$$

What about divertor heat loads?



$$q_{wall} = \gamma M_{\parallel} n c_s T_e \sin(\theta)^{[2]}, \quad \gamma = \gamma_e + \gamma_i + \phi + \frac{\chi_i + \chi_m}{T_e}, \quad R_E = 0$$

$$\gamma_e = 2, \quad \gamma_i = 3(1 + 0.5T_i/T_e) \approx 3.5, \quad \phi \approx 2.9, \quad \chi_i = 13.6, \quad \chi_m \approx 2.2$$

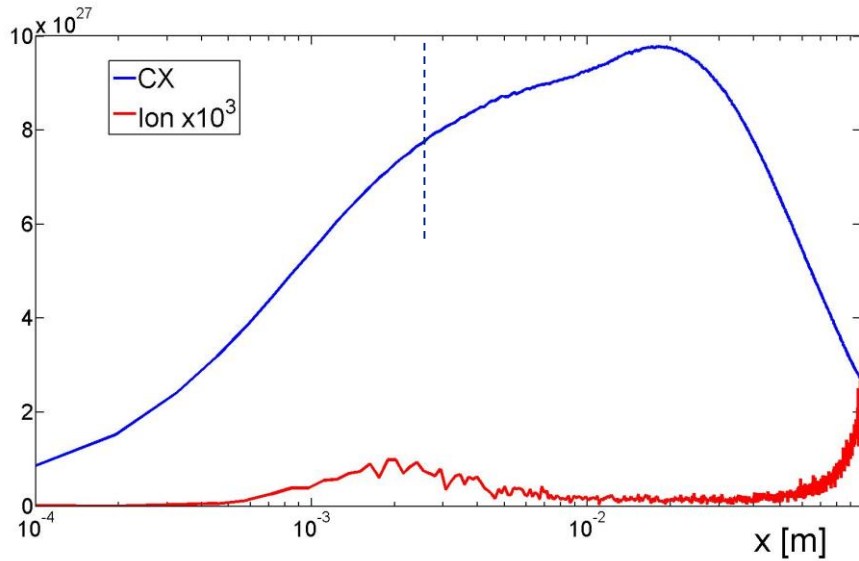
$$q_{wall} = \left(8.4 + \frac{15.8}{T_e} \right) J T_e, \quad \gamma_0 = 8.4, \quad J = M_{\parallel} n c_s \sin(\theta)$$

Contribution of neutrals

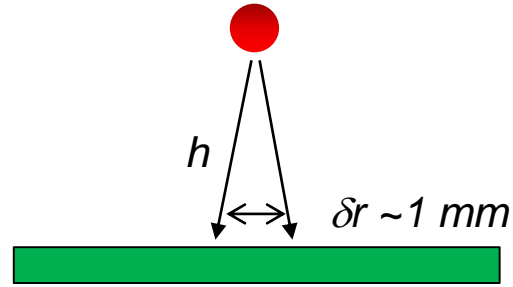
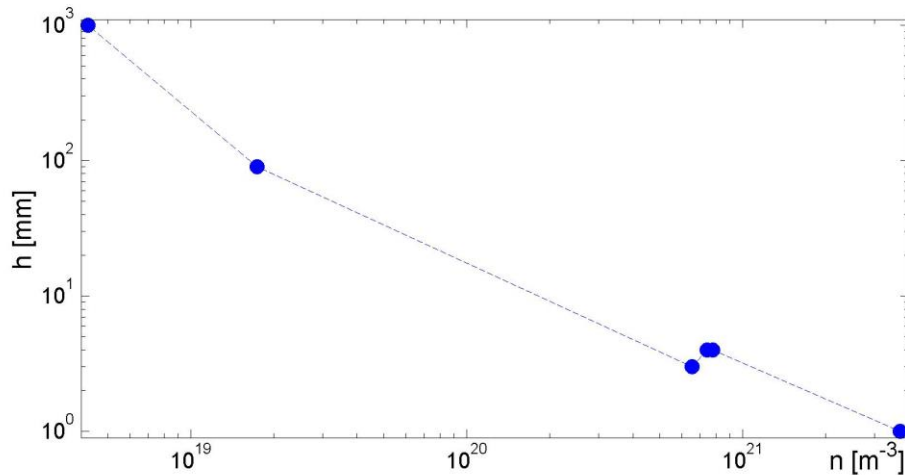


$$q_{wall} = \left(8.4 + \frac{15.8}{T_e} + \gamma_n \right) J T_e, \quad \gamma_n = \frac{q^n}{J T_e} + 2.2 \frac{F^n}{J T_e}$$

[2] P. Stangeby, book, sec. 5 (2000)

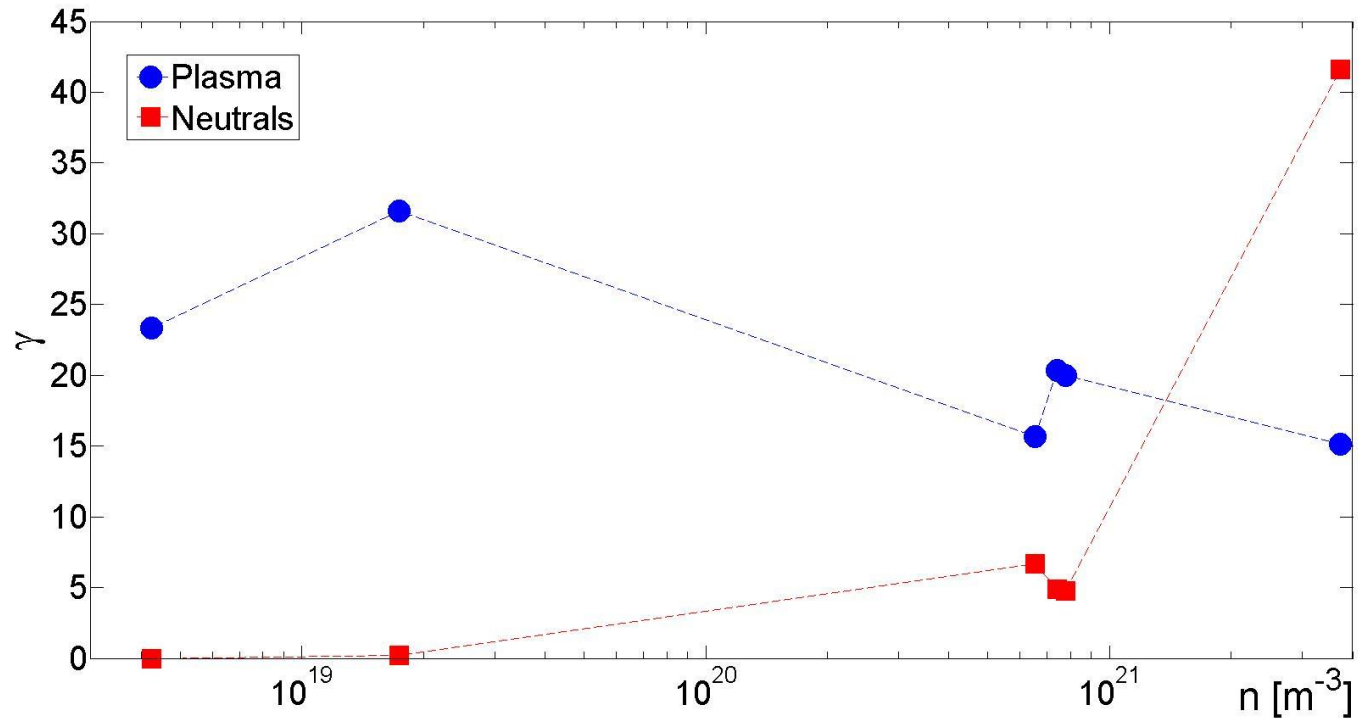


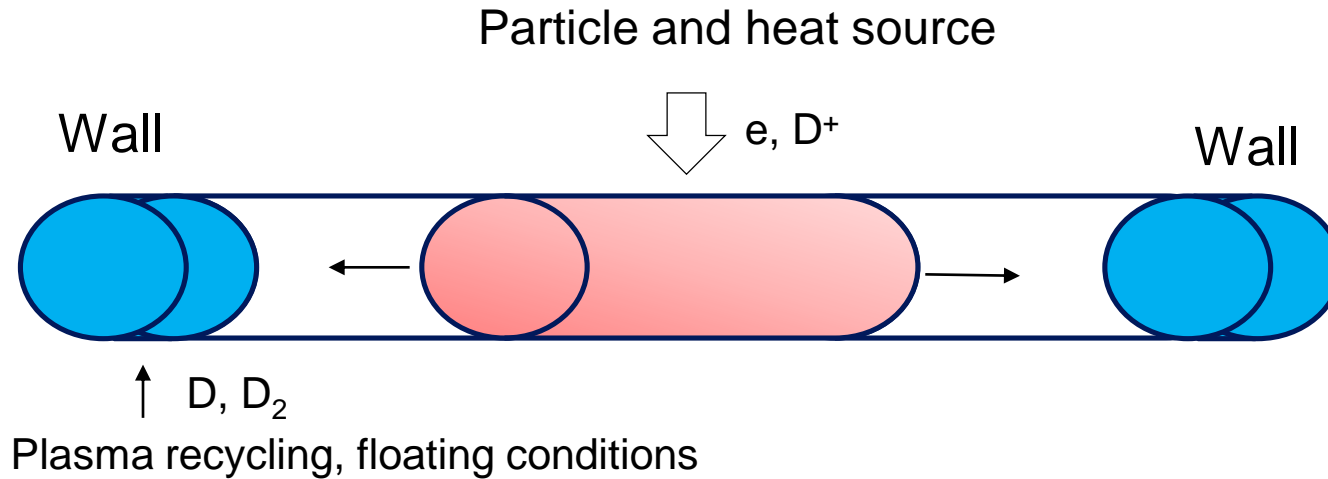
Profiles of CX and ionization collision events across the collisional sheath



$$\delta F = \frac{\arcsin(\delta r / h)}{\pi} F_0$$

In the DEMO divertor sheath the neutrals can be the main heat carriers





Each simulation takes up to 5 M core hours, 10^{10} particles, 10^6 (1D) spatial cells

Needs:

- to speed up the simulation (reduce memory usage)
- Incorporate multi-step atomic processes

Particle memory allocation in the original PIC code

Species 1

Species 2

⋮

Species N_{sp}

Memory is uniformly allocated for different particle species. **Simple implementation**, but can lead to significant fraction of **unused memory**.

Particle memory allocation in the updated PIC

Sp. 1

Species 2

⋮

Sp. N_{sp}

Allocated memory is **proportional** to the concentration of given particle species. **More optimized memory usage**, but requires **significant update** of the original code. 10% - 30% **faster** than the original code.

Dynamic memory allocation in **the future** code

Sp. 1

Species 2

⋮

Sp. N_{sp}

Time



Species. 1

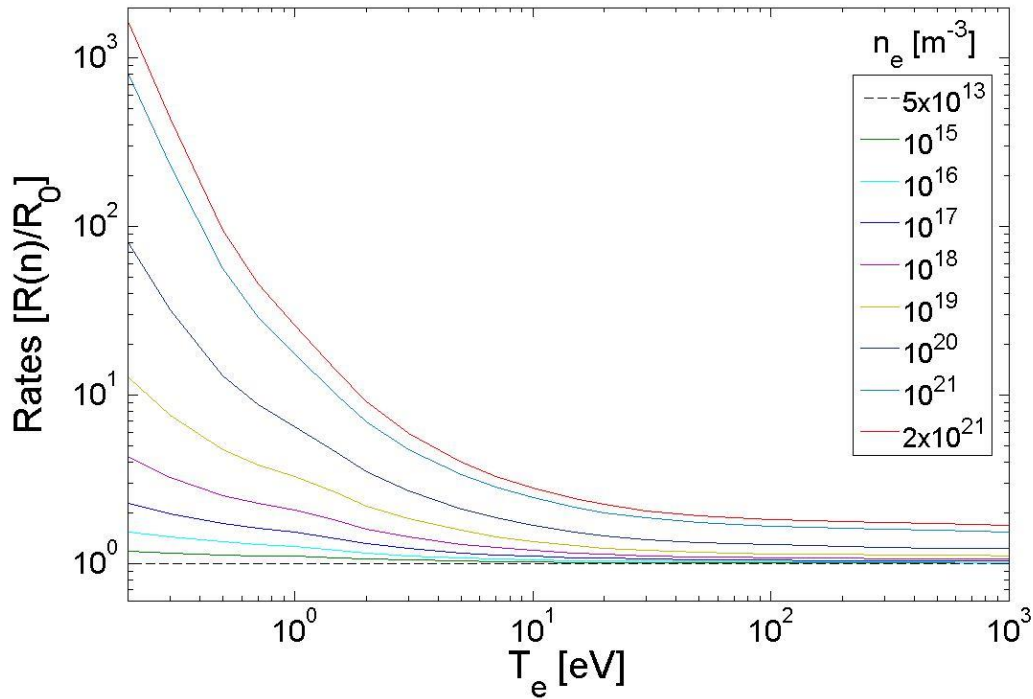
Sp. 2

⋮

Sp. N_{sp}

Species memory is allocated dynamically. **Fully optimized memory usage**. Requires **major update** of the code.

Update for exascale modelling



Normalized effective D ionization rate coefficients^[2].

Example from ADAS: $e + \text{Ne}^{+i} \rightarrow e + \text{Ne}^{+i}, (\nu)$

Target	states	Number of CS
Ne	89	$(N+3)N/2 = 4\,096$
Ne ⁺	279	39\,339
Ne ⁺²	554	154\,289
Ne ⁺³	668	224\,114
Ne ⁺⁴	564	159\,894
Total	2\,154	$\sim 5.8 \times 10^5$

„Dressed“ cross-section method

Kinetic collisional-radiative model?

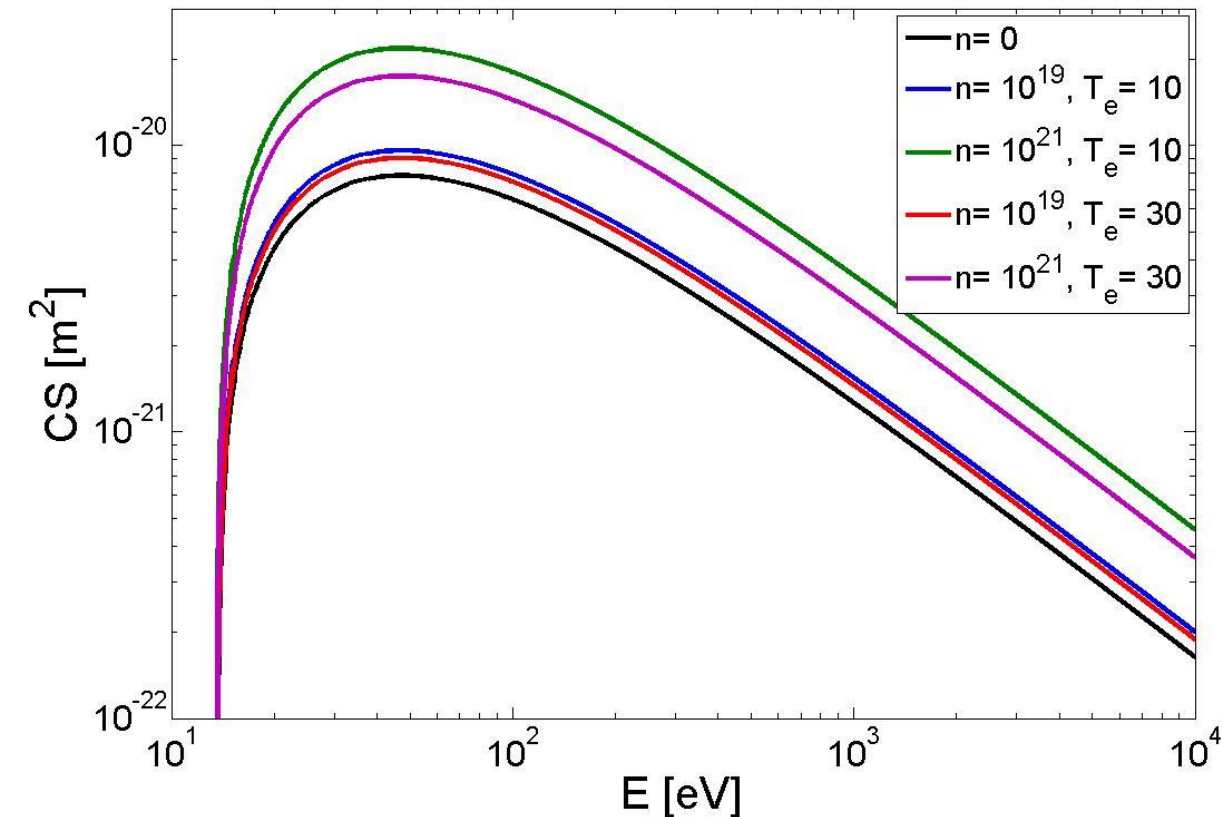
[2] <https://open.adas.ac.uk/>

$$\sigma(E, T, n) = \sigma(E) \frac{R(T, n)}{R_{n=0}(T)}$$



$$\int f_m V \sigma(E, T, n) d\vec{V} = R(T, n)$$

$$\sigma(E, T, n \rightarrow 0) = \sigma_{n=0}(E)$$

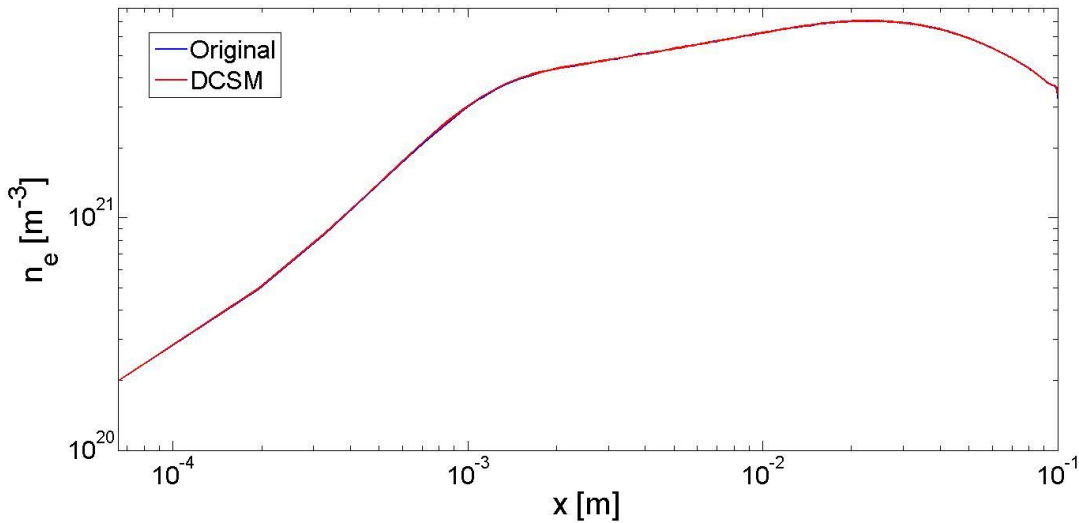
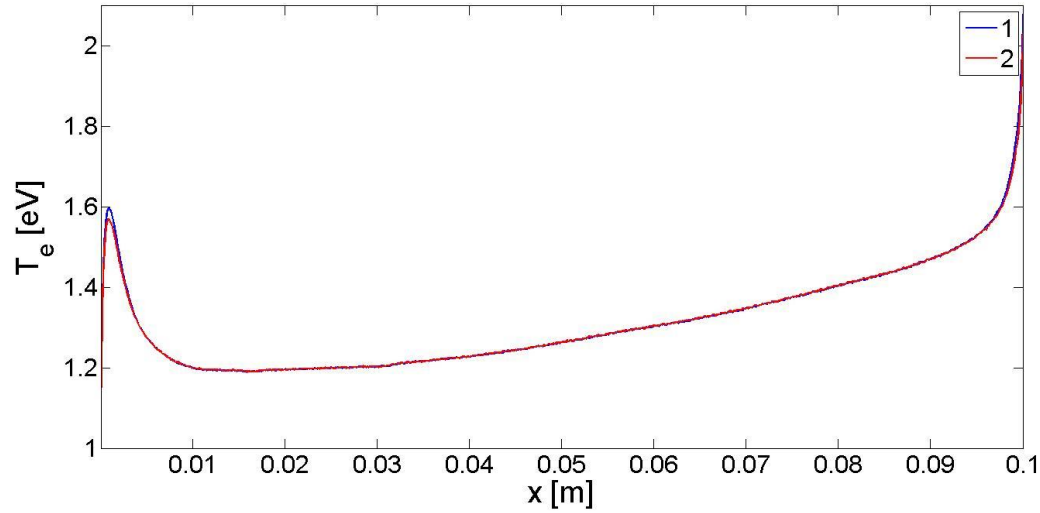


Advantage

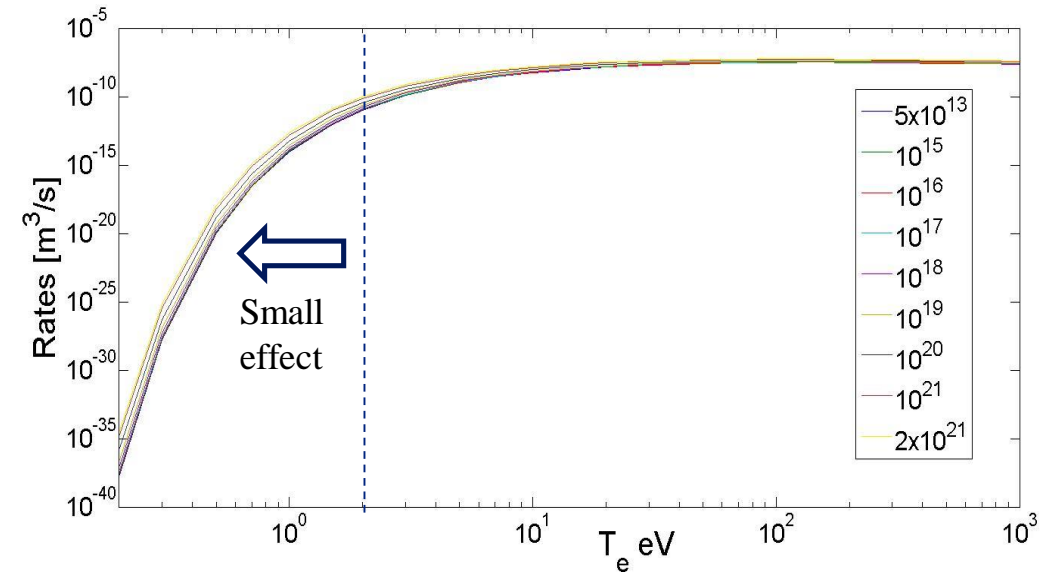
- i. large number of interaction channels are effectively incorporated
- ii. cross-sections and rate coefficients are available

Disadvantage

- i. needs calculation of temperature → reduction of the run speed (<10%)
- ii. Threshold energies E_{th} are density and temperature independent
- iii. EDFs assumed to be near-Maxwellian



Plasma density and temperature in the DEMO-relevant plasma sheath^[4]



Low ionization rate for < 2 eV plasma

[4] D. Tskhakaya, ICAMDATA 2022