Water you waiting for? - A Complete and Consistent Set of Electron-H_2O Collision Cross Sections for Plasma Modelling

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1. Introduction

Water is an omnipresent impurity in electric discharges where H_2O molecules interact with free electrons e^-. The characterisation of the e^- kinetics by the electron energy distribution function (EEDF) requires a complete and consistent set of electron collision cross sections (CSs). By the e^- swarm method, such a set is derived that considers the anisotropy of the rotational scattering through individual differential, integral and momentum transfer cross sections (DCSs, ICSs and MTCSs, respectively) based on the Born approximation [1, 2]. Assuming isotropic scattering simplifies the proposed set, allows for its application in freely accessible space-homogeneous codes and still yields better agreement with experiments compared to other established CS sets.

$$\mathrm{DCS}_i(\varepsilon,\theta) = \sqrt{\frac{\varepsilon'}{\varepsilon}}\frac{4D^2}{6(2J'+1)}\frac{S_i}{\varepsilon'+\varepsilon-2\sqrt{\varepsilon'\varepsilon}\cos\theta} \quad \text{such that} \quad \mathrm{ICS}_i(\varepsilon) = 2\pi\int_0^\pi \mathrm{DCS}_i(\varepsilon,\theta)\sin\theta\mathrm{d}\theta \quad \text{and} \quad \mathrm{MTCS}_i(\varepsilon) = 2\pi\int_0^\pi \mathrm{DCS}_i(\varepsilon,\theta)(1-\cos\theta)\sin\theta\mathrm{d}\theta$$

2. Cross Section Set

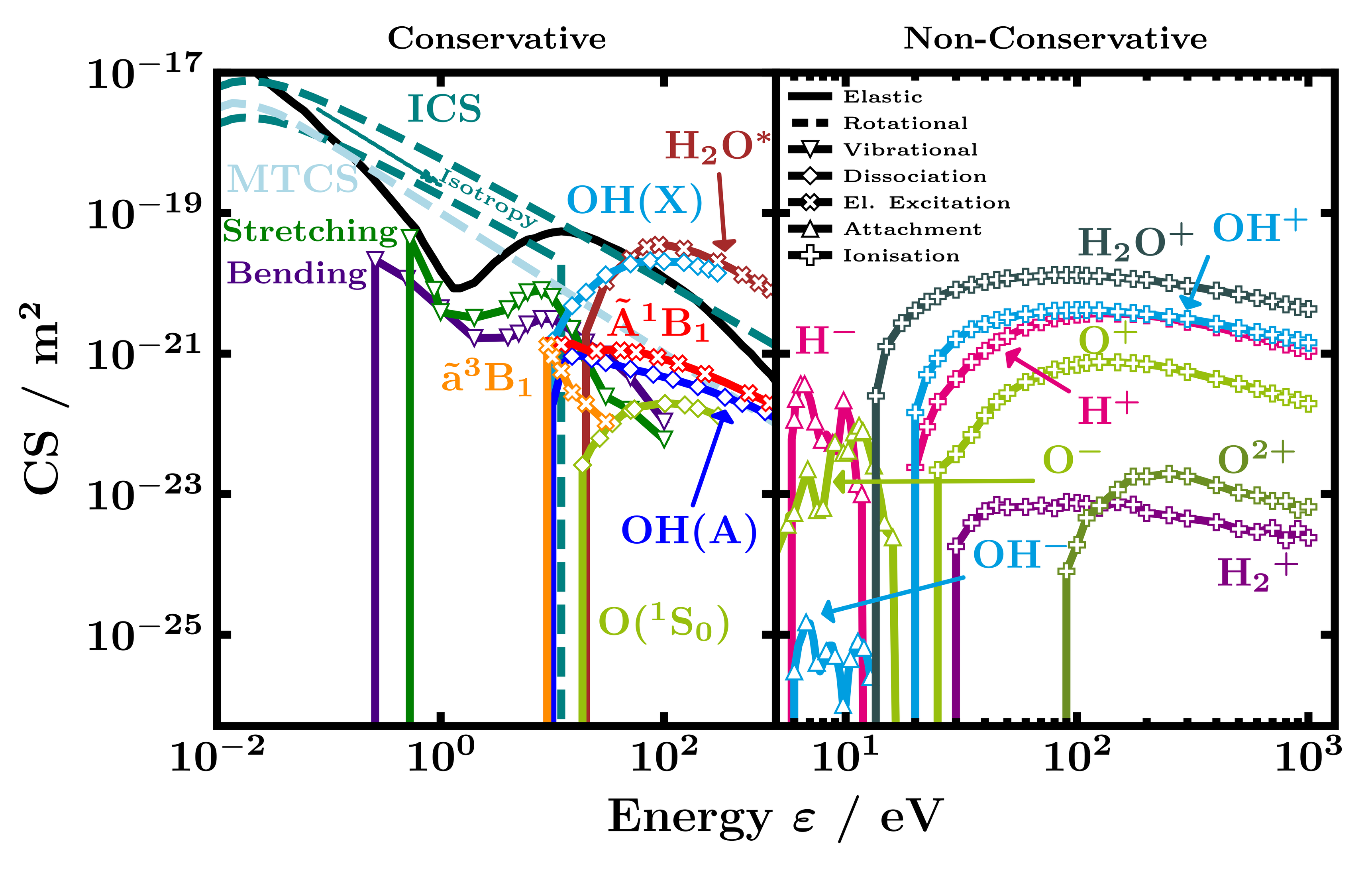

Fig. 1: Proposed complete and consistent electron collision cross section set for water molecules divided in conservative (number of electrons is constant) and non-conservative (ionisation and attachment) collisions. When assuming isotropy, the rotational ICSs and MTCSs are adjusted or discarded, respectively [3].

3. Validation

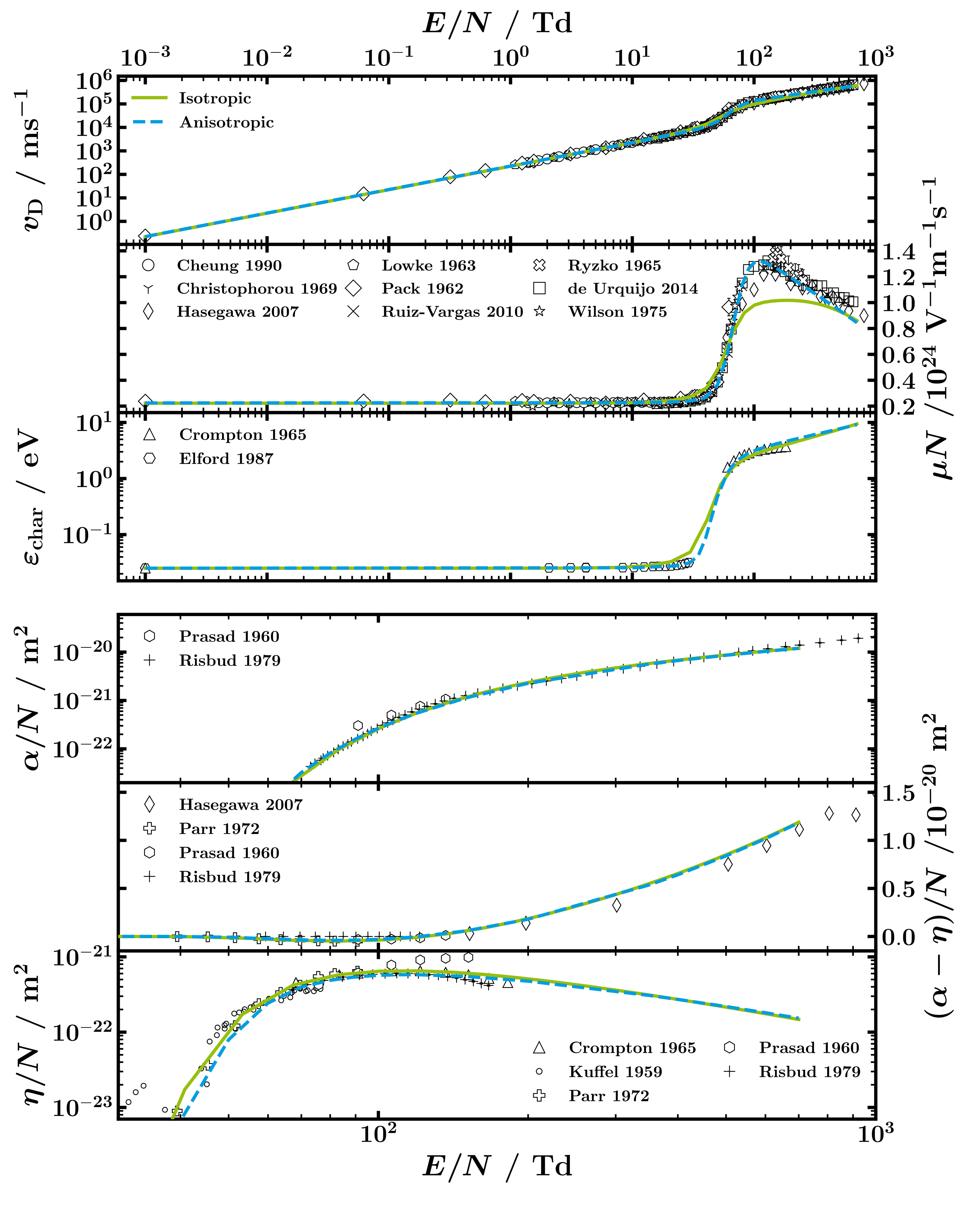

Fig. 2: Comparison of experimental electron swarm parameters - from top to bottom: drift velocity, red. mobility, char. energy, red. Townsend coef., red. eff. Townsend coef. and red. attachment coef. - with LoKI-B [4] results either assuming isotropy or including anisotropy vs. the red. el. field E/N.

4. Applicability

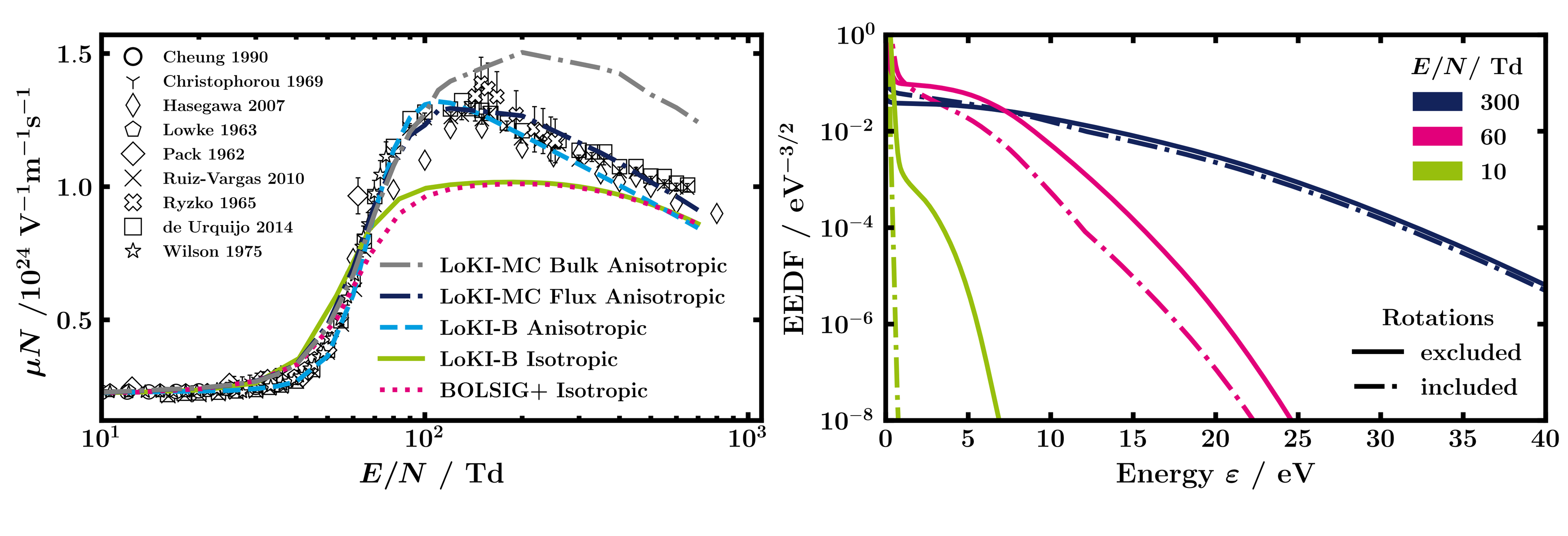

Fig. 3: Agreement of two-term solvers LoKI-B and BOLSIG+ [5] as well as Monte Carlo code LoKI-MC [6] shown by means of the red. mobility (left), EEDFs at representative E/N with and without included rotations (right).

5. Conclusion

- Proposition of complete and consistent set of electron CSs for H_2O
- Simplification by assuming isotropy allows for wide-spread applicability
- Inclusion of anisotropy improves results (even beyond two-term solvers)
- Release of both sets in the IST-LISBON database on LXCat [7]

6. Literature

1. Y. Itikawa, *J. Phys. Soc. Jpn.* **32**, 217–226 (1972).
2. L. Vialetto *et al.*, *Plasma Sources Sci. Technol.* (2021).
3. M. Budde *et al.*, *J. Phys. D: Appl. Phys.* **55**, 445205 (2022).
4. A. Tejero-del-Caz *et al.*, *Plasma Sources Sci. Technol.* **28**, 043001 (2019).
5. G. J. M. Hagelaar *et al.*, *Plasma Sources Sci. Technol.* **14**, 722–733 (2005).
6. T. C. Dias *et al.*, *Comput. Phys. Commun.*, Accepted (2022).
7. L. L. Alves, *J. Phys.: Conf. Ser.* **565**, 012007 (2014).

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