The LisbOn KInetics Boltzmann solver

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This work presents the LisbOn KInetics Boltzmann solver (LoKI-B), a simulation tool to model non-equilibrium low-temperature plasmas, produced from different gas mixtures for a wide range of working conditions. LoKI-B (to become open-source) provides the solution to the homogeneous and stationary two-term electron Boltzmann equation including: first and second-kind collisions, electron-electron collisions and spatial or temporal electron density growth models to account for the production of secondary electrons born in ionisation events. On output, it yields the electron energy distribution function and different electron macroscopic parameters. The tool can handle simulations for any gas mixture, accounting for the electronic, vibrational and rotational internal degrees of freedom of the atomic / molecular excited states present in the plasma.

Introduction

Predictive tools for non-equilibrium low-temperature plasmas (LTPs) should properly describe the kinetics of electrons, which are responsible for inducing plasma reactivity. A microscopic description of the electron kinetics provides essential information for global / fluid models, such as electron impact rate coefficients and macroscopic electron transport parameters. It also provides the power transferred from the electric field to the different electron collisional channels.

Here, we focus on plasma-based environmental and biological applications, which have recently attracted the interest of pure and applied research. In this context, we have launched a research project for delivering a KInetic Testbed for PLASMa Environmental and Biological Applications (KIT-PLASMEBA) [1] that includes a simulation tool, the LisbOn KInetics (LoKI), with a Boltzmann solver (LoKI-B).

Code implementation

LoKI-B is a simulation tool, developed under MATLAB® with an object-oriented design, that describes the electron kinetics by solving the homogeneous and stationary electron Boltzmann equation under the classical two-term approximation, for continuous (DC) or high-frequency (HF) applied electric fields. It includes:

- inelastic direct/stepwise and superelastic collisions with all types of excited states (electronic, vibrational and rotational), with distributions defined in a proper and user-friendly way;
- the continuous approximation for rotations with a Chapman-Cowling corrective term, simplifying the handling of rotational inelastic/superelastic collisions for some gases [2];
- secondary electrons born in ionization events, allowing for an electron density spatial or temporal growth, with an energy sharing described by a single differential cross section or taken in one of the limiting cases “equal energy sharing” or “no energy sharing”;
- electron-electron collisions (impact upon the isotropic part only).

LoKI-B users must provide information about: the working conditions, the electron scattering cross sections (directly obtainable from the open-access platform LXCat [3]), some atomic and molecular data, and the populations of the different excited states present in the gas mixture. On output, LoKI-B yields: the electron energy distribution function (EEDF) and the corresponding first anisotropy, the electron macroscopic quantities (rate coefficients and transport parameters) and a detailed description of the power density transferred to the different electron collisional channels. Alternatively, LoKI-B can

consider a generalized prescribed EEDF, ranging in the limits of the Maxwellian and the Druyvestyen EEDFs, in order to evaluate electron macroscopic quantities.

The development team of LoKI-B is currently engaging verification and validation (V&V) procedures, to ensure the quality of the tool and the results it provides, before its public release (late 2018) as an open-source tool. LoKI-B can be used as a standalone tool, but it can also be easily coupled, due to its open-source nature, to macroscopic global / fluid models (subject of a companion contribution [4]).

Results

We show examples of some results obtained with LoKI-B during its V&V. In Fig. 1 we compare the values of the reduced mobility obtained with LoKI-B, against the values provided by BOLSIG+(03/2016) [5] and obtained from experiment. For both tools we used the same complete set of Helium cross section, obtained from the IST-Lisbon database on LXCat [6]. In Fig. 2 we show an analogous comparison for a rather more complex simulation, in dry air (a mixture of Nitrogen (80%) and Oxygen (20%)), taking into account the rotational distributions of both gases. A very good agreement is found between the different simulations and the experimental results.

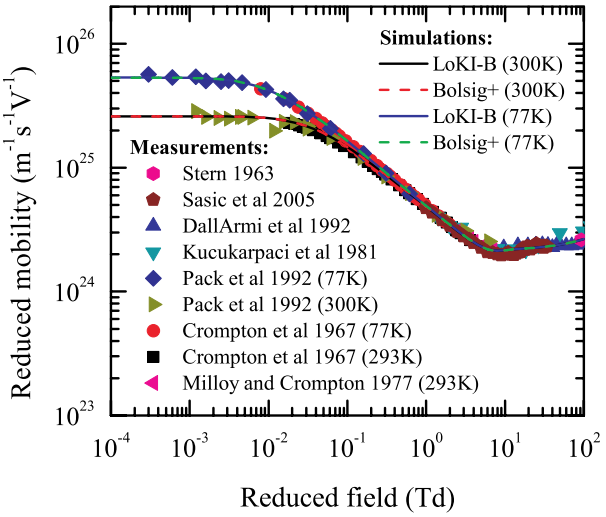

Fig. 1: Comparison of reduced mobility for He

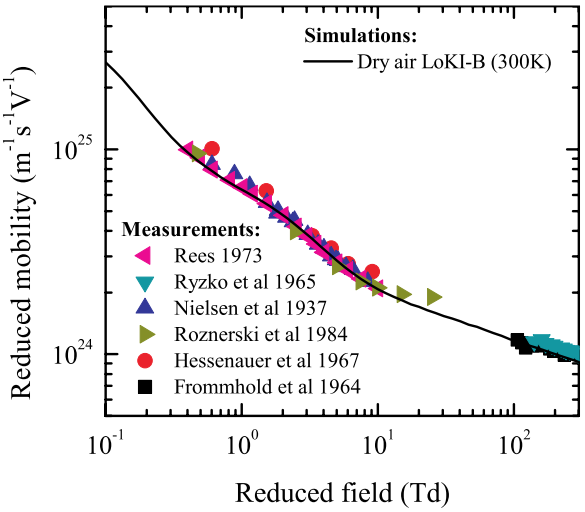

Fig. 2: Comparison of reduced mobility for dry air

Conclusion

LoKI-B is a user-friendly, scalable and upgradable open-source tool, that enables researchers to easily study the electron kinetics for any gas mixture. This work discussed its current status of development, presenting the basic structure, evidencing the functionality and introducing test cases along with first results of benchmarking. The development of LoKI-B will continue focusing on its graphical user interface and the introduction of V&V procedures. The tool will be publicly released by the end of 2018.

Acknowledgments

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