Development of the LisbOn KInetics (LoKI) tool

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This work presents the current status of development of LisbOn KInetics (LoKI), a computational tool to model non-equilibrium low-temperature plasmas, produced from different gas mixtures for a wide range of working conditions. LoKI comprises a Boltzmann module (LoKI-B) and a chemistry module (LoKI-C), coupled in a self-consistent way, yielding the electron energy distribution function, the electron swarm parameters, the concentrations of the various plasma species, and the corresponding gain/loss reaction rates. The tool can handle simulations including any gas mixture, accounting for the electronic, vibrational and rotational internal degrees of freedom of the atomic / molecular excited states present in the discharge.

1. Introduction

Predictability in plasma science and engineering based on fundamental modelling has been considered a requirement for the progress in the field, and the model-based design of plasma processes has been identified as a necessary capability to achieve industrial goals. Therefore, there is general agreement on the intellectual and technological importance of modelling low-temperature plasmas (LTPs).

Predictive tools for non-equilibrium LTPs should describe the kinetics of both electrons and heavy-species, the former responsible for inducing plasma reactivity and the latter providing the paths for industrial applications. 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), embodying a MATLAB® computational tool (LisbOn KInetics, LoKI) linked to a web-platform (KIT) containing state-of-the-art kinetic schemes.

2. Code implementation

LoKI comprises two modules (LoKI-B and LoKI-C) that can run self-consistently coupled or as standalone tools. The foundations for developing this tool were stablished years ago [1]. LoKI-B (to become open-source) provides the solution to the homogeneous two-term electron Boltzmann equation [2] (for a pure gas or a gas mixture, including first and second-kind collisions, as well as electron-electron collisions), using the LXCat open-access website [3] for obtaining electron scattering cross section data; LoKI-C gives the solution to the system of zero-dimensional (volume average) rate balance equations for the most relevant charged and neutral species in the plasma. The simulations can include any gas mixture, accounting for the electronic, vibrational and rotational internal degrees of freedom of the atomic / molecular excited states present in the discharge. On output, LoKI yields the electron energy distribution function, the electron swarm parameters, the concentrations of the various plasma species, and the corresponding gain/loss reaction rates.

The results are obtained either for a prescribed constant pressure, ensured by varying the gaseous mixture composition, or at fixed mass density. For stationary discharges, the reduced maintenance electric field is self-consistently calculated as an eigenvalue solution to the problem, under the assumption of quasi-neutrality.

3. Discussion and conclusions

LoKI is a user-friendly, scalable and upgradable tool. This work discusses its current status of development, presenting basic structure, evidencing functionality and introducing test cases along with first results of benchmarking against other codes. LoKI development will continue focusing on its graphical user interface and on the introduction of verification and validation procedures.

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5. References

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