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The LisbOn KInetics tool suit

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This work presents the LisbOn KInetics (LoKI) tool suit, a set of simulation tools to model non-equilibrium low-temperature plasmas, produced from different gas mixtures for a wide range of working conditions. LoKI comprises two modules: a Boltzmann solver, LoKI-B (to become open-source), and a chemistry solver, LoKI-C. Both modules can run as standalone tools or coupled in a self-consistent manner. LoKI-B provides the solution to the homogeneous and stationary two-term electron Boltzmann equation, while LoKI-C solves the system zero-dimensional rate balance equations for the most relevant charged and neutral species in the plasma. When coupled, 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.

Introduction

Predictive tools for non-equilibrium low-temperature plasmas (LTPs) should properly describe the kinetics of both electrons and heavy-species, the former responsible for inducing plasma reactivity and the latter providing the paths for reaction mechanisms. 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, LisbOn KInetics (LoKI), linked to a web-platform (KIT) containing state-of-the-art kinetic schemes.

Code implementation

LoKI is a simulation tool, developed under MATLAB® with an object-oriented design. It comprises two modules, a Boltzman solver, LoKI-B (the subject of a companion contribution [2]), and a chemistry solver, LoKI-C, that can run self-consistently coupled or as standalone tools. In Fig. 1 we can see the workflow when one or both modules are activated. LoKI-B (to become open-source) solves the electron kinetics [2], 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 heavy species, charged and neutral, present in the plasma, using the ode15s time-dependent MATLAB® solver for stiff differential equations. The simulations can include any gas mixture, accounting for the electronic, vibrational and rotational internal degrees of freedom of the atomic / molecular excited states. For stationary discharges, when both modules are activated, the reduced maintenance electric field (or an equivalent parameter, such as

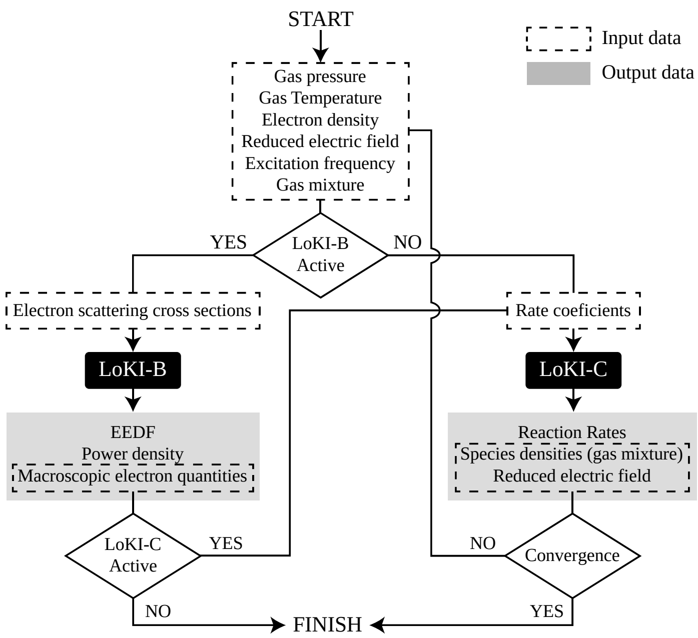

Fig. 1: LoKI workflow when one or both of its modules are active

the electron temperature) is self-consistently calculated as an eigenvalue solution to the problem, under the assumption of quasi-neutrality [4].

The development team of LoKI is currently engaging verification and validation (V&V) procedures, to ensure the quality of the tool and the results it provides.

Results

We show the results of a set of simulations for a pure oxygen DC discharge, obtained using the reaction mechanism presented in [4] with both LoKI modules self-consistently coupled. The simulations where performed for an infinitely long tube of radius 1 cm, pressures varying in the range of 0.1-10 Torr, a gas temperature of 300 K and an electron density of 1.7×10^{16} m^{-3}. In Fig. 1 we show the discharge characteristic, corresponding to the plot of the maintenance reduced electric field, *E/N*, versus the product of the pressure, *p*, and the tube radius, *R*. In Fig. 2 we show the evolution of the densities of some representative species, relative to the gas density, as a function of *pR*.

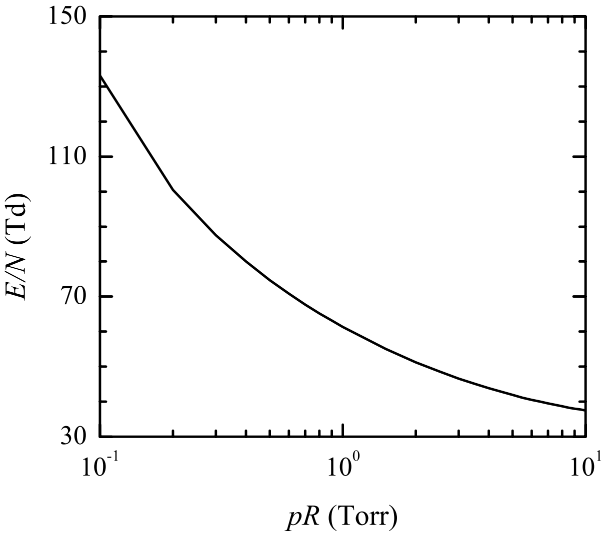

Fig. 1: Discharge characteristic for a DC oxygen plasma

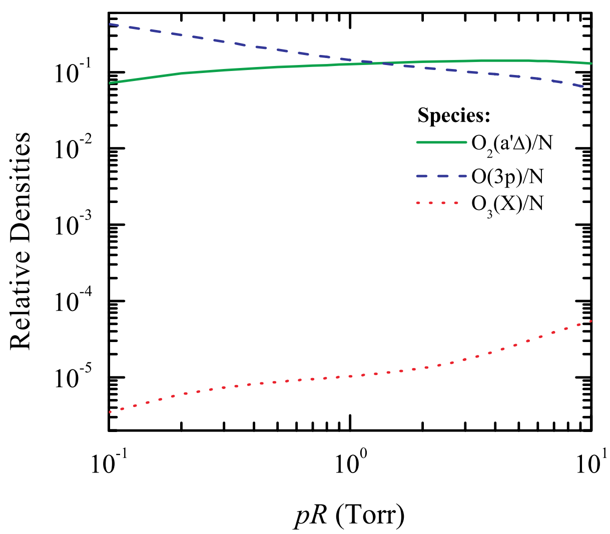

Fig. 2: Relative densities of some representative species

Conclusion

LoKI is a user-friendly, scalable and upgradable tool suit. It enables the user to easily couple a global model, with the possibility of including transport losses for neutrals and/or charged particles, along with a detailed description of the electron kinetics. This work discussed its current status of development, presenting the basic structure, evidencing the functionality and displaying first results. The development of the LoKI tool suit will continue, focusing on its graphical user interface and on the introduction of V&V procedures.

Acknowledgments

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