Updates on the LisbOn KInetics tool suite

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This work presents the latest evolutions of the LisbOn KInetics (LoKI) tool suite, for the modeling of non-equilibrium low-temperature plasmas, produced from different gas mixtures for a wide range of working conditions. LoKI comprises two modules: LoKI-B (open-source), that provides the solution to the two-term electron Boltzmann equation, and LoKI-C, that solves the system of zero-dimensional rate balance equations for the most relevant plasma species. When coupled, the reduced maintenance electric field is self-consistently calculated, under the assumption of quasi-neutrality. LoKI-C now includes the possibility of coupling the particle rate balance equations to the gas thermal balance equation, as well as to a mesoscopic surface kinetic model.

Introduction

With the advent of powerful hardware and readily available software, computer simulations have become almost indispensable in all fields of research. Low-Temperature Plasma (LTP) physics is no different, and we can find codes with approaches ranging from first-principles to model-based, running on multi-node clusters or mobile hardware.

Global models [1] represent a simple yet powerful tool that allows the study of LTPs. Among the advantages of global models, we can highlight the relative simplicity of implementation and fast run times, as well as the availability of ready-to-use software (sometimes even open-source). These advantages allow: i) using available tools by non-expert modelers to straighforwardly obtain computational results that give useful insight on the plasma behavior, or to backup experimental data; ii) using highly optimized codes by expert modelers to explore plasma chemistry in complex gas mixtures, studying the reaction pathways and their interplay in state-to-state simulations, accounting for thousands of reactions.

In this context, we started years ago the development of a set of simulation tools addressing quick and simple simulations for large and complex plasma systems: the LisbOn KInetics (LoKI) tool suite, comprising a Boltzmann solver (LoKI-B) [2, 3, 4] and a chemistry solver (LoKI-C) that can run self-consistently coupled or as standalone tools (see Fig. 1).

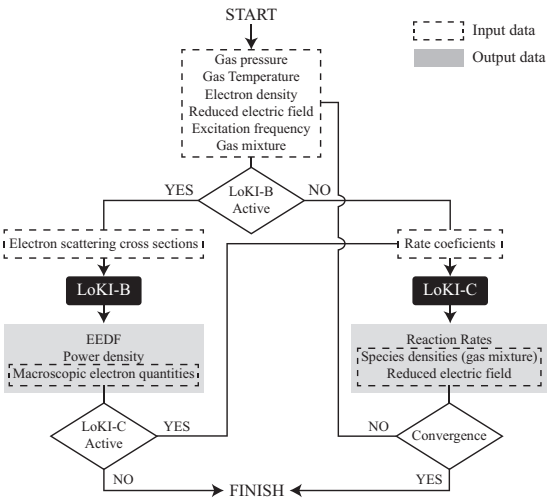

Fig. 1: LoKI workflow, showing input/output data.

New code features

Following the previous roadmap, LoKI has been recently updated with new models that enrich the code and enlarge the type of simulations of interest for users. In particular, we have implemented the following models:

a) Thermal model: that solves the gas thermal balance equation [5], coupled with the particle rate balance equations for the densities of the heavy species and the electron Boltzmann equation, yielding the time evolution of the (average) gas temperature, T_g.

b) Mesoscopic surface kinetic model: that adopts a deterministic description to solve a set of coupled "rate-balance like" equations [6], accounting for the different plasma-surface interaction processes, yielding the coverage of available/occupied sites at the surface while describing the interplay between surface and volume kinetics.

To illustrate the previous models, we show the results of simulations for a pure nitrogen DC discharge, obtained using a simplified reaction mechanism similar to the one presented in [7] including a surface kinetics describing atom recombination at the walls [6]. The simulations were performed for an infinitely long tube with 1.0 cm radius, pressures $p \sim$10-100 Pa and electron densities $n_e \sim 10^{16}$-10^{17} m^{-3}. In Fig. 2 we show: a) the average gas temperature, as a function of n_e, for $p = 13.3$ Pa; b) the fractional coverage of physisorption sites (θ_F), as a function of p, for $n_e = 10^{16}$ m^{-3}.

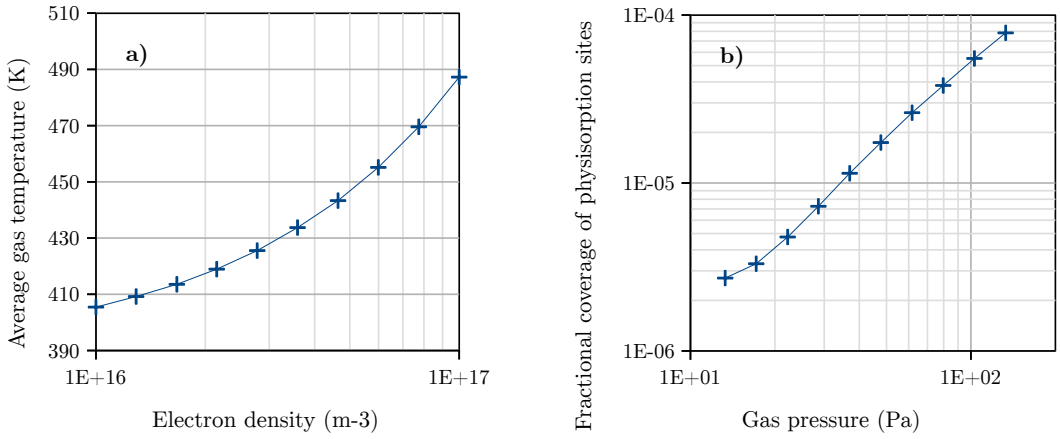

Fig. 2: a) T_g vs. n_e for $p = 13.3$ Pa. b) θ_F vs. p for $n_e = 10^{16}$ m^{-3}.

Conclusion

LoKI is a user-friendly, scalable and upgradable tool suite. It enables the user to easily solve a global model, including: state-of-the-art chemistry schemes (with a detailed description of the electron kinetics), transport losses for neutrals and/or charged particles, the self-consistent evaluation of the gas temperature, and the description of a surface kinetics. This work discussed the current status of development of LoKI, presenting new features, evidencing its functionality and displaying results.

Acknowledgments

This work was partially funded by the European Union (NextGenerationEU), the Spanish Ministerio de Universidades (Plan de Recuperación, Transformación y Resiliencia) and by the Portuguese Foundation for Science and Technology under projects UIDB/50010/2020 and UIDP/50010/2020.

Funded by the European Union NextGenerationEU

GOBIERNO DE ESPAÑA MINISTERIO DE UNIVERSIDADES Plan de Recuperación, Transformación y Resiliencia

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