The LisbOn KInetics tool suit

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Introduction

Predictive tools for non-equilibrium low-temperature plasmas should properly describe the **kinetics of electrons and heavy species**, the former responsible for **inducing plasma reactivity** and the latter **providing the paths for reaction mechanisms**. Both descriptions should be properly coupled in order to provide a self-consistent description of the system.

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], embodying a MATLAB® computational 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** [2], and a **chemistry solver, LoKI-C**, that can run self-consistently coupled or as standalone tools.

- **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**.

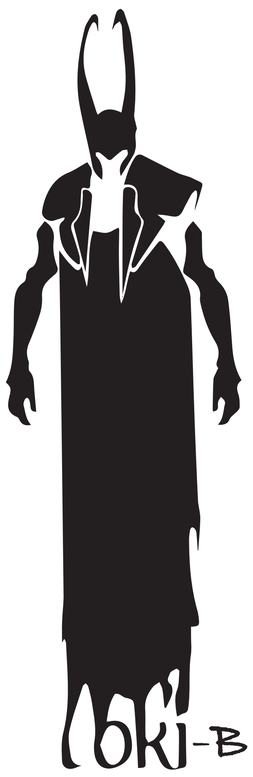
The simulations can include **any gas mixture**, accounting for the **electronic, vibrational and rotational internal degrees of freedom** of the atomic / molecular excited states. For stationary discharges, when both modules are activated, the reduced maintenance electric field (or an equivalent parameter, such the electron temperature) is self-consistently calculated as an eigenvalue solution to the problem, under the assumption of quasi-neutrality [4].

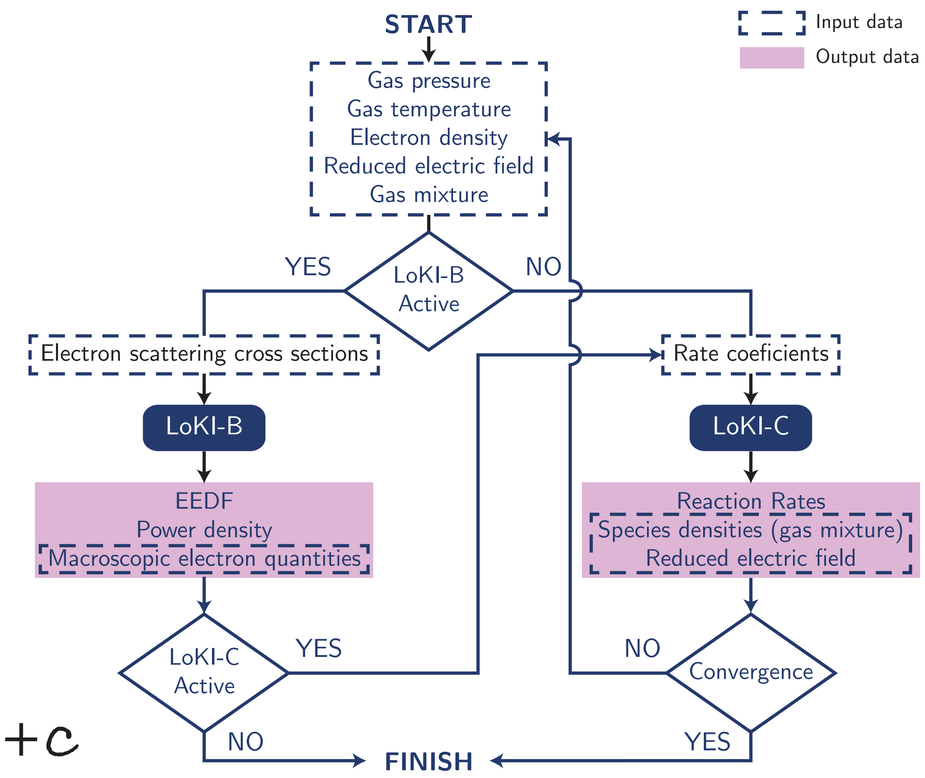
The development team of LoKI is currently engaging **verification and validation** (V&V) procedures, to ensure the quality of the tool and the results it provides.

Code workflow

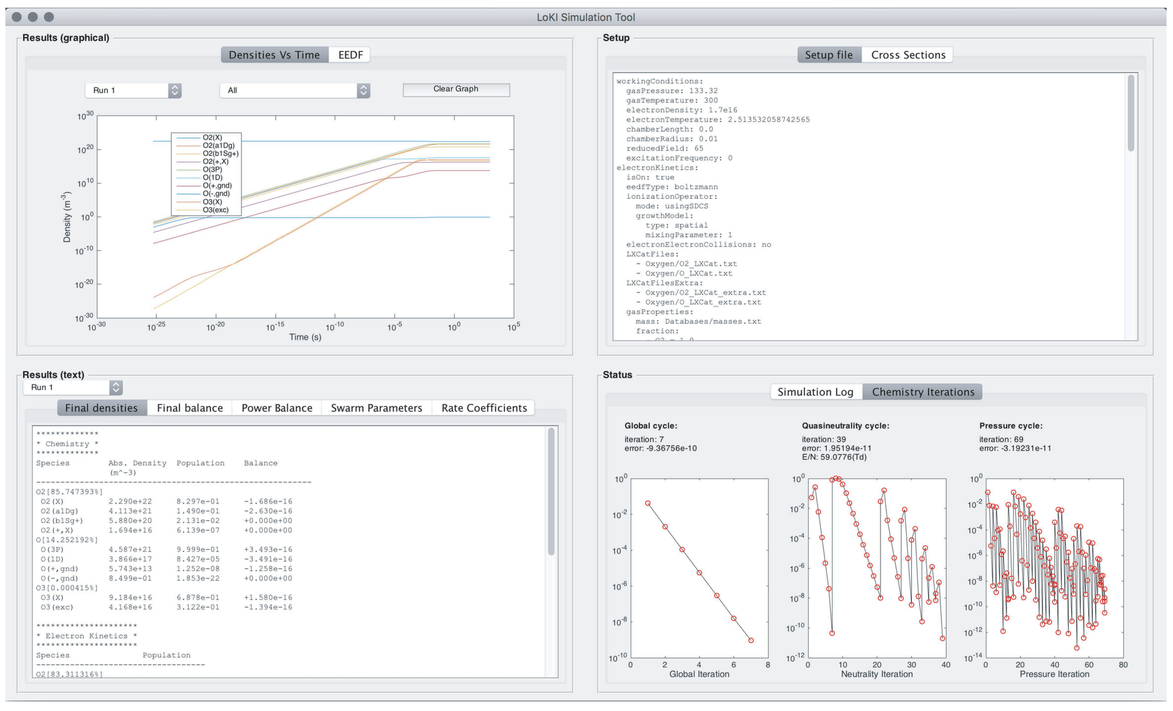
The following flow chart describes the **workflow of LoKI**. When **both modules are self-consistently coupled**, the code:

1.- solves the **electron kinetics** (LoKI-B)
2.- sends electron macroscopic quantities (electron impact rate coefficients) to LoKI-C
3.- solves the **heavy species kinetics** (LoKI-C) ensuring the prescribed pressure (**pressure cycle**)
4.- ensures the neutrality prescribing a new value for the reduced electric field (or electron temperature). If neutrality is obtained proceeds to step 5, otherwise goes back to step 1 (**neutrality cycle**)
5.- ensures consistency between the gas mixture used in LoKI-B and LoKI-C. If electron macroscopic quanti-





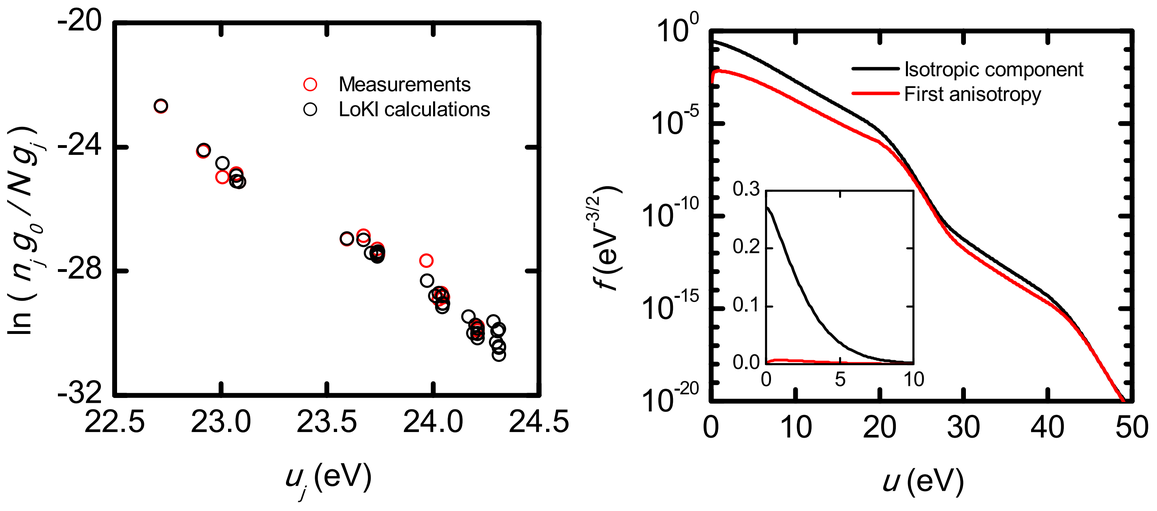
The **LoKI graphical user interface** helps understanding the **status of convergence** as well as **visualising the final results**.



Helium simulations

We show the results of a **simulation for a pure Helium DC discharge**, obtained using the **reaction mechanism presented in [5]** with both LoKI modules self-consistently coupled.

The simulation was performed for an **infinitely long tube of radius 3x10^{-3} m**, a **gas pressure of 10^5 Pa**, a **gas temperature of 1800 K** and an **electron density of 1.7x10^{19} m^{-3}**. We can see that the calculated spectrum for the densities of the main species is in **very good agreement with the experiment** [5]. The results show also the **electron distribution function** obtained for the final self-consistent value of the **reduced maintenance electric field *E/N* ~ 5 Td**.

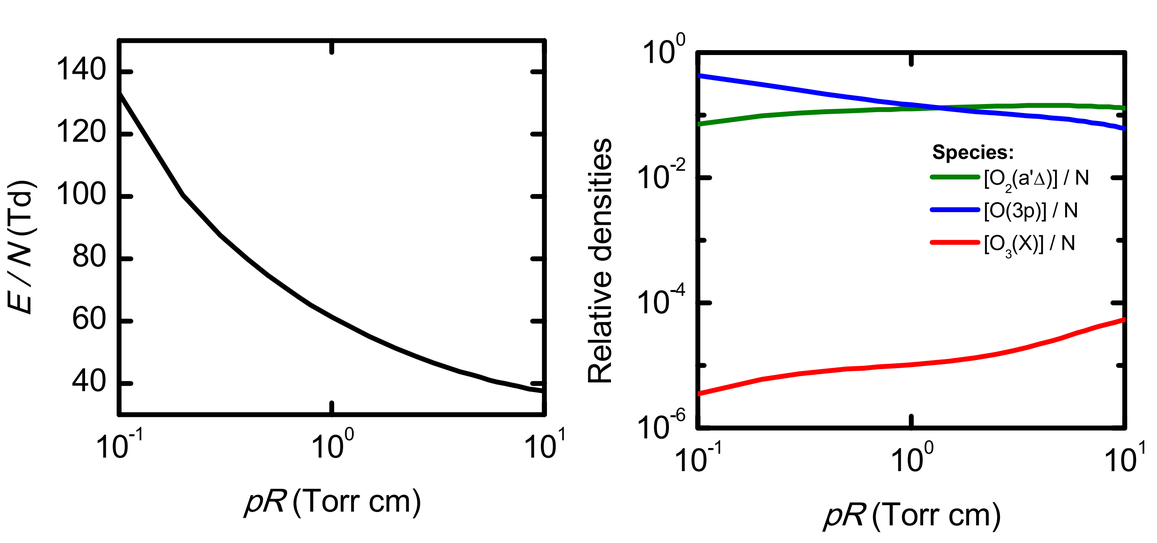


The previous graphs show results that are part of an ongoing **validation exercise for a reaction mechanism in Helium**.

Oxygen simulations

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 were 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 1.7x10^{16} m^{-3}**. 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*. Also, we show the evolution of the **densities of some representative species**, relative to the gas density, as a function of *pR*.



The previous graphs show results that are part of an ongoin **validation exercise for a reaction mechanism in Oxigen**.

Conclusions

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.

References

[1] KIT-PLASMEBA project webpage: http://plasmakit.tecnico.ulisboa.pt.
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[3] LXCat webpage: http://www.lxcat.net.
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[5] M Santos et al., *J. Phys. D: Appl. Phys.*, **47,** 265201 (2014)

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