The LisbOn KInetics (LoKI) computational tool

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There is general agreement on the intellectual and technological importance of modelling low-temperature plasmas (LTPs). Predictive models have 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 [1].

LisbOn KInetics (LoKI) is a computational tool, currently under development, to model non-equilibrium LTPs, produced from different gas mixtures for a wide range of working conditions. The foundations for developing this tool were stablished years ago [2].

LoKI comprises two modules (LoKI-B and LoKI-C) that can run self-consistently coupled, or as standalone tools [3]. LoKI-B (to become open-source) provides the solution to the homogeneous two-term electron Boltzmann equation [4] 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 out of ionisation events. LoKI-C gives the solution to the system of zero-dimensional, *i.e.* 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 plasma. On output, LoKI yields the electron energy distribution function, the electron swarm parameters, the electron power transferred to the different collisional channels, the concentrations of the various plasma species, and the corresponding gain/loss reaction rates. The results are obtained for a prescribed constant pressure, ensured by varying the gaseous mixture composition. 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.

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References

[1] National Research Council. *Plasma Science: Advancing Knowledge in the National Interest*. The National Academies Press, Washington, DC, 2007. ISBN 978-0-309-10943-7. doi:10.17226/11960.

[2] V Guerra and J Loureiro. Self-consistent electron and heavy-particle kinetics in a low-pressure - glow discharge. *Plasma Sources Science and Technology*, 6(3):373–385, aug 1997. ISSN 0963-0252. doi:10.1088/0963-0252/6/3/014.

[3] A. Tejero-del-Caz *et al.* The LisbOn KInetics tool suit. Submitted to *24th Europhysics Conference on Atomic and Molecular Physics of Ionized Gases (ESCAMPIG)*, Glasgow, Scotland, July 17-21, 2018.

[4] A. Tejero-del-Caz *et al.* The LisbOn KInetics Boltzmann solver. Submitted to *24th Europhysics Conference on Atomic and Molecular Physics of Ionized Gases (ESCAMPIG)*, Glasgow, Scotland, July 17-21, 2018.

[5] Project webpage. `http://plasmakit.tecnico.ulisboa.pt`. Accessed: 2018-16-23.