The LisbOn KInetics Global Model (LoKI-GM) for plasma chemistry studies

L. L. Alves[1], A. Tejero-del-Caz[2], P. Pereira[1], M. Lino da Silva[1], L. Marques[3], N. Pinhão[1], C. D. Pintassilgo[1,4], T. Silva[1], P. Viegas[1], V. Guerra[1]

[1] *Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Universidade de Lisboa, Lisboa, PORTUGAL*
[2] *Departamento de Física, Facultad de Ciencias, Universidad de Córdoba, Córdoba, SPAIN*
[3] *Centro de Física das Universidades do Minho e do Porto, Universidade do Minho, Braga, Portugal*
[4] *Faculdade de Engenharia, Universidade do Porto, Porto, Portugal*

Introduction and LoKI-GM description

The **LisbOn KInetics LoKI-GM** [1] is a simulation tool that embodies the software implementation of the expertise in plasma chemistry modelling accumulated over many years by the N-PRiME group in Lisbon [2]. The tool, **released in July 2026 as open-source software** (licensed under the GNU GPL v3.0) [3], solves the global kinetic model for pure gases and gas mixtures [4], providing a self-consistent chemical and transport description of charged/neutral species, both in volume and surface phases, for user-defined working conditions: mixture composition, pressure, dimensions, and excitation features (glow (DC/HF), post-discharge, pulsed). LoKI-GM handles simulations in any atomic/molecular gas mixture, considering collisions with any volume/surface target states, featuring any type of internal degrees of freedom: electronic, vibrational and rotational. The code has been tested under many different plasma conditions.

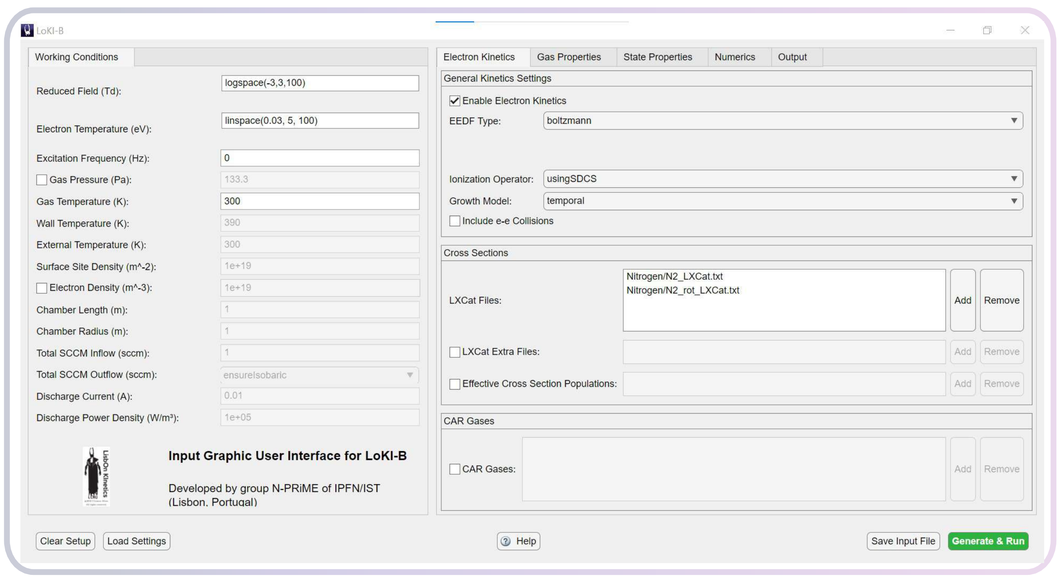
LoKI-GM has two modules, that can run self-consistently coupled or as standalone tools:

- LoKI-B: a Boltzmann solver [5,6], which solves the space independent form of the two-term EBE to calculate the isotropic and the anisotropic parts of the electron distribution function, and the corresponding electron macroscopic parameters;

- LoKI-C: a Chemical solver [7], which solves the system of zero-dimensional (volume average) rate balance equations for the most relevant charged and neutral species in the plasma, and calculates the densities of species, the reaction creation/destruction rates, and the reduced electric field (and any related quantity, such as the discharge current or the discharge power-density).

LoKI-GM is implemented using a flexible and extensible object-oriented architecture in MATLAB® [8], leveraging its matrix-based framework and high-performance ODE solvers.

The supported input/output formats comprise both graphical user interfaces (see figure) and text-based files in **ASCII, JSON and HDF5 formats**. In the HDF5 format, all output data are stored in a single, structured file.



LoKI-GM supports the following types of simulations:

- **Steady-state:** LoKI-C and LoKI-B run coupled until steady-state is reached;

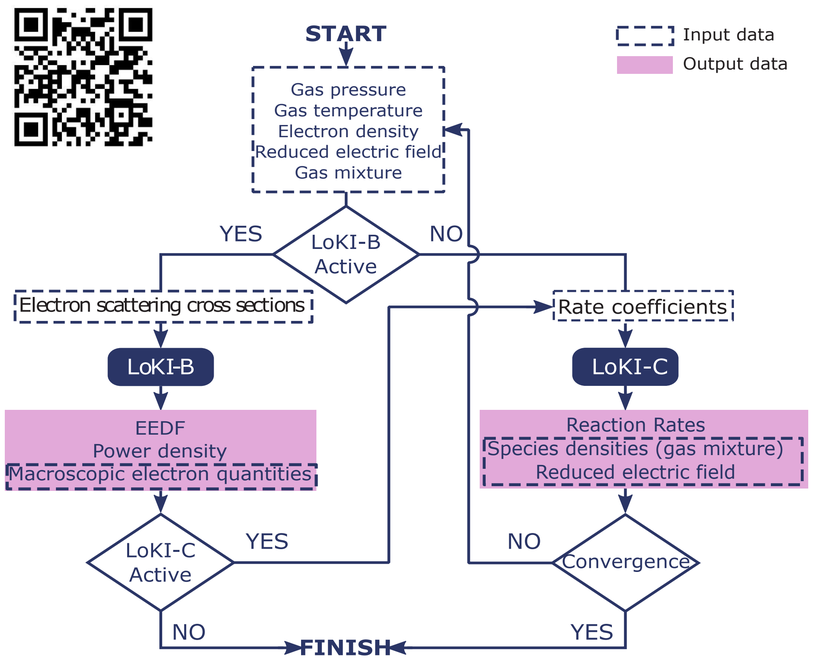
- **Post-discharge:** start with a coupled LoKI-C/LoKI-B steady-state calculation, followed by a standalone LoKI-C simulation at E/N=0 to describe the time-dependent post-discharge;

- **Quasi-stationary:**, LoKI-C runs as a standalone tool using precomputed lookup tables to obtain electron swarm parameters, rate coefficients, and power transfer as functions of the electric field (Local Field Approximation, LFA) or electron mean energy (Local Mean Energy Approximation, LEA).

LoKI-GM workflow

The self-consistent coupling between LoKI-B and LoKI-C is achieved via an iterative workflow embedding two (or three) cycles:
(i) **Pressure cycle** (optional, running within LoKI-C) to ensure calculations at constant gas-pressure specified by the user;
(ii) **Neutrality cycle**, to ensure calculations at constant electron density (or any related quantity, such as the discharge current or discharge power density);
(iii) **Global cycle**, to converge over the populations of the heavy species considered in the solution of the EBE.

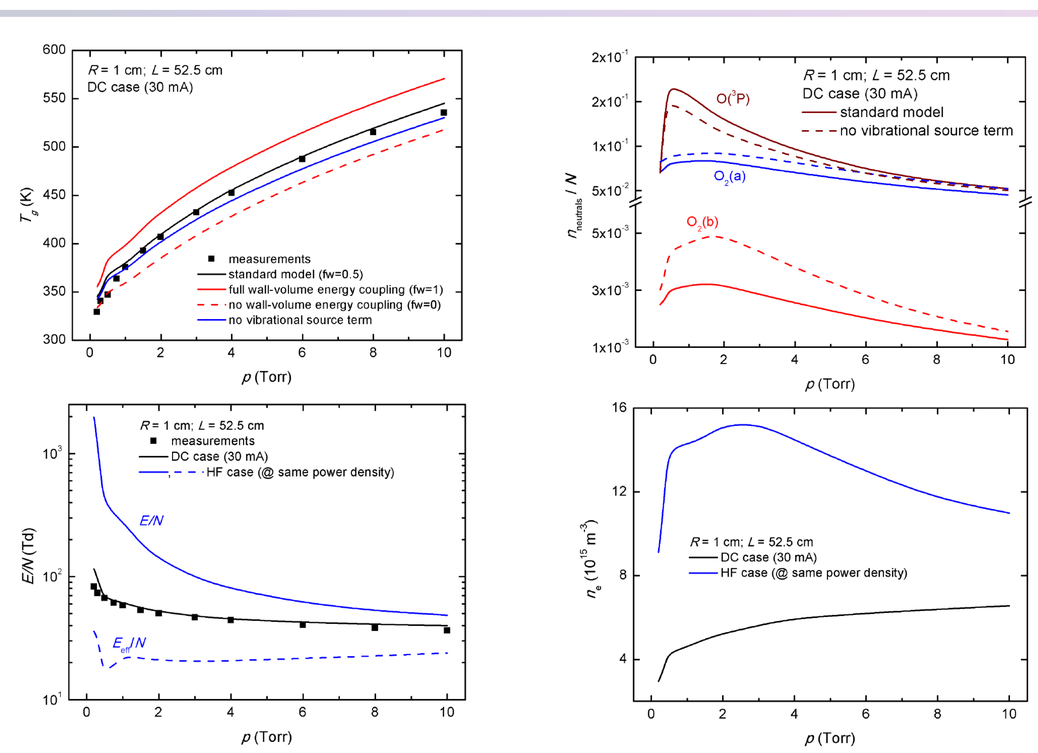
Download the code



Simulations in oxygen DC/HF plasmas

- Simulations for oxygen DC plasmas show that the self-consistent gas temperature decreases when the contribution of gas-heating mechanisms to the thermal balance is reduced. Tests were made by varying the fraction of energy (fw) that returns to the volume after a wall-recombination event, as well as by neglecting the contribution of vibrational excitation.

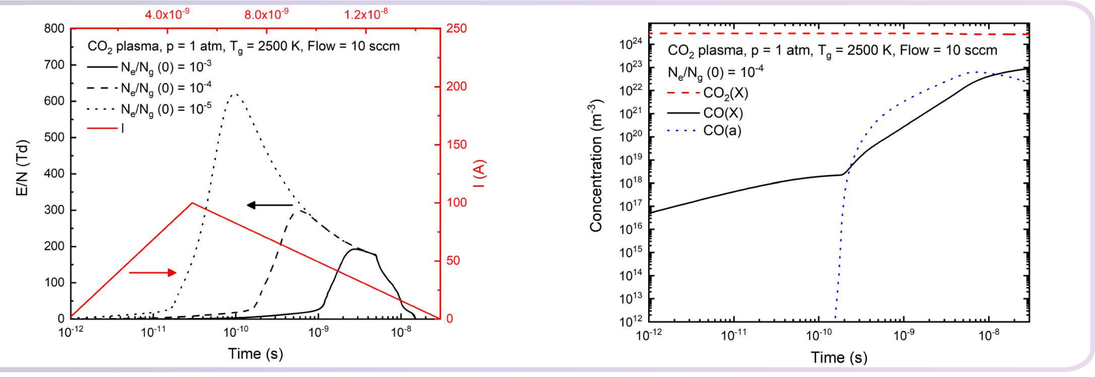
- Simulations for oxygen HF plasmas (2.45GHz) adopted the same discharge power-density obtained for the DC case. Under these conditions, the power coupling occurs through a lower effective electric field and, consequently, through a lower power transferred from the electric field to the electrons. As a result, a higher electron density is required to sustain the prescribed discharge power-density.



Simulations in CO_2 pulsed plasmas

- Simulations in CO_2 pulsed plasmas illustrate LoKI-GM's capability to couple electron and heavy-species kinetics, handle time-dependent excitation, and incorporate gas flow.

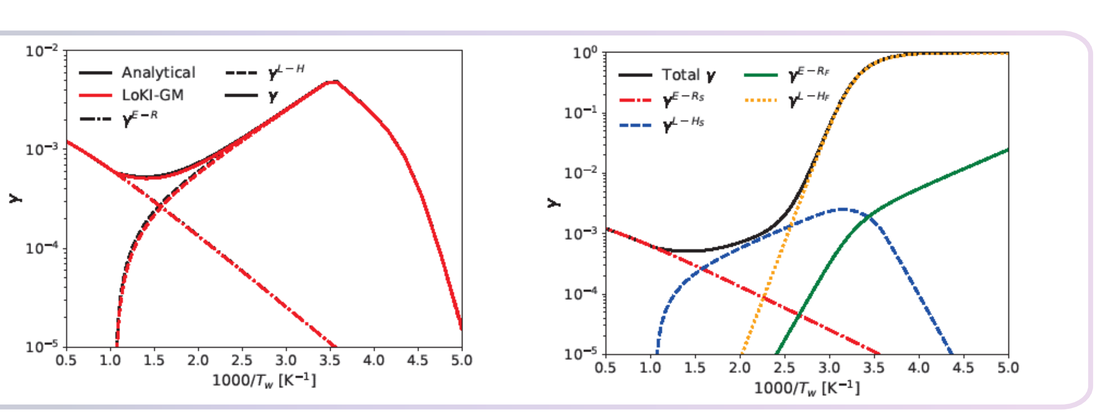
- The concentration of CO(X) increases due to electron-impact dissociation processes and the subsequent chemical conversion of CO_2, whereas the concentration of CO(a) increases rapidly only once the reduced electric field becomes sufficiently large.



Microkinetic mesoscopic surface model in N_2

- Simulations for a pure mesoscopic microkinetic model in N_2 yield a wall-recombination probability γ almost in exact agreement with the analytical model of [9]. Note that, at high wall temperatures, Eley-Rideal (E-R) recombination becomes dominant with respect to Langmuir-Hinshelwood (L-H), where the recombination energy barrier can be more easily overcome.

- The possibility of E-R and L-H recombination involving physisorbed atoms have also be exploited. As expected, the contribution of these mechanism becomes significant as the wall temperature decreases.



References

[1] https://nprime.tecnico.ulisboa.pt/loki/
[2] https://www.ipfn.tecnico.ulisboa.pt/nprime/
[3] https://github.com/LoKI-Suite
[4] L. L. Alves *et al., Plasma Sources Sci. Technol.* **27** (2018) 023002.
[5] A. Tejero-del-Caz *et al., Plasma Sources Sci. Technol.* **28** (2019) 043001
[6] A. Tejero-del-Caz *et al., Plasma Sources Sci. Technol.* (2021) **30** 065008
[7] V. Guerra *et al., Plasma Sources Sci. Technol.* **28** (2019) 073001
[8] https://www.mathworks.com/help/matlab/creating-help.html
[9] V. Guerra IEEE *Trans. Plasma Sci.* **35** (2007) 1397

Acknowledgements

The authors acknowledge Dr. T. C. Dias and MSc. A. Gonçalves for their support and dedication to the development of LoKI-GM.
This work was supported by the FCT - Fundação para a Ciência e Tecnologia, I.P., under projects UID/50010/2025 (https://doi.org/10.54499/UID/50010/2025), UID/PRR/50010/2025 (https://doi.org/10.54499/UID/PRR/50010/2025), UID/PRR2/50010/2025 (https://doi.org/10.54499/UID/PRR2/50010/2025), LA/P/0061/2020 (https://doi.org/10.54499/LA/P/0061/2020) and 2022.04128.PTDC (doi.org/10.54499/2022.04128.PTDC).

Fundação para a Ciência e a Tecnologia

Multimedia

Scan the following links with your smartphone to access multimedia content.

Go to our website

20th International Conference on Plasma Surface Engineering (PSE 2026), 31 August - 3 September 2026, Erfurt, Germany