Release of LoKI-GM
The LisbOn Kinetics Global Model

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Global models

Popular choice to study plasma chemistry

Adopt a **0D / spatially averaged description**, hence reducing computational effort

- allow describing in detail the plasma chemistry in complex gas mixtures
- should include transport effects especially at low to intermediate pressures

Usually involve the coupled solution of

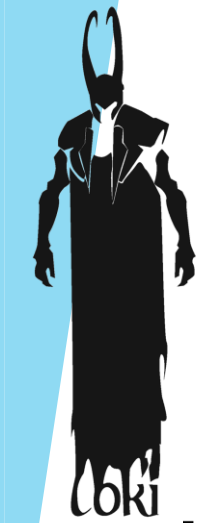
- **Chemistry solver** (to solve the “plasma chemistry”)
- **Boltzmann solver** (to describe the “electron kinetics”)

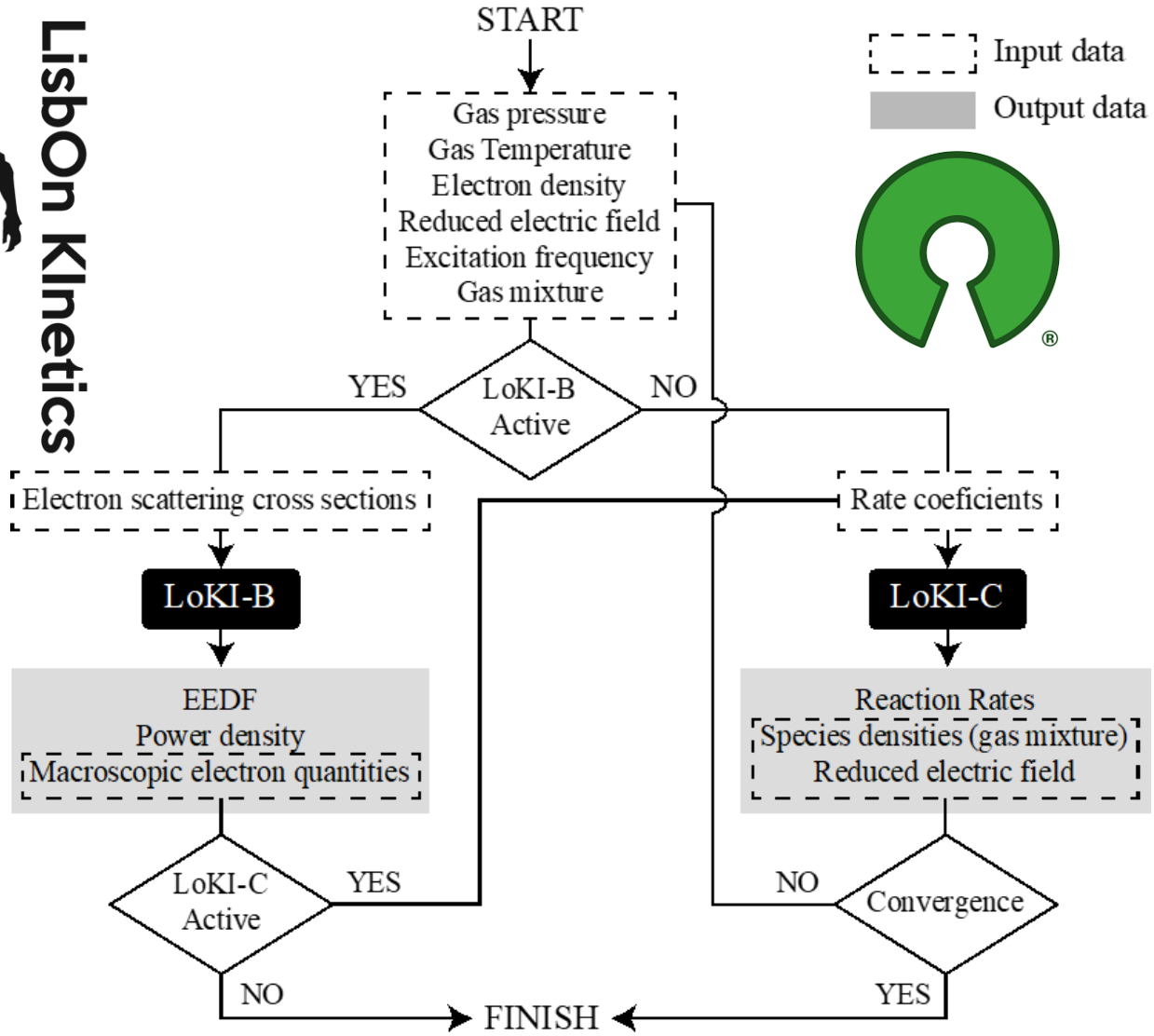
  The non-equilibrium features of the eedf can significantly change (> 20-30%) the values of the electron parameters

L L Alves *et al.* 2018 *Plasma Sources Sci. Technol.* **27** 023002

The LisbOn KInetics (LoKI-GM) simulation tool

(developed under MATLAB®)





LoKI-B

- solves the space independent form of the two-term electron Boltzmann equation, for DC/HF or time-dependent (non-oscillatory) electric fields.
- includes e-e collisions, CAR operator, and growth models for the electron density.

LoKI-C

- solves the system of 0D rate balance equations for the heavy particles of pure gases or gaseous mixtures.
- includes modules to describe

(i) the collisional, radiative and transport mechanisms controlling the creation / destruction of volume and surface species

(ii) the thermal heating of the neutral gas

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https://github.com/LoKI-suite

Outline

- **The LisbOn KInetics Global Model : main features**
  - Description
  - Type of simulations supported
  - Chemistry model (LoKI-C)
  - Workflow
- **Showcase of results**
  - Oxygen plasmas (steady-state simulations)
  - CO_2 plasmas (quasi-stationary simulations)
  - Nitrogen plasmas (surface kinetics only simulations)
- **Final remarks**
- **Release of LoKI-GM**

LoKI-GM : main features

LoKI-GM: description

Software features

- **Developed under MATLAB®** to benefit from its matrix-based architecture
- **C++ version of LoKI-B** is also available **(integrated in PLASIMO)**
- Adopts flexible and upgradable object-oriented programming
- Distributed under the GNU General Public License 3.0.

Guiding principles

- **Clear ontology** that privileges the separation between tool and data
- **Flexibility** to host any volume/surface plasma chemistry scheme, with full state-to-state description
- **Consistency** in the coupling between electron kinetics and heavy-species kinetics
- **Clarity** in defining the working conditions relevant for comparing simulations with measurements.

LoKI-GM: description (cont)

History / status / roadmap

- First closed beta version of LoKI-B was **released early 2017**
- First public release of LoKI-B: **March 2019**
- **Verification and Validation** during development (only the most recent studies are mentioned)

  DC glow discharges sustained in O_2, CO_2, CO_2-N_2, CO_2-O_2 and CO_2-CH_4
  inductively coupled discharges sustained in O_2
  DC glow discharges, radio-frequency discharges and afterglows in N_2–O_2
  microwave discharges sustained in N_2–O_2
  pulsed glow discharges sustained in O_2, N_2-O_2, and CO_2
  analysis of spatially-average transport models; comparison between 1D radial and 0D global models benchmarked against BOLSIG+ (various gases) and QGM in O_2

- Current versions (October 2025 / July 2026)
  `LoKI-B_v25.10 / LoKI-B++_v25.10`
  `LoKI-GM_v26.07` **(TO RELEASE IN THIS SATELLITE EVENT)**

LoKI-GM: type of simulations supported

Steady-state simulations

- LoKI-C and LoKI-B are run in a coupled manner
- DC/HF excitations
- the reduced electric-field amplitude *E/N* is self-consistently calculated by imposing charge neutrality for a prescribed electron density, n_e, or discharge current, I_{dc}, or discharge power-density, *dP/dV.*

Quasi-stationary simulations

- LoKI-C runs as a standalone tool
- *E(t)* (or $I_{dc}(t)$ or *dP(t)/dV*) are defined by the user
- use precomputed lookup tables of electron macroscopic parameters
- impose charge neutrality, and can be applied to pulsed discharges

Post-discharge simulations

- steady-state calculation + standalone LoKI-C simulation at $E = 0$
- impose charge neutrality and $T_e = T_g$

LoKI-C: chemistry model

The spatially-average particle balance equation

$$\frac{\partial n_j}{\partial t} = S_j^{\text{chem}} + S_j^{\text{transp}} + S_j^{\text{flow}}$$

Kinetic scheme

$$\sum_l a_{l,r}^{(1)} \mathrm{X}_l \longrightarrow \sum_{l'} a_{l',r}^{(2)} \mathrm{X}_{l'}$$

Includes rate coefficients for

- volume reactions: electron collisions, heavy-species collisions, radiative transitions
- surface reactions: physisorption, chemisorption, desorption, surface diffusion, recombination

Includes rate coefficients for

Electron kinetics

- multicomponent diffusion + thermal flux transport of neutral states
- transport of charged species (ambipolar-like, h-factor) accounting for multiple pos./neg. ions

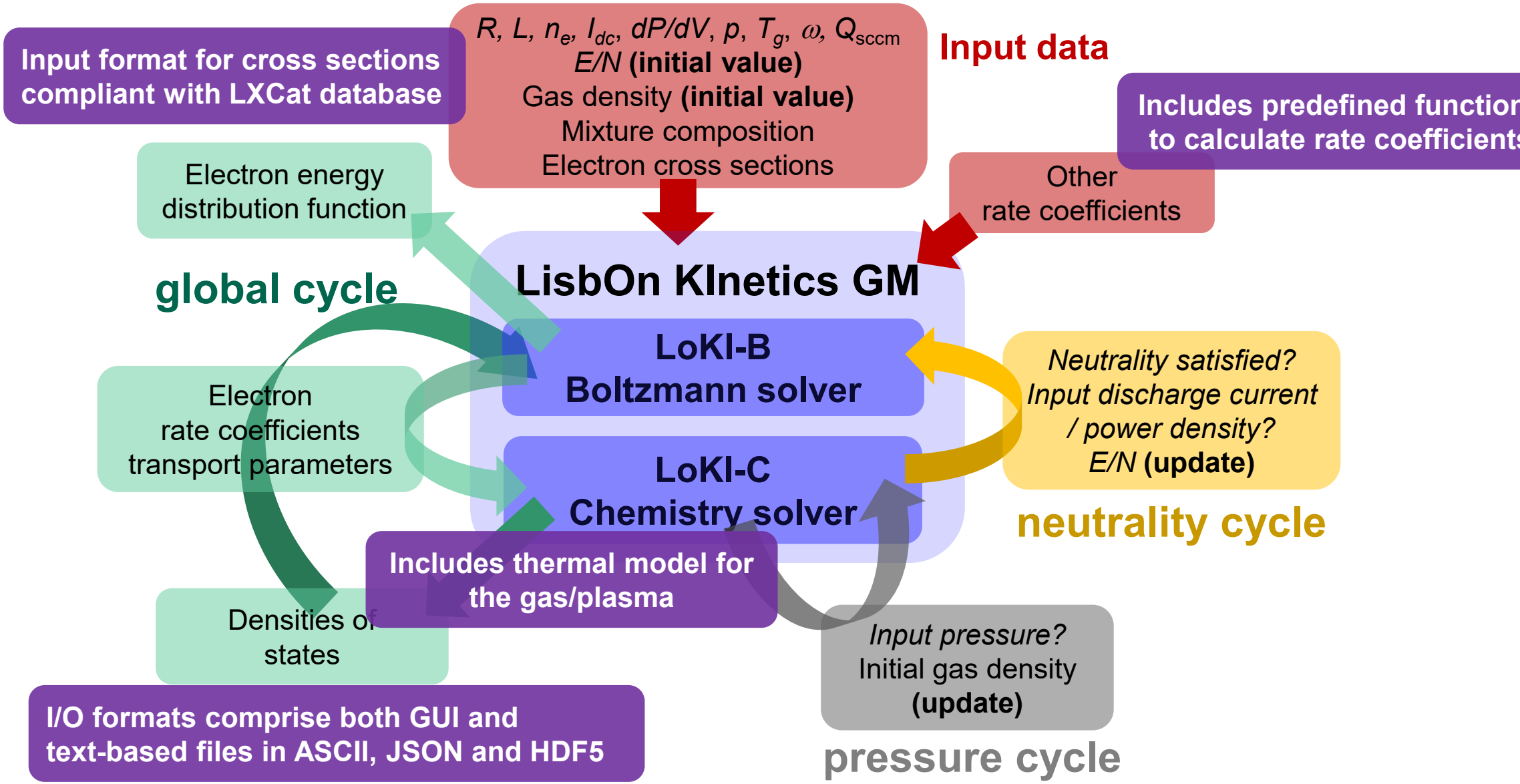
Includes rate coefficients for

- in/out flow, allowing for: numerical values or isobaric model

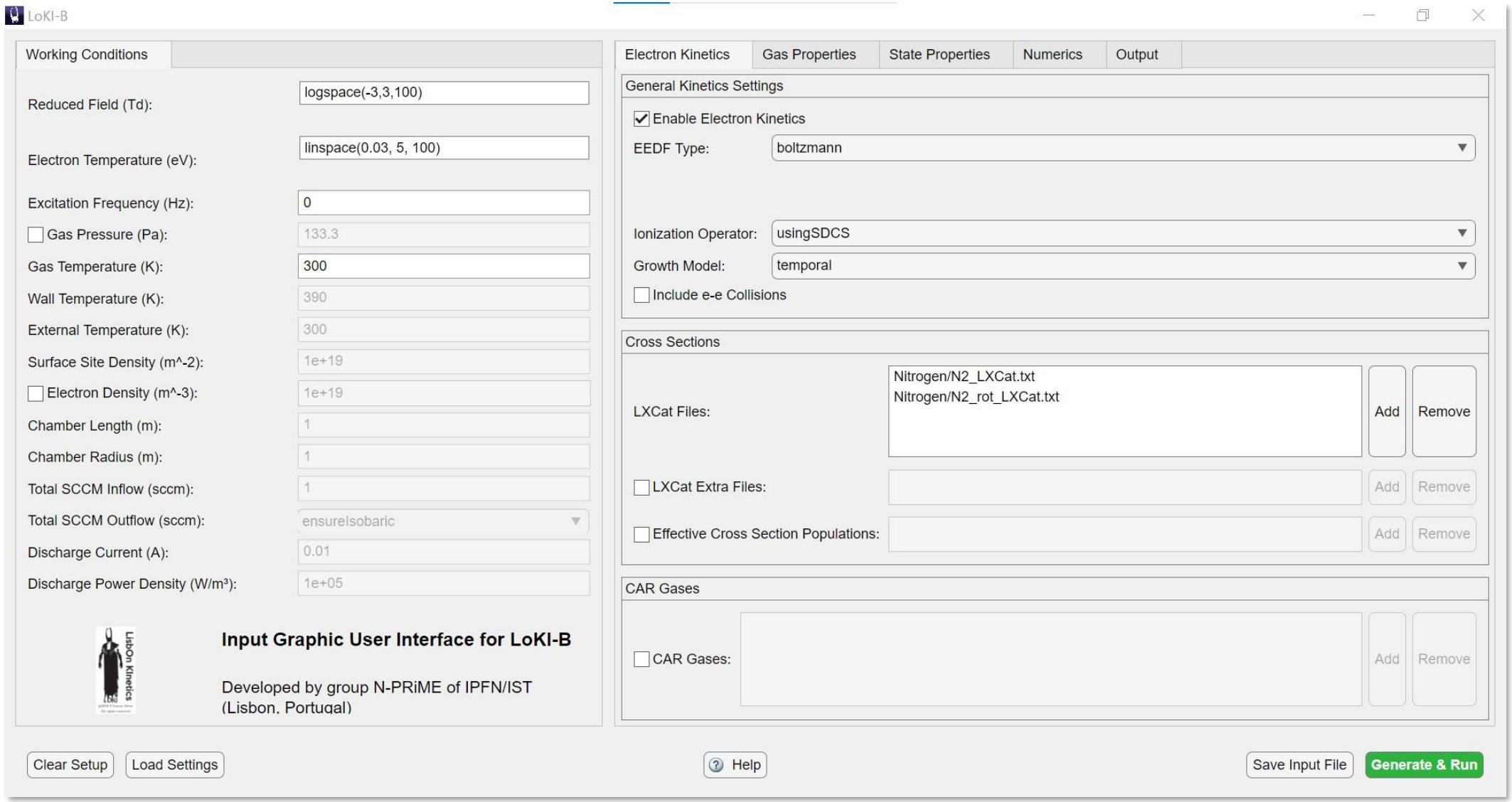
L L Alves *et al.* 2018 *Plasma Sources Sci. Technol.* **27** 023002
L. L. Alves et al. 2018 Plasma Sources Sci. Technol. **27** 023002
D. Marinov et al. 2017 Plasma Process Polym. **14** 1600175

P Coche *et al.* 2016 *J. Phys. D: Appl. Phys.* **49** 235207
V Guerra and J Loureiro 1999 *Plasma Sources Sci. Technol.* **8** 110
J Tennyson *et al.* 2022 *Plasma Sources Sci. Technol.* **31** 095020
P Chabert 2016 *Plasma Sources Sci. Technol.* **25** 025010

LoKI-GM: workflow



LoKI-B: input GUI



LoKI-GM: run testcase (speed 8x)

N_2 plasma

DC discharge, 133 Pa, 20 mA, 1 cm, 1 sccm

Thermal model activated

Species considered

$N_2(X,v)$, $N_2(A^3\Sigma_u^+)$, $N_2(B^3\Pi_g)$, $N_2(C^3\Pi_u)$, $N_2(w^1\Delta_u)$, $N_2(a^1\Pi_g)$, $N_2(a'^1\Sigma_u^-)$

$N(^4S)$, $N(^2P)$, $N(^2D)$

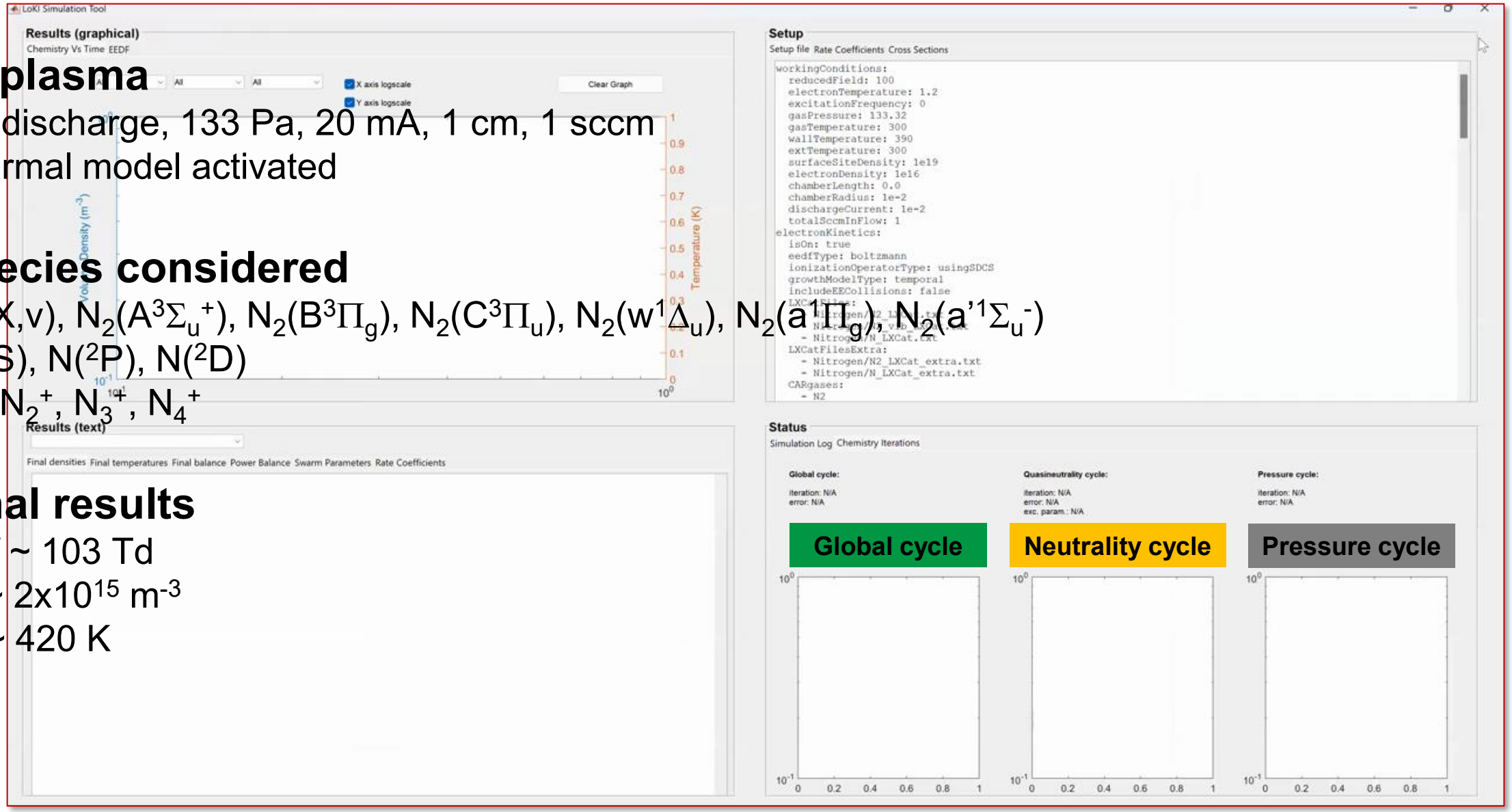
N^+, N_2^+, N_3^+, N_4^+

Final results

E/N ~ 103 Td

n_e ~ 2x10^{15} m^{-3}

T_g ~ 420 K



LoKI-GM : showcase of results

Oxygen plasmas: validation of reaction mechanism

(steady-state simulations)

Plasmas produced by cylindrical DC glow discharges

- R = 1 cm; L = 52.5 cm
- p = 30 – 1000 Pa
- I_{dc} = 10 – 40 mA

Benchmark experiments

- probe measurements for E/N
- radially averaged VUV; actinometry; on-axis CRDS
  for densities of species [$O_2(X^3\Delta_g^-)$, $O_2(a^1\Delta_g)$, $O_2(b^1\Sigma_g^+)$ and $O(^3P)$]
- OES of $O_2(b^1\Sigma_g^+)$ and TALIF for T_g

Main creation / destruction mechanisms

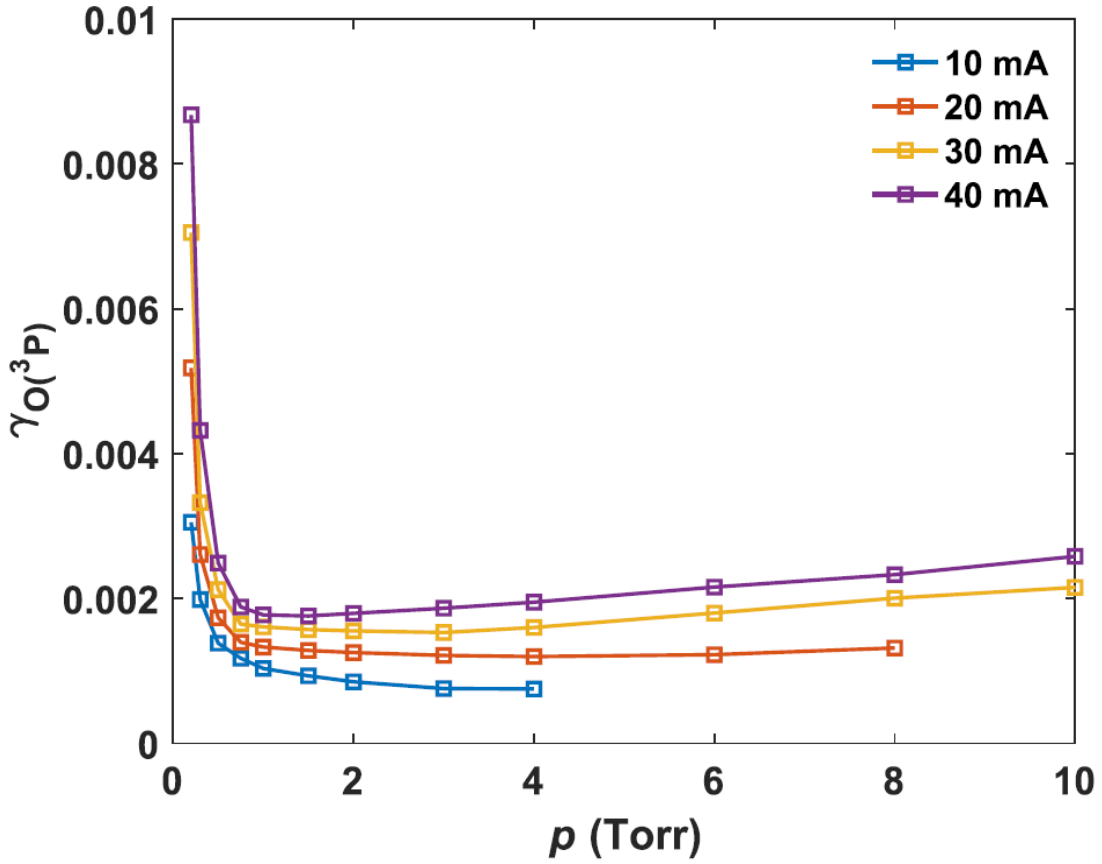
- electron-impact excitation/dissociation
- two- and three-body quenching
- wall recombination

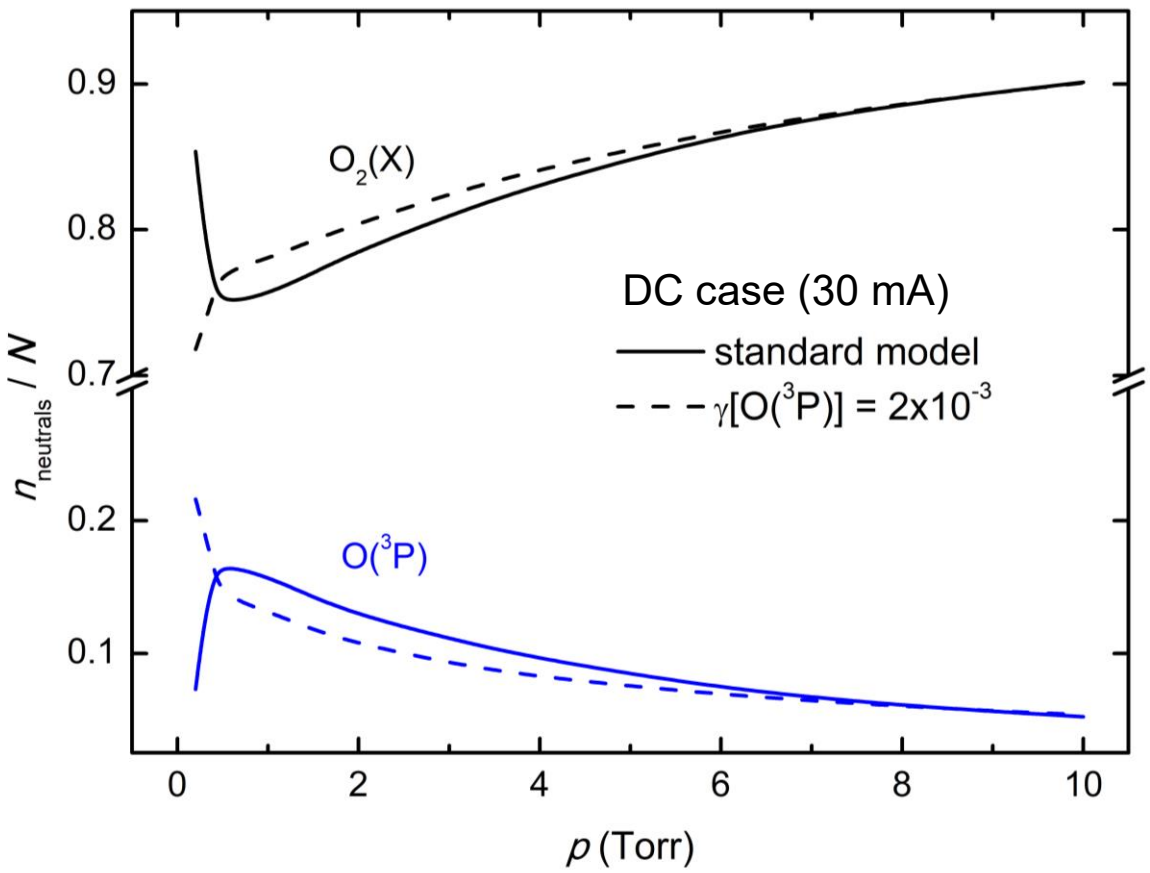
Laboratoire de Physique des Plasmas (LPP), France
Lomonosov Moscow State University (MSU), Russia

T C Dias *et al.* 2023 *Plasma Sources Sci. Technol.* **32** 084003

Oxygen plasmas: surface recombination

O(^{3}P) wall-recombination probability



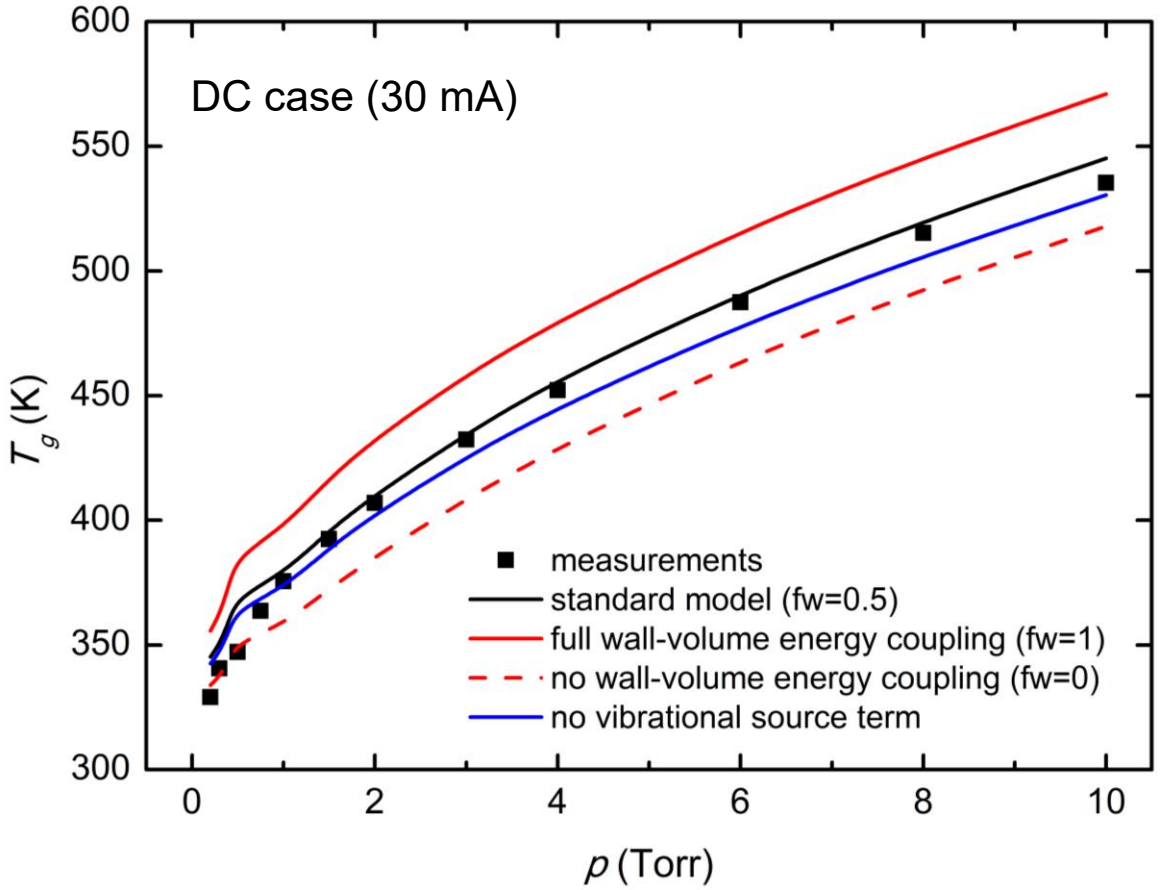


J-P Booth *et al.* 2020 *Plasma Sources Sci. Technol.* **29** 115009

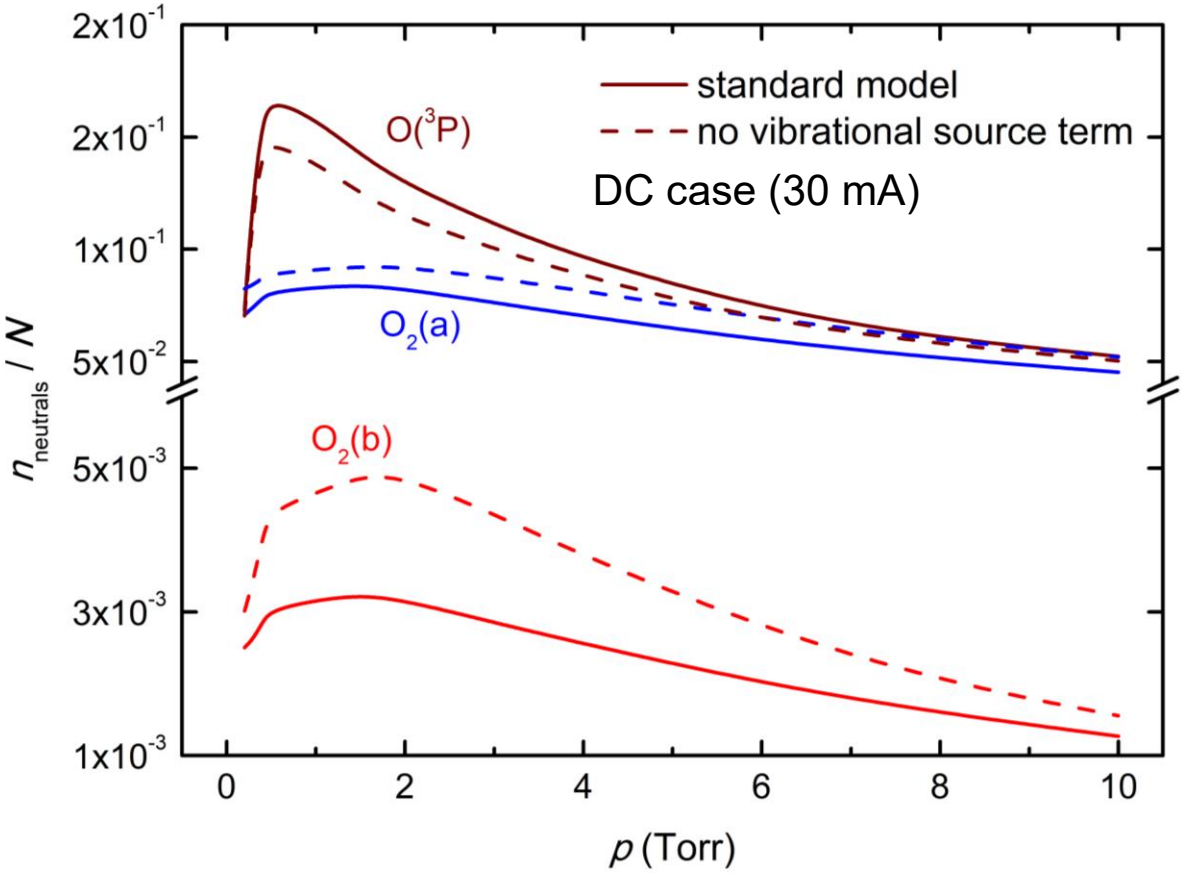
Oxygen plasmas: thermal model parameters

Influence of

- **wall-volume energy coupling**
- **vibrational source-term**

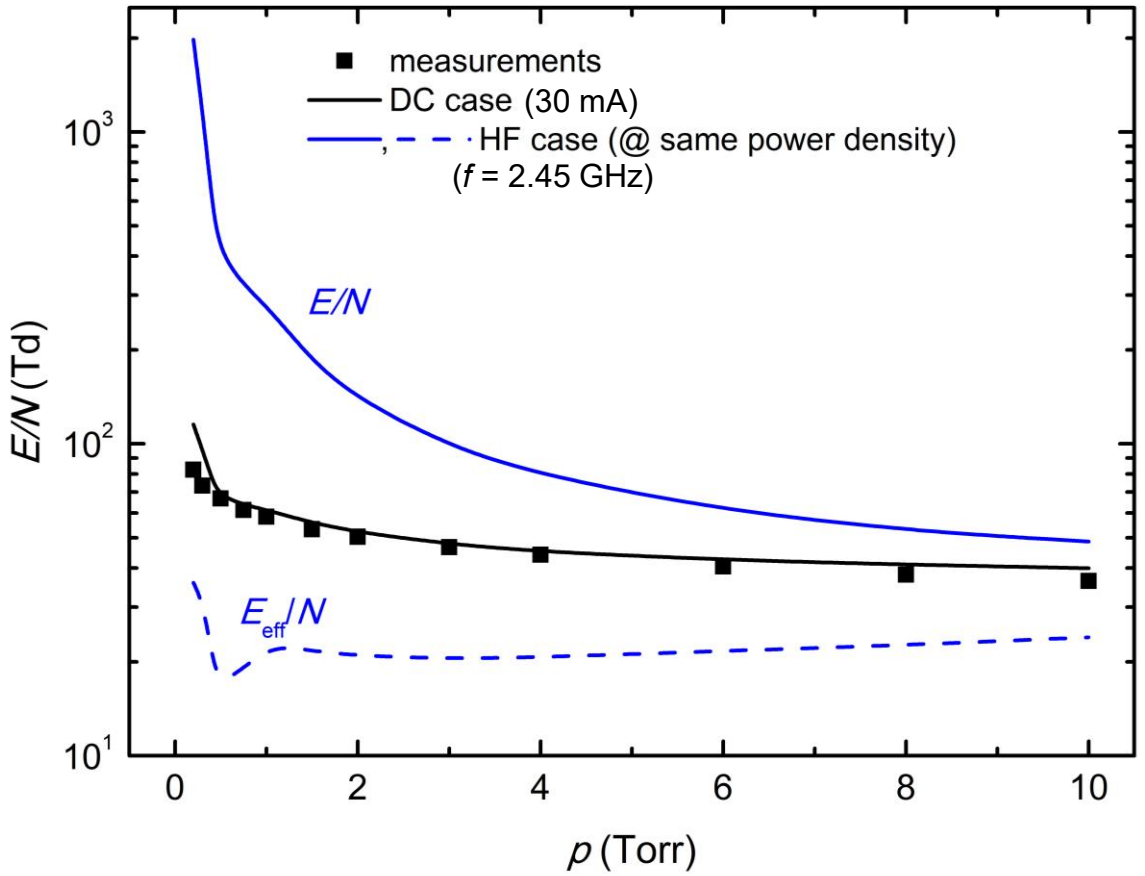


The wall-volume energy coupling can also change the density of $O_2(b)$ by up to 20%

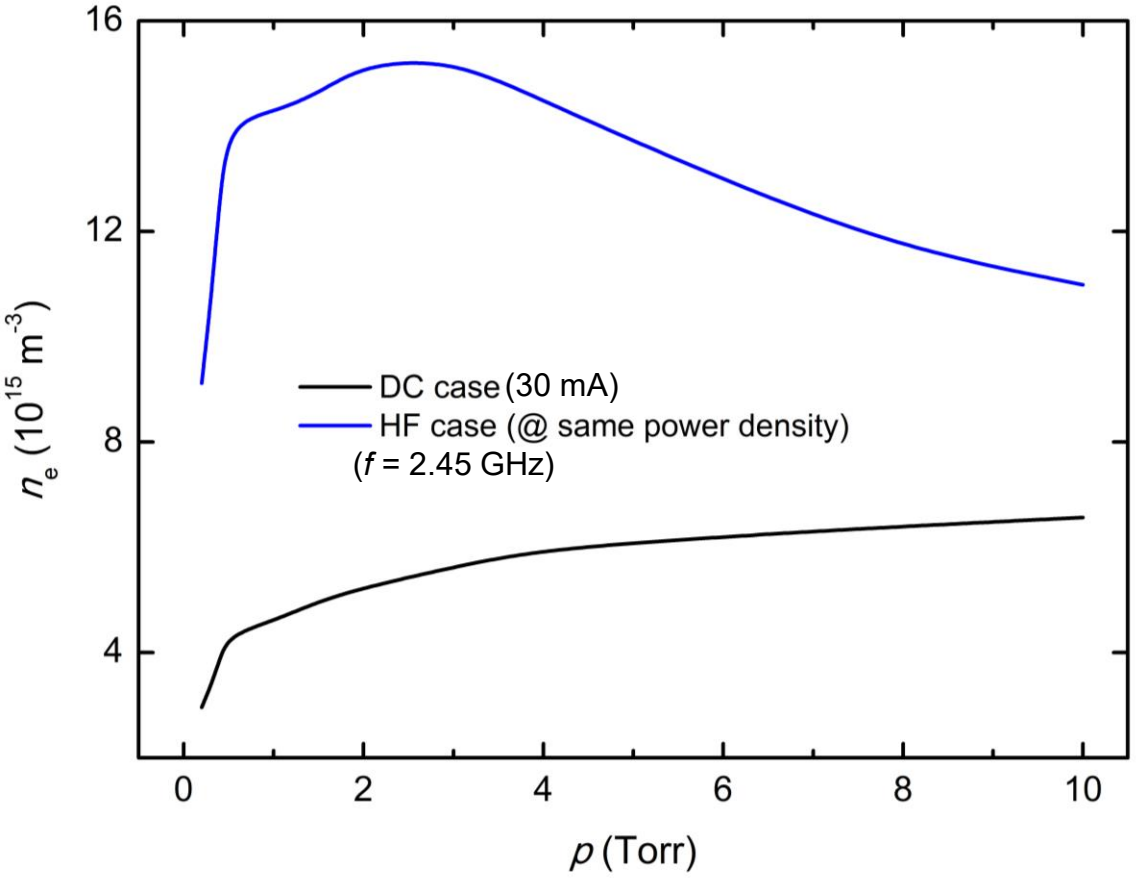


Oxygen plasmas: DC vs HF discharges

Discharge characteristics



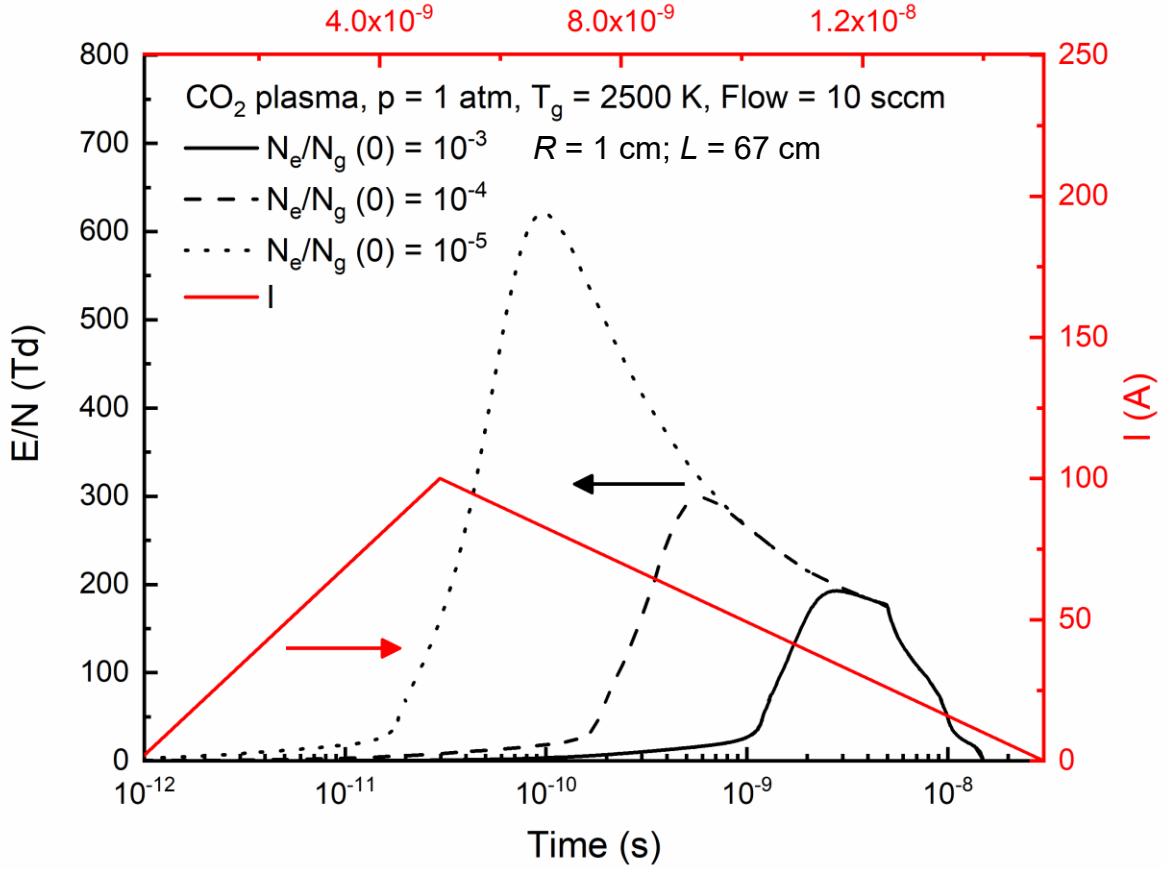
Electron density



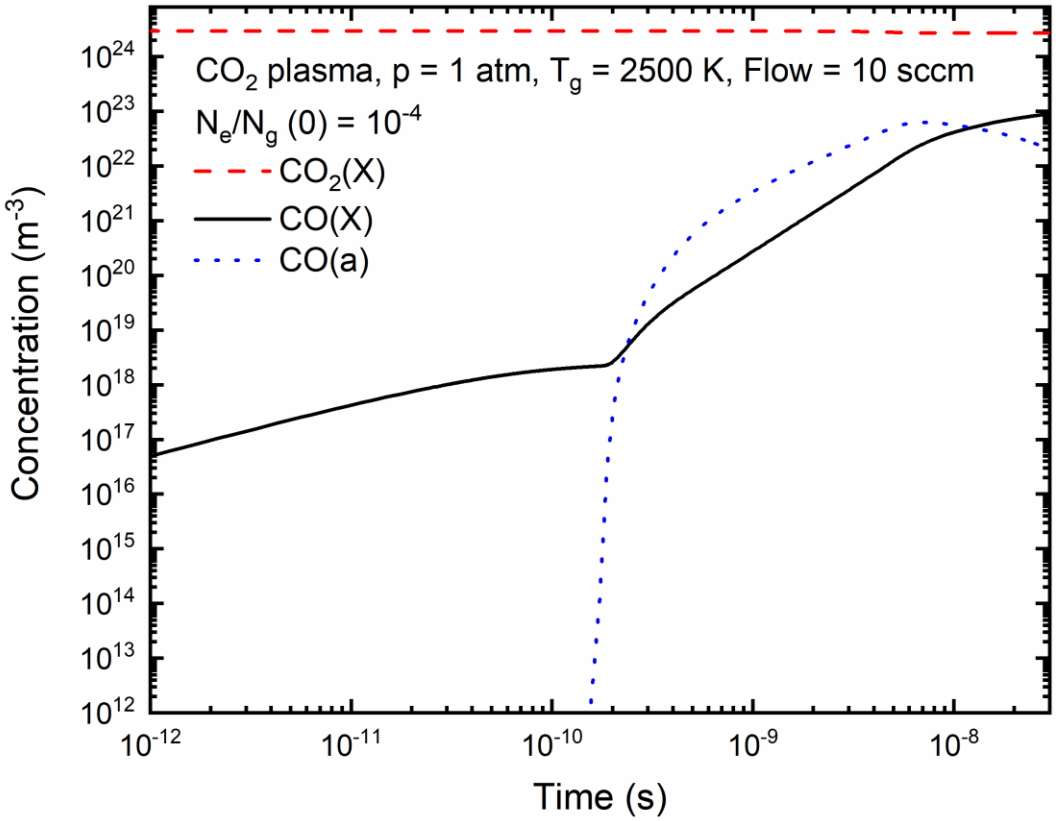
The decrease in the effective electric-field is associated with an increase in the electron density

CO_2 plasmas: excitation by current pulse

(quasi-stationary simulations)



CO_2 dissociation remains at ~4%



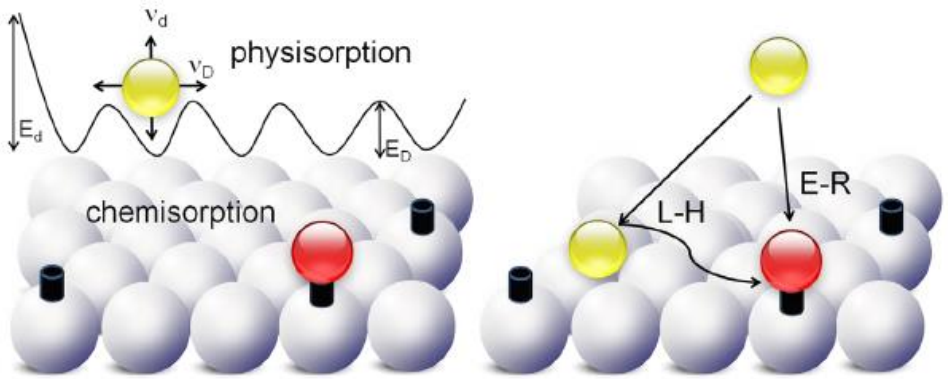
Results highlight the role of electron-impact mechanisms and electronically excited species also in atmospheric-pressure plasmas

Nitrogen plasmas: verification of surface kinetics

(surface kinetics only simulations)

Analysis of plasma-surface interaction

- T_w = 200 – 2000 K
- [N(^{4}S)] = 10^{21} m^{-3} (in the volume)
- [wall_empty(F)] + [wall_empty(S)] = 10^{20} m^{-2}
- [wall_empty(S)] / [wall_empty(F)] ~ 2x10^{-3}

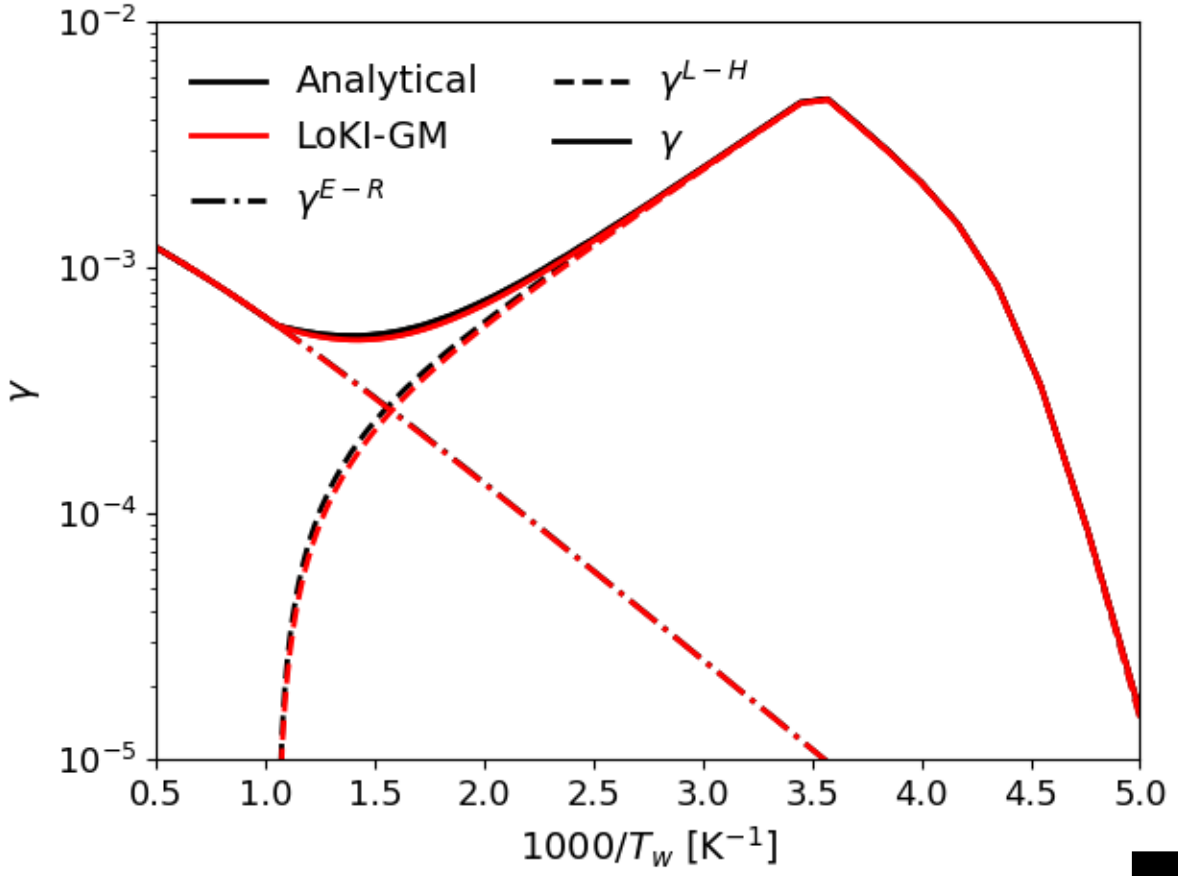


Surface microkinetic mesoscopic model

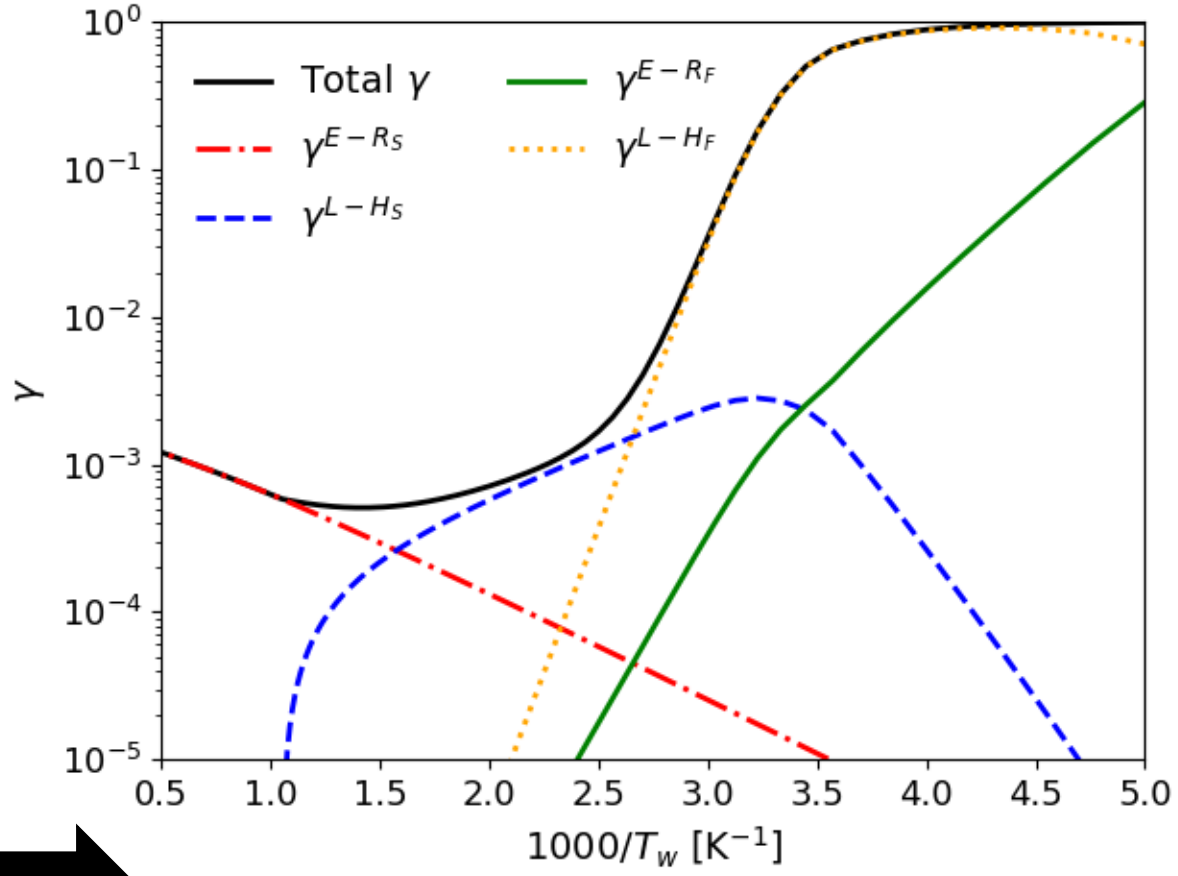
N(^{4}S) + wall_empty(F) -> N(F)	**physisorption**
N(F) -> wall_empty(F) + N(^{4}S)	**desorption**
N(^{4}S) + wall_empty(S) -> N(S)	**chemisorption**
N(F) + wall_empty(S) -> N(S) + wall_empty(F)	**surface diffusion**
N(^{4}S) + N(S) -> wall_empty(S) + 2N(^{4}S)	**Eley-Rideal recomb.**
N(F) + N(S) -> wall_empty(S) + wall_empty(F) + 2N(^{4}S)	**Langmuir- Hinshelwood recomb.**
N(^{4}S) + N(F) -> wall_empty(F) + 2N(^{4}S)	**Eley-Rideal recomb. (phys.)**
N(F) + N(F) -> wall_empty(F) + wall_empty(F) + 2N(^{4}S)	**Langmuir- Hinshelwood recomb. (phys.)**

Nitrogen plasmas: surface kinetics

Verification of standard kinetics



Influence of extra mechanisms



Low T_w

+ Release of chemical schemes (to publish on ChemCat)

- **Oxygen** (both with/without vibrational excitation)
- **CO_2** (without vibrational excitation)
- **Nitrogen** (simplified chemistry scheme)

Extensive documentation available

```
%---- electron impact excitation ----
e + O2(X) <-> e + O2(a1Dg)                  | eedf |  |  % Phelps 1985
e + O2(X) <-> e + O2(b1Sg+)                 | eedf |  |  % Phelps 1985
e + O2(a1Dg) <-> e + O2(b1Sg+)              | eedf |  |  % Tashiro 2006
e + O(3P) <-> e + O(1D)                     | eedf |  |  % Laher 1990
e + O2(X) <-> e + O2(A3Su+_C3Du_c1Su-)      | eedf |  |  % Phelps 1985
```

```
%---- neutral species collisions ----
O2(a1Dg) + O(3P) -> O2(X) + O(3P)                | constantRateCoeff        | 7e-22                              | level  % Kossyi 1992
O2(a1Dg) + O(3P) + O2(X) -> O2(X) + O(3P) + O2(X) | constantRateCoeff        | 3E-44                              | level  % Braginskiy 2005, rateCoeff: 1-3E-44
2O2(a1Dg) -> O2(b1Sg+) + O2(X)                   | modifiedArrheniusGasTemp | 1.81e-24*300^(-3.8), 3.8, 700      | level  % Heidner 1981
O2(a1Dg) + O2(X) -> O2(X) + O2(X)                | powerGasTemp             | 2.20E-24*300^-0.8, 0.8             | level  % Kossyi 1992
O2(b1Sg+) + O(3P) -> O2(a1Dg) + O(3P)            | constantRateCoeff        | 4e-20                              | level  % Ionin 2007
O2(b1Sg+) + O(3P) -> O2(X) + O(3P)               | offsetArrheniusGasTemp   | 4e-20, 1e-16, -3700                | level  % Ionin 2007 + Booth 2022
O2(b1Sg+) + O(3P) -> O2(X) + O(1D)               | modifiedArrheniusGasTemp | 3.39E-17*300^0.1, -0.1, -4201      | level  % Zinn 1982
O2(A3Su+_C3Du_c1Su-) + O(3P) -> O(3P) + O2(X)    | constantRateCoeff        | 4.95e-18                           | level  % Vasiljeva 2004
```

```
%---- Ion transport ----
O2(+,X) + wall -> O2(X)          | classicalAmbipolarDiffNegIon |  | level
O(+,gnd) + wall -> O(3P)         | classicalAmbipolarDiffNegIon |  | level

%---- Neutral transport --
O2(a1Dg) + wall -> O2(X)         | multicomponentTransportChantry | 2.2e-4, nearWallTemperature | level  % Booth 2020
O2(b1Sg+) + wall -> O2(X)        | multicomponentTransportChantry | 0.135, nearWallTemperature  | level  % Booth 2022
O2(A3Su+_C3Du_c1Su-) + wall -> O2(X) | multicomponentTransportChantry | 1, nearWallTemperature | level  % Vasiljeva 2004
```

Final remarks

Final remarks

Check posters
P2+92 (LoKI-GM)
P2+102 (LoKI-B++)
Poster Session 2

LoKI-GM is able to perform several types of simulations
relevant for the assessment of plasma chemistry schemes

- **Steady-state simulations**, including a thermal model, self-consistent calculating the reduced maintenance field, the gas temperature, and the densities of species
- **Quasi-stationary simulations,** coupling electron and heavy-species kinetics, handling time-dependent excitation, and incorporating gas flow
- **Surface kinetics only** simulations, based on microkinetic mesoscopic models
- …

The potential of modelling as a predictive tool can only be achieved after a **validation process**, by comparing modelling results with experimental measurements, a step that requires **collaborative work within the community**

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Release of LoKI-GM

Release of LoKI-GM_27.07

https://github.com/LoKI-Suite/LoKI-GM

Thank you !

If you have difficulties, if you find bugs, or if you have requests

- open issues in LoKI-GM repository
- contact us at loki@tecnico.ulisboa.pt

Enjoy LoKI-GM