

The LisbOn Kinetics Global Model (LoKI-GM)

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Modelling activities

Fundamental component in any research domain

- **complementing** and/or aiding experimental diagnostics
- providing **predictions** on the behavior of significant quantities (especially when experimental access is limited)
- contributing to a deeper **understanding** of the field's fundamental knowledge

LTP models prove particularly valuable and challenging given the inherent complexity of the medium

- often characterized by **different material phases**
- **composed** by charged particles and by neutral species in different excited states
- intrinsically in **non-equilibrium**

I Adamovich *et al.* 2022 *J. Phys. D: Appl. Phys.* **55** 373001

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

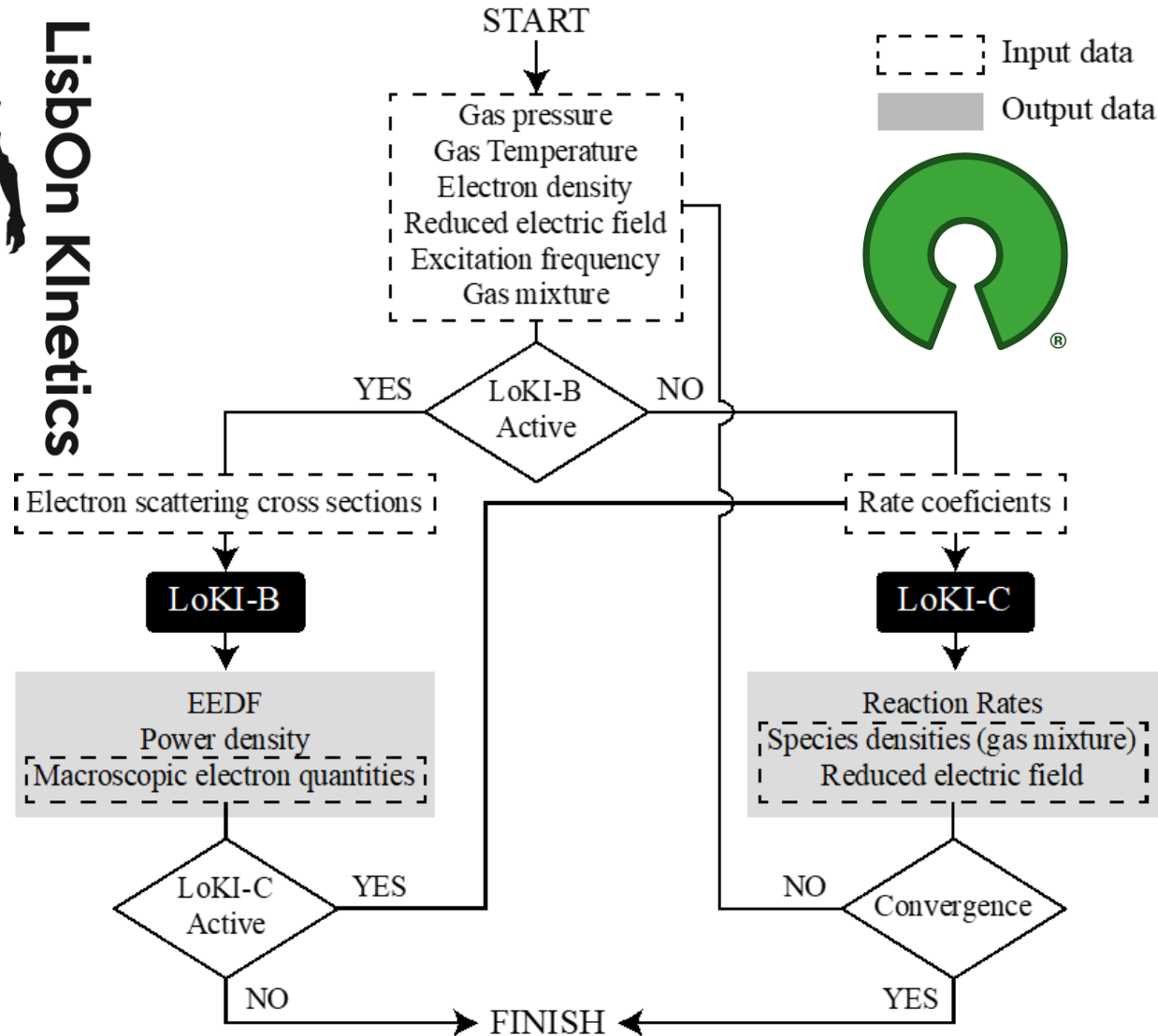
L L Alves *et al.* 2018 *Plasma Sources Sci. Technol.* **27** 023002

The LisOn Knetics (LoKI-GM) simulation tool

(developed under MATLAB®)



LisOn Knetics



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
 - the collisional, radiative and transport mechanisms controlling the creation / destruction of volume and surface species
 - the thermal heating of the neutral gas

- **The LisbOn Knetics Global Model : main features**

- Description

- Type of simulations supported

- Chemistry model (LoKI-C)

- Workflow

- **Show case of results**

- Oxygen plasmas

- surface recombination
 - thermal model parameters
 - (DC vs HF discharges)

- Nitrogen plasmas

- surface kinetics

- **Final remarks**



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_v10.25 / LoKI-B++_v10.25
 - LoKI-GM_v26.07 (to be released @ ESCAMPIG)



LoKI-GM: type of simulations supported

Steady-state simulations

- LoKI-C and LoKI-B are run in a coupled manner
- DF/HF excitations
- the electric-field amplitude E (or the discharge current I_{dc} or the discharge power-density dP/dV) are self-consistently calculated by imposing charge neutrality

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

$$\sum_l a_{l,r}^{(1)} X_l \longrightarrow \sum_{l'} a_{l',r}^{(2)} X_{l'}$$

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

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

Electron kinetics

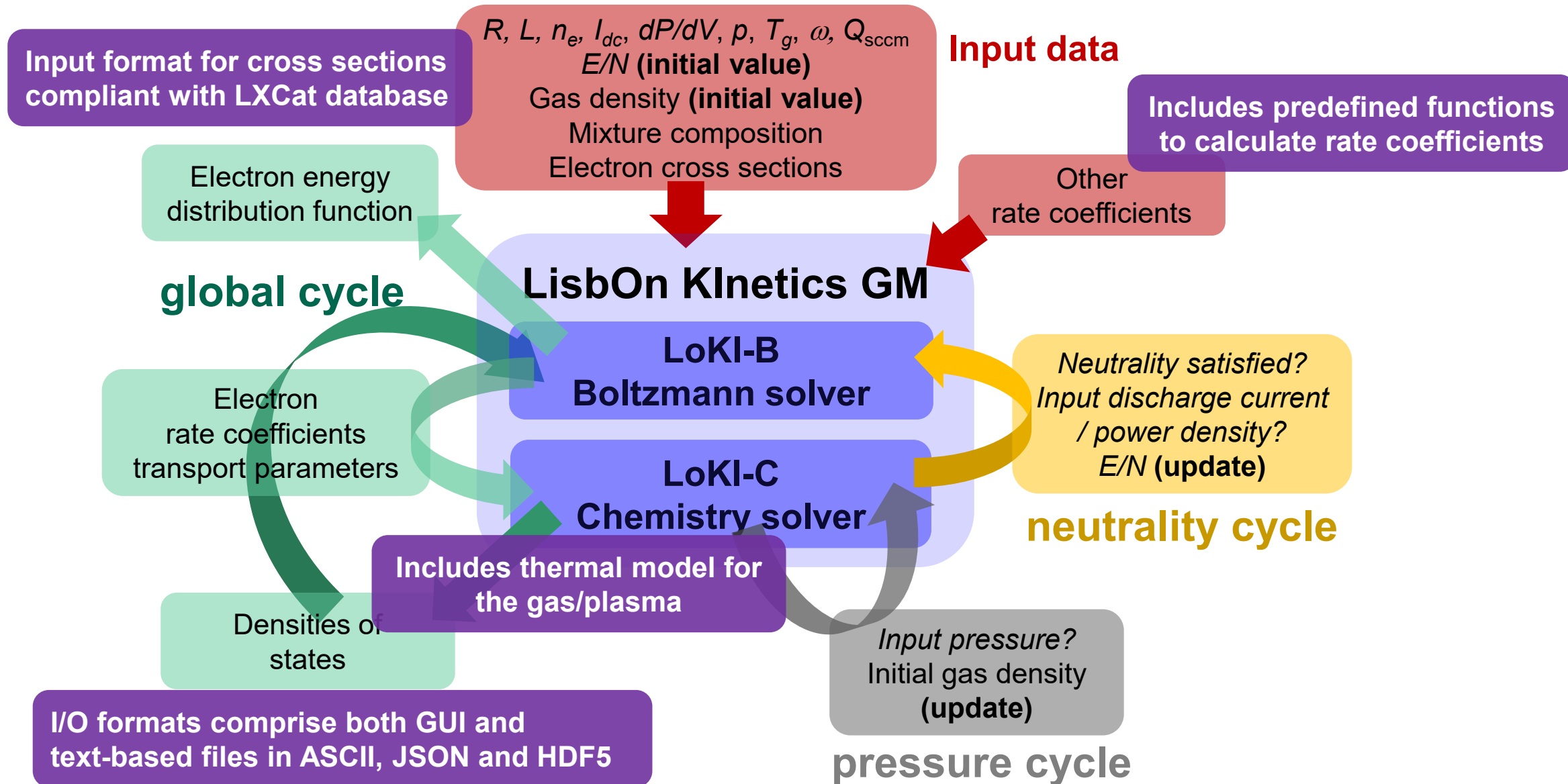
Includes rate coefficients for

- 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-B

Working Conditions

Reduced Field (Td):

logspace(-3,3,100)

Electron Temperature (eV):

linspace(0.03, 5, 100)

Excitation Frequency (Hz):

0

☐ Gas Pressure (Pa):

133.3

Gas Temperature (K):

300

Wall Temperature (K):

390

External Temperature (K):

300

Surface Site Density (m⁻²):

1e+19

☐ Electron Density (m⁻³):

1e+19

Chamber Length (m):

1

Chamber Radius (m):

1

Total SCCM Inflow (sccm):

1

Total SCCM Outflow (sccm):

ensureIsobaric

Discharge Current (A):

0.01

Discharge Power Density (W/m³):

1e+05



Developed by group N-PRiME of IPFN/IST
(Lisbon, Portugal)
Build hash: 0x4D522D41525047

Load Settings

Save Input File

Generate & Run

Electron Kinetics

Gas Properties

State Properties

Numerics

Output

General Kinetics Settings

☒ Enable Electron Kinetics

EEDF Type: boltzmann

Ionization Operator: usingSDCS

Growth Model: temporal

☐ Include e-e Collisions

Cross Sections

LXCat Files:

Nitrogen/N2_LXCat.txt
Nitrogen/N2_rot_LXCat.txt

AddRemove

☐ LXCat Extra Files:

AddRemove

☐ Effective Cross Section Populations:

AddRemove

CAR Gases

☐ CAR Gases:

AddRemove

LoKI-GM: run testcase (speed 8x)

N₂ plasma

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

Thermal model activated

Species considered

N₂(X,v), N₂(A³Σ_u⁺), N₂(B³Π_g), N₂(C³Π_u), N₂(w¹Δ_u), N₂(a¹Π_g), N₂(a¹Σ_u⁻)

N(⁴S), N(²P), N(²D)

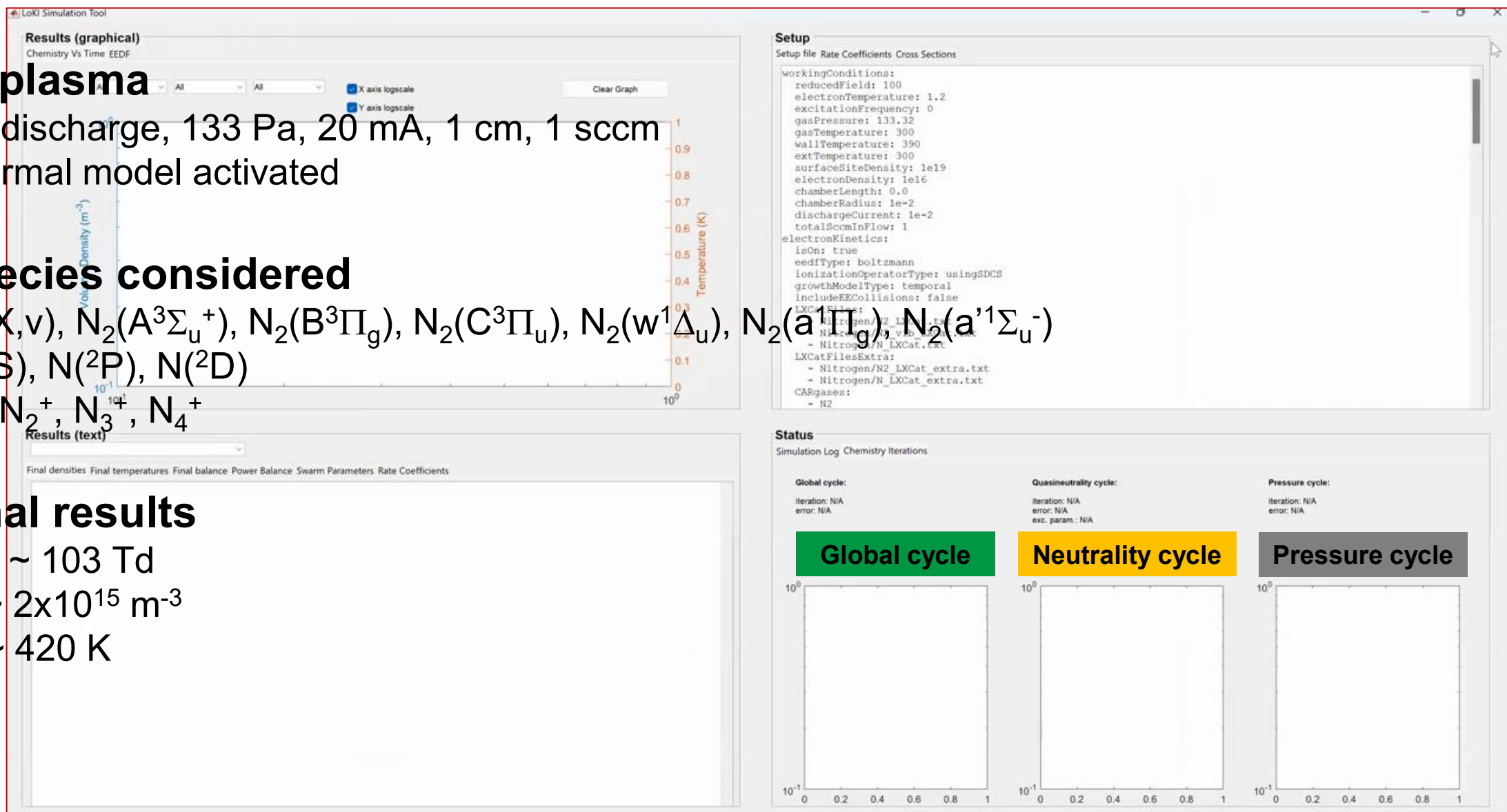
N⁺, N₂⁺, N₃⁺, N₄⁺

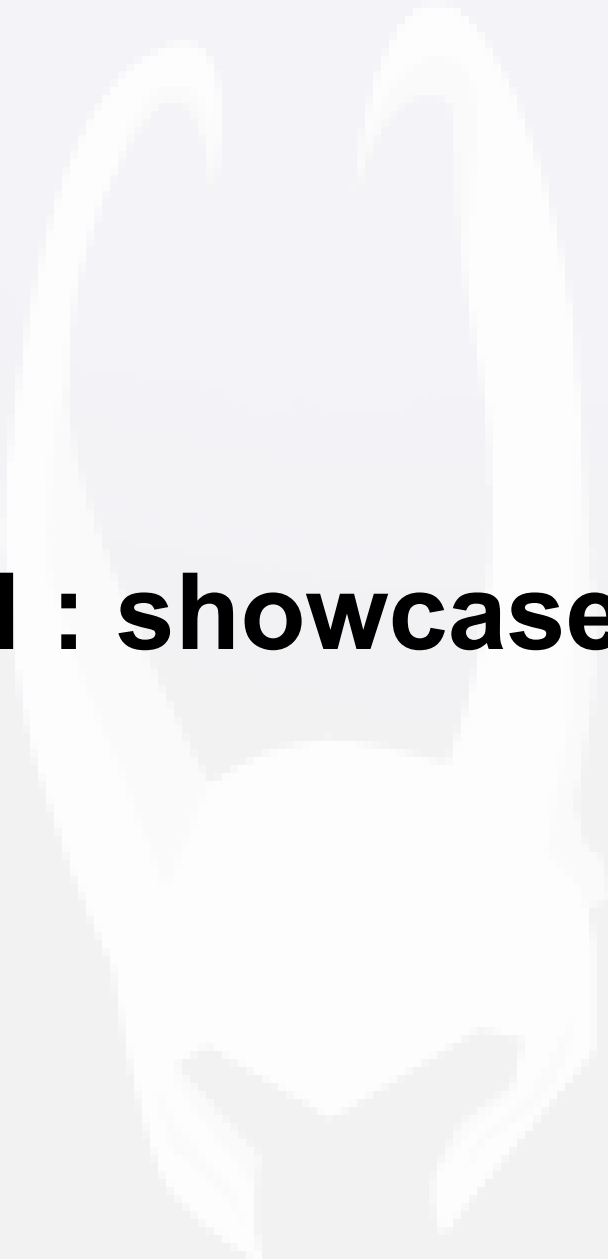
Final results

E/N ~ 103 Td

n_e ~ 2x10¹⁵ m⁻³

T_g ~ 420 K





LoKI-GM : showcase of results

Oxygen plasmas: validation of reaction mechanism

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

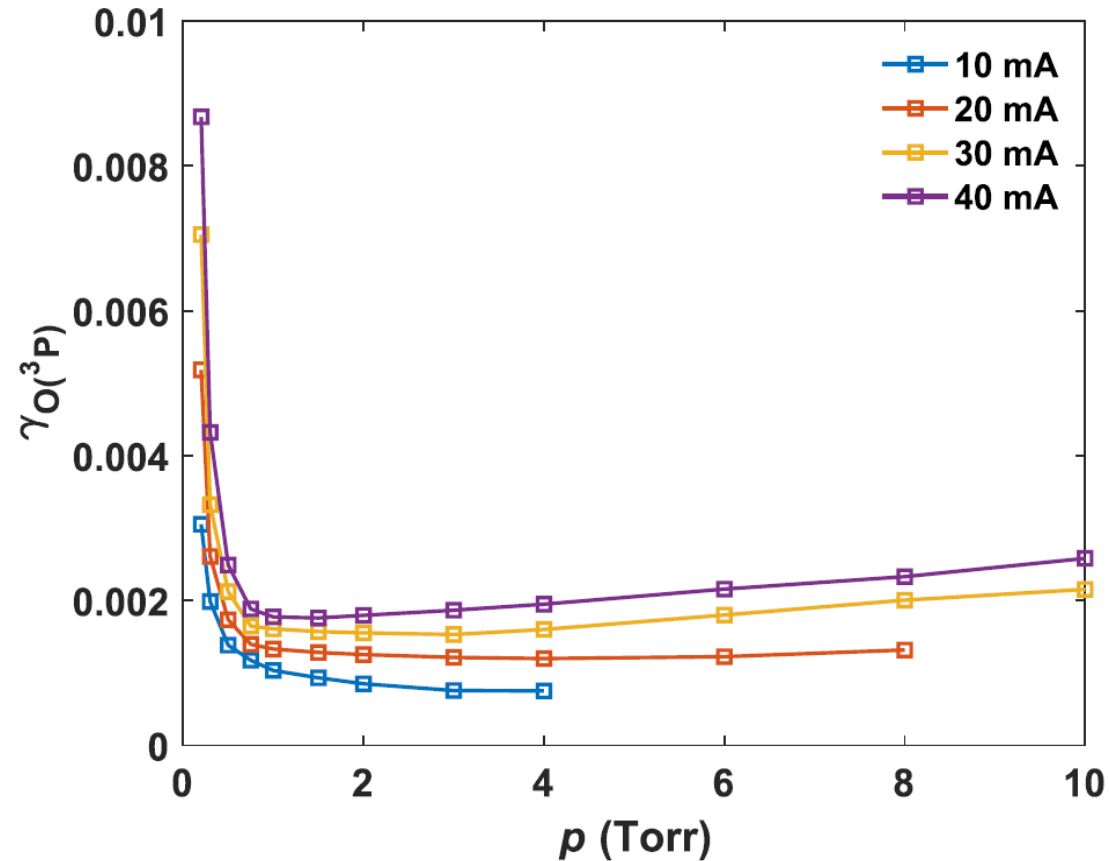
- electron-impact excitation/dissociation
- two- and three-body quenching
- wall recombination

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

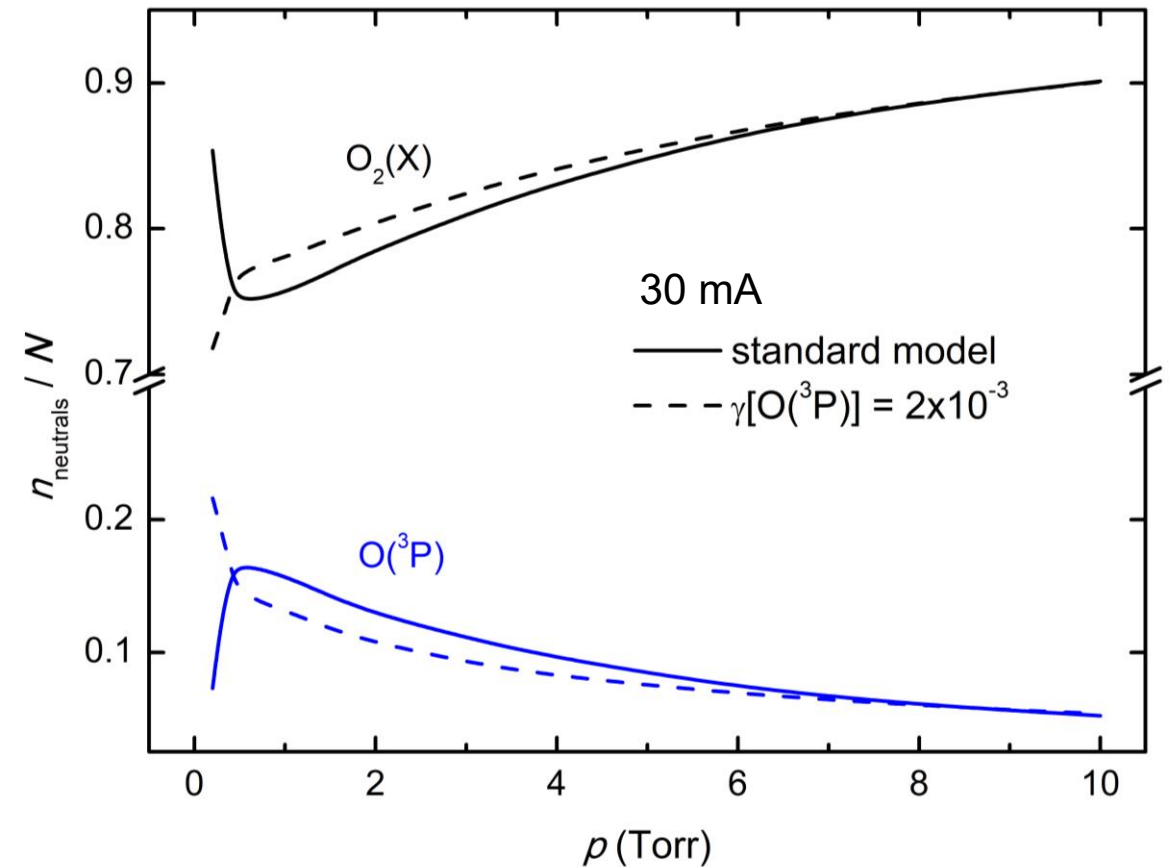
T C Dias *et al.* 2023 *Plasma Sources Sci. Technol.* **32** 084003

Oxygen plasmas: surface recombination

$O(^3P)$ wall-recombination probability



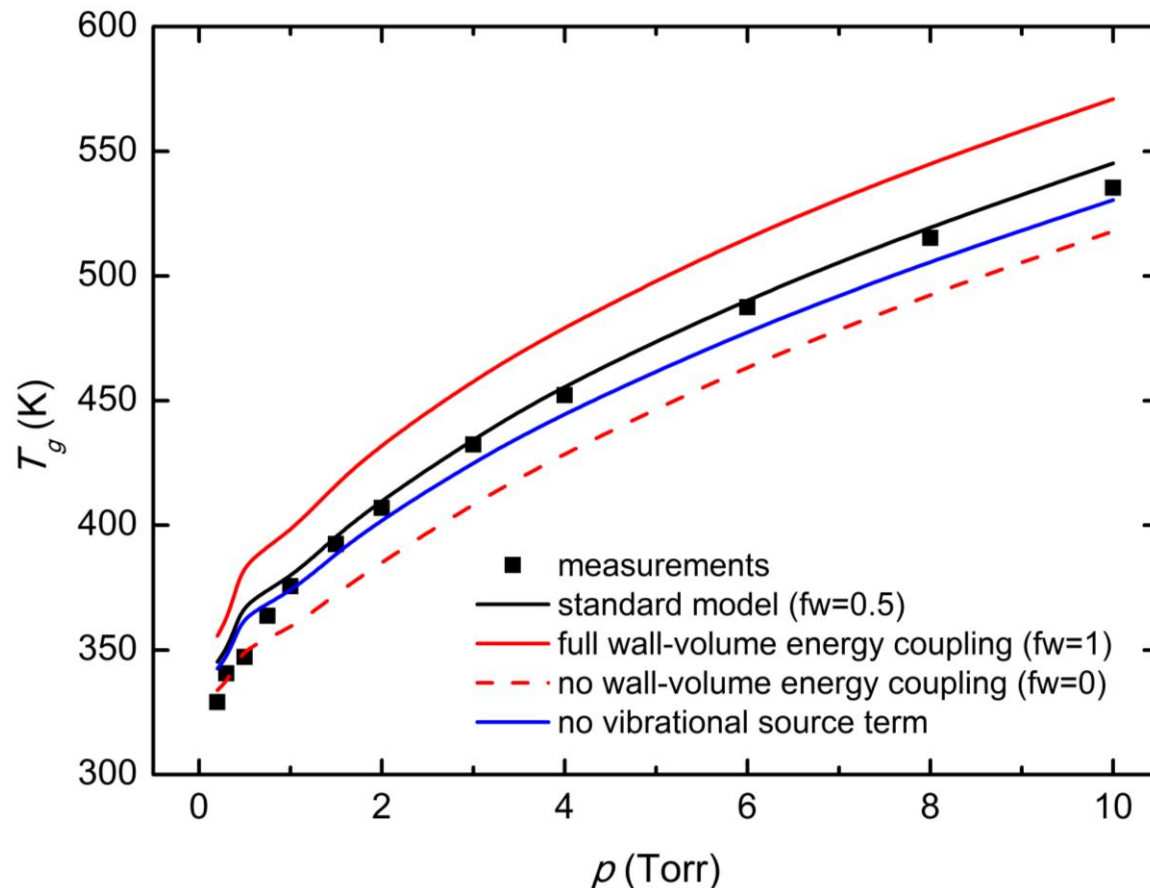
J-P Booth *et al.* 2020 *Plasma Sources Sci. Technol.* **29** 115009



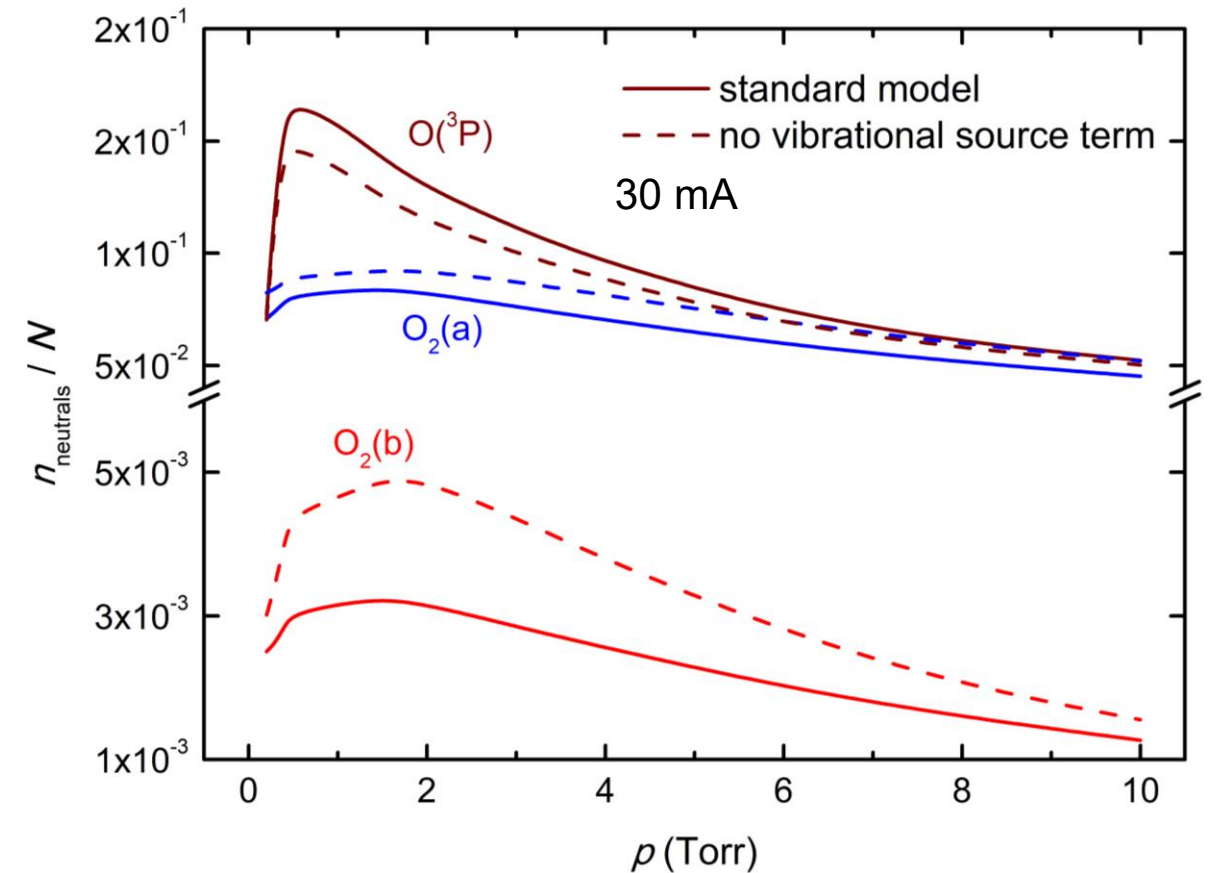
Oxygen plasmas: thermal model parameters

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%

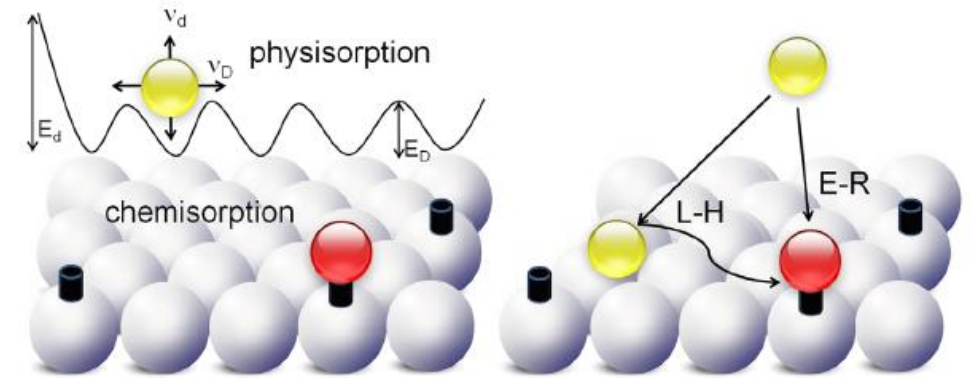
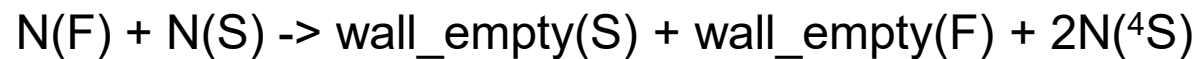


Nitrogen plasmas: verification of surface kinetics

Analysis of plasma-surface interaction

- $T_w = 200 - 2000$ K
- $[N(^4S)] = 10^{21} \text{ m}^{-3}$ (in the volume)
- $[\text{wall_empty}(F)] + [\text{wall_empty}(S)] = 10^{20} \text{ m}^{-2}$
- $[\text{wall_empty}(S)] / [\text{wall_empty}(F)] \sim 2 \times 10^{-3}$

Surface microkinetic mesoscopic model



physisorption

desorption

chemisorption

surface diffusion

Eley-Rideal recomb.

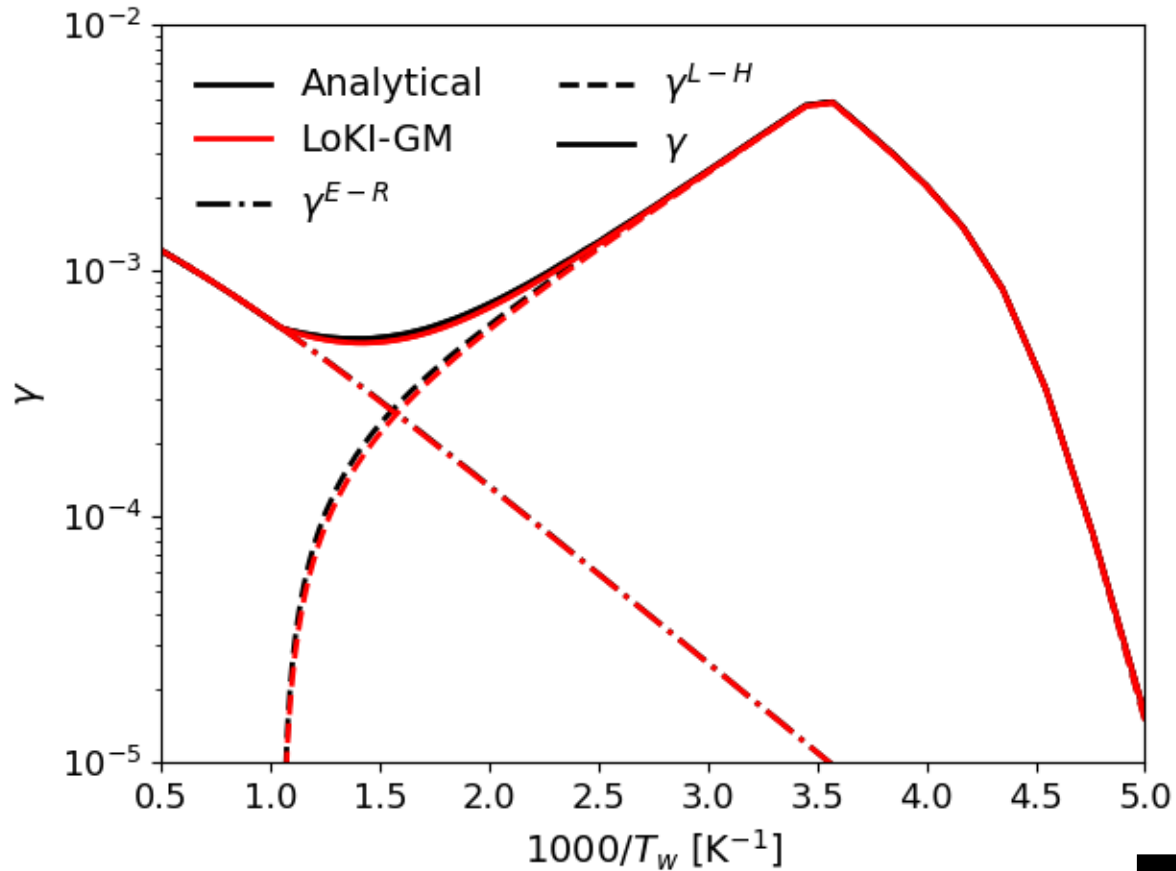
Langmuir- Hinshelwood recomb.

Eley-Rideal recomb. (phys.)

Langmuir- Hinshelwood recomb. (phys.)

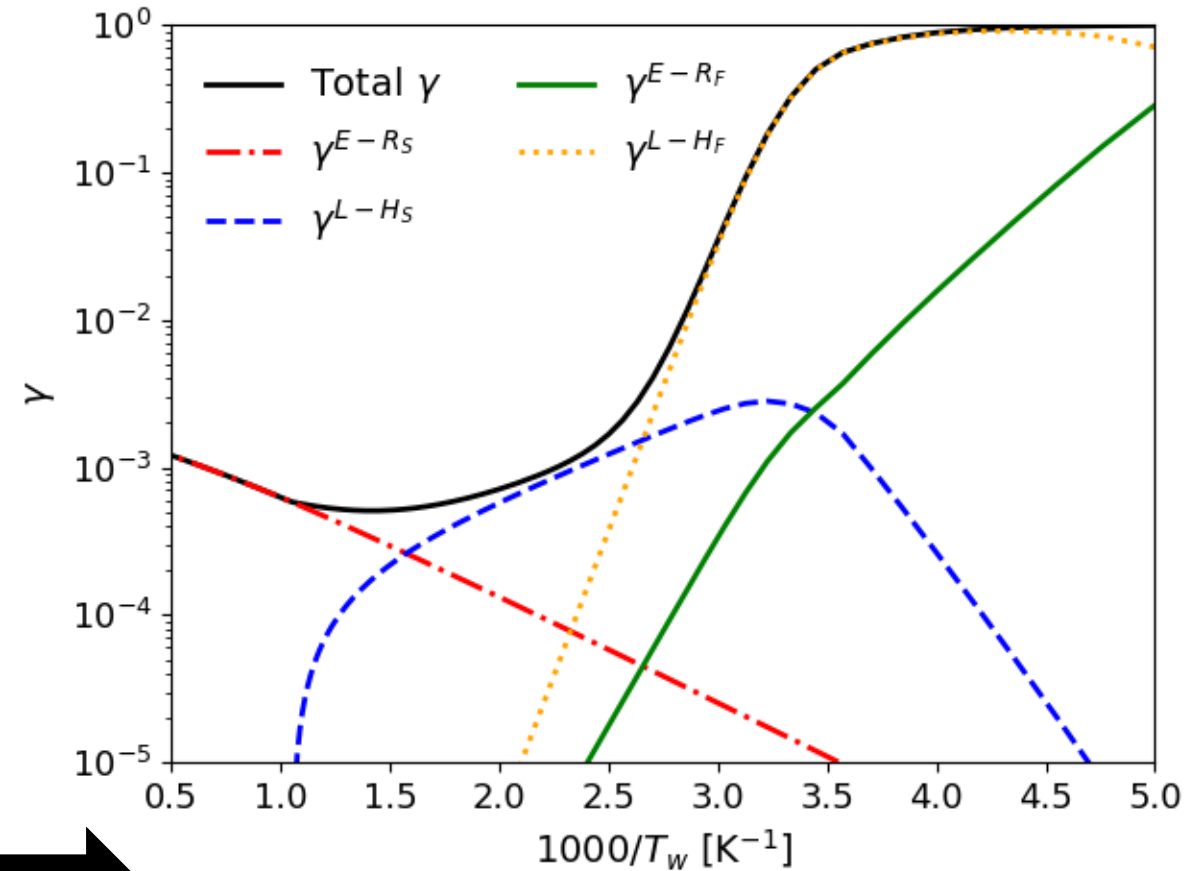
Nitrogen plasmas: surface kinetics

Verification of standard kinetics



Low T_w

Influence of extra mechanisms



Final remarks

- **Global models** are powerful predictive tools for the modelling of LTPs, particularly when the primary goal is the **assessment of plasma chemistry schemes**
- 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**

LoKI-GM (open-source in July 2026), will be employed within project **GREENFAB-X (HORIZONS-JU-CHIPS-2025-IA)**, which aims to foster innovation in green technologies and digital solutions for semiconductor manufacturing



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