Electron kinetics in fast-pulsed discharges

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1st Frontiers in Low-Temperature Plasma Simulations

Introduction

Predictive tools for non-equilibrium low-temperature plasmas (LTPs) should describe properly the **kinetics of electrons**, responsible for **inducing plasma reactivity**. Here, we focus on plasmas produced in N_2-O_2 gaseous mixtures, aiming to deliver a **KInetic Testbed for PLASMa Environmental and Biological Applications (KIT-PLASMEBA)** [1], comprising the development of simulation tools and the critical assessment of collisional-radiative data.

In this framework, we have developed the **LisbOn KInetics Boltzmann solver (LoKI-B)** [2,3], an **open-source** MATLAB® simulation tool that solves a time and space independent form of the **two-term electron Boltzmann equation** (EBE), for non-magnetized non-equilibrium LTPs created from different gases or gas mixtures. The simulation tool gives a microscopic description of the electron kinetics and calculates macroscopic quantities, such as **electron impact rate coefficients and electron transport parameters**.

Recently, there has been increasing interest in non-equilibrium LTPs created by **fast-pulsed discharges**, because of their potential advantages in different technological applications [4]. In this work, we present the recent developments introduced in LoKI-B in order to **improve the description of the electron kinetics in fast-pulsed discharges**.

Fast-pulsed discharges

The typical timescale of the breakdown, for gases at elevated pressures, ranges from the **nanosecond to the microsecond scale**. Changing the applied voltage during this crucial process greatly affects the plasma parameters and composition. With the advent of non-equilibrium plasmas at atmospheric pressures for many applications, discharges generated by voltage pulses with rise times up to hundreds of volts per nanosecond (or even higher) have become a **promising technique to tune the plasma for each specific application** [4].

Here, **global models** represents a simple, yet powerful, tool to study and understand plasmas produced by fast-pulsed discharges. One of the main pieces of information that are needed in a global model refers to electron parameters (rate coefficients, transport parameters, etc). This information can be obtained by **coupling the chemistry solver to an electron Boltzmann equation (EBE) solver**, typically adopting the classical two-term expansion.

In most cases this coupling involves several approximations (possibly due to the **lack of readily available time-dependent EBE solvers**): introducing **effective source terms** [5] that account for the electron-impact creation of excited species, or considering a **quasi-stationary situation for electrons** [6,7] solving a time-independent form of the EBE for the different (and time varying) values of the reduced electric field, E/N.

LisbOn KInetics

Time dependent EBE (two-term expansion)

Under the **classical two-term expansion**, and considering an **exponential temporal growth for the electron density**, the time dependent **equation for the isotropic component** can be writen as follows:

$$\frac{\partial f(u,t)}{\partial t}+\sqrt{\frac{m_e}{2eu}}\frac{\langle\nu_{eff}\rangle(t)}{N}uf(u,t)+\frac{1}{N}\sqrt{\frac{m_e}{2e}}\frac{\partial(G_{\rm el}(u,t)+G_E(u,t))}{\partial u}=S(u,t)$$

The total **inelastic collision operator**, $S(u,t)$, corresponds to the sum of all the single operators for the inelastic transitions:

$$S_{i,j}(u,t)=\delta_i\left[(u+V_{i,j})\sigma_{i,j}(u+V_{i,j})f(u+V_{i,j},t)-u\sigma_{i,j}(u)f(u,t)\right]+\delta_j\frac{g_i}{g_j}\left[u\sigma_{i,j}(u)f(u-V_{i,j},t)-(u+V_{i,j})\sigma_{i,j}(u+V_{i,j})f(u,t)\right]$$

The continuous operators that account for the **elastic collisions**, $G_{el}(u,t)$, and the interation with the **electric field**, $G_E(u,t)$, can be written as:

$$G_{\rm el}(u,t)=-\sum_k 2\gamma_k\nu^{\rm el}_{k/c}(u)u^{3/2}\left[f(u,t)+\frac{k_BTg}{e}\frac{\partial f(u,t)}{\partial u}\right]$$

$$G_E(u,t)=N\sqrt{\frac{2e}{m_e}}\frac{u}{3}\frac{E(t)}{N}f^1(u,t)$$

Finally the **equation for the anisotropic component**, $f^1(u,t)$, can be obtained as:

$$f^1(u,t)=-\frac{1}{\sigma_c(u)+\sqrt{\frac{m_e}{2eu}}\frac{\langle\nu_{eff}\rangle(t)}{N}}\frac{E(t)}{N}\frac{\partial f(u,t)}{\partial u}$$

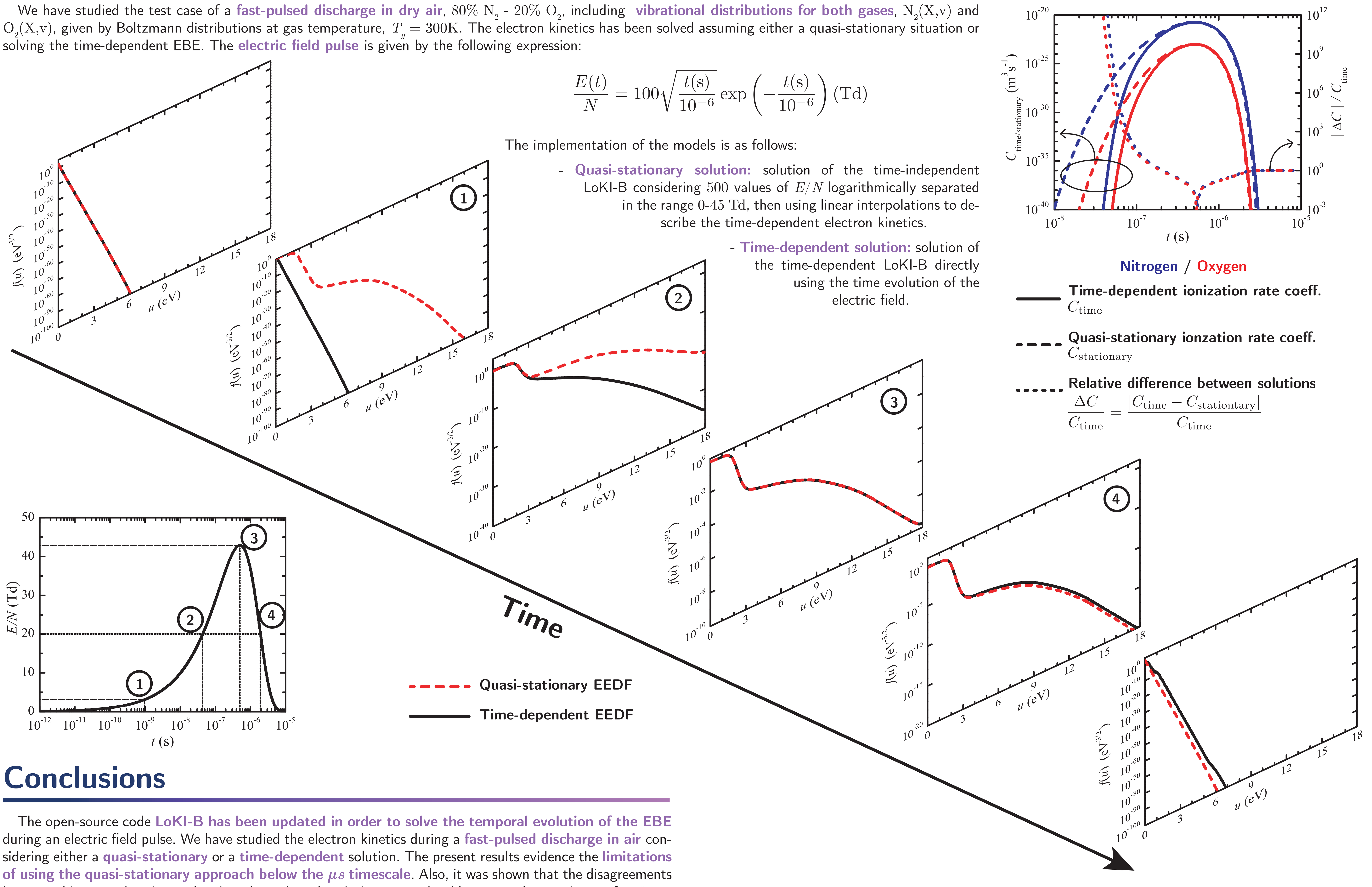
Comparison of quasi-stationary and time dependent calculations

We have studied the test case of a **fast-pulsed discharge in dry air**, 80% N_2 - 20% O_2, including **vibrational distributions for both gases**, N_2(X,v) and O_2(X,v), given by Boltzmann distributions at gas temperature, $T_g=300$K. The electron kinetics has been solved assuming either a quasi-stationary situation or solving the time-dependent EBE. The **electric field pulse** is given by the following expression:

$$\frac{E(t)}{N}=100\sqrt{\frac{t(\mathrm{s})}{10^{-6}}}\exp\left(-\frac{t(\mathrm{s})}{10^{-6}}\right)(\mathrm{Td})$$

The implementation of the models is as follows:

- **Quasi-stationary solution:** solution of the time-independent LoKI-B considering 500 values of E/N logarithmically separated in the range 0-45 Td, then using linear interpolations to describe the time-dependent electron kinetics.
- **Time-dependent solution:** solution of the time-dependent LoKI-B directly using the time evolution of the electric field.



Conclusions

The open-source code **LoKI-B has been updated in order to solve the temporal evolution of the EBE** during an electric field pulse. We have studied the electron kinetics during a **fast-pulsed discharge in air** considering either a **quasi-stationary** or a **time-dependent** solution. The present results evidence the **limitations of using the quasi-stationary approach below the μs timescale**. Also, it was shown that the disagreements between this approximation and a time-dependent description are noticeable even at longer times, of $\sim 10\mu s$.

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Acknowledgments

This work was funded by Portuguese FCT, Fundação para a Ciência e a Tecnologia, under projects UID/FIS/50010/2019 and PTDC/FISPLA/1243/2014 (KIT-PLASMEBA).

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1st Frontiers in Low-Temperature Plasma Simulations, 13 - 16 May (2019), Bad Honnef (Germany)