Electron kinetics in fast-pulsed discharges

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

[1] Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, Lisboa, Portugal
[2] Centro de Física da Universidade do Minho, Campus de Gualtar, Braga, Portugal
[3] Faculdade de Engenharia da Universidade do Porto, Porto, Portugal

This work presents a comparative study of the electron kinetics in fast-pulsed discharges produced in dry air (80% N_2 – 20% O_2), considering a quasi-stationary and a time-dependent solution of the electron Boltzmann equation (EBE), written under the classical two-term approximation. The simulations were performed using the open-source LisbOn KInetics Boltzmann solver (LoKI-B), which handles simulations in any atomic / molecular gas mixture, considering first and second kind collisions with any target state (electronic, vibrational and rotational), characterized by any user-prescribed population. The original capabilities of LoKI-B have been extended in order to obtain the time-dependent solution of the EBE for a pulsed electric field. Important deviations are found between the quasi-stationary and the time-dependent approaches, below the microsecond scale.

1. Introduction

Predictive tools for non-equilibrium low-temperature plasmas (LTPs) should describe properly the kinetics of electrons, responsible for stimulating the 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], an open-source 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 rate coefficients and transport parameters, which are key for solving global models [3]. Indeed, LoKI-B is coupled to a Chemistry solver (LoKI-C), that receives these parameters as input data.

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]. However, due to the lack of readily available time-dependent EBE solvers, several assumptions are usually made to incorporate the electron kinetics into the corresponding chemistry models: introducing effective source terms that account for the electron-impact creation of excited species [5], or considering a quasi-stationary description for electrons [6,7] by solving a time-independent form of the EBE for the different values of the reduced electric field, *E/N*, over the duration of the pulse.

2. Simulations of fast-pulsed discharges

We have studied the temporal evolution of the electron kinetics in a pulsed discharge, excited by a reduced electric field given as a function of time, *t*, by:

$$E/N\,(t) = 100\sqrt{\frac{t(\mathrm{s})}{10^{-6}}}\exp\left(-\frac{t(\mathrm{s})}{10^{-6}}\right)\ (\mathrm{Td}). \quad (1)$$

Figure 1 shows the time evolution of the pulse given by equation (1). The maximum value of *E/N* is ~45Td, which falls within the accepted limits of applicability of the two-term approximation for the EBE. The rise and fall times of the pulse are ~1μs and ~10μs respectively, and these somewhat long times were chosen to evidence the limitations of the quasi-stationary approach when compared with a full time-dependent description.

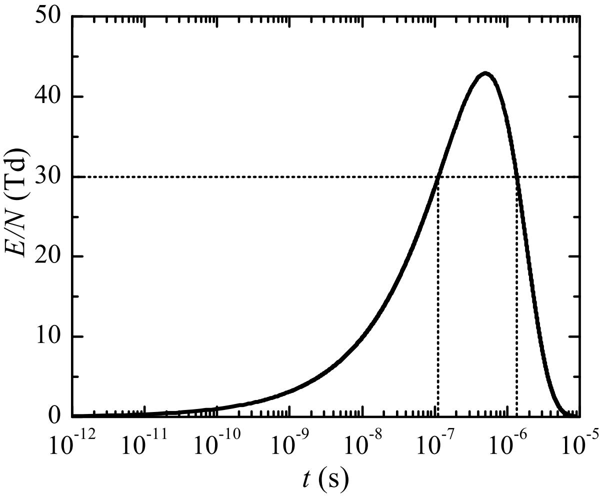

Fig. 1. Reduced electric field pulse given by equation (1).

In the quasi-stationary approach, LoKI-B was used to evaluate a lookup table for the electron macroscopic parameters, with 500 values of *E/N* logarithmically separated in the range 0 – 45 Td. Then, by using linear interpolation and the time dependence given in equation (1), we have obtained the temporal evolution of the macroscopic parameters. To perform the time-dependent calculations, we have extended the capabilities of LoKI-B by including the time derivative of the electron energy distribution function (EEDF) in the the EBE. The simulations have been carried out for a dry air discharge (80% N_2 – 20% O_2), including vibrational populations $N_2(X,v)$ and $O_2(X,v)$ given by Boltzmann distributions at the gas temperature, T_g = 300K.

3. Results

Figure 2 shows the temporal evolution of the electron-impact ionisation rate coefficients of N_2 and O_2, calculated for the time-dependent, C_{time}, and the quasi-stationary, $C_{\text{stationary}}$, approaches. In this figure, it is also shown the relative difference between the solutions, evaluated as $\frac{\Delta C}{C_{\text{time}}} = \frac{|C_{\text{time}}-C_{\text{stationary}}|}{C_{\text{time}}}$.

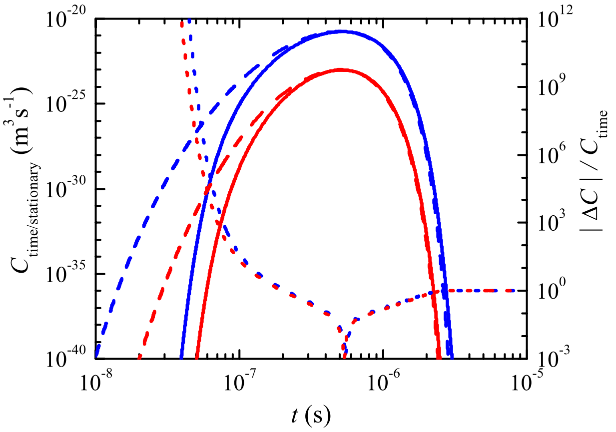

Fig. 2. Electron-impact ionisation rate coefficients of N_2 (blue) and O_2 (red), as a function of time, considering a time-dependent (solid) or a quasi-stationary (dashed) solution of the EBE (left axis). Relative difference between the solutions (dotted, right axis).

Around the peak of the pulse, ~5×10^{-7} s, the relative difference between the solutions drops to a minimum, this is caused because the time derivative of the reduced field vanishes, approaching a stationary situation. However, the difference between both solutions increases rapidly as we leave a narrow region around the maximum of the reduced field. For times above 10^{-6} s, both solutions are in reasonable agreement, yet reaching a non-negligible relative difference of ~100% (corresponding to a factor of 2 difference in the corresponding rate coefficients). Below 10^{-6} s, the results of the quasi-stationary solution deviate considerably from those obtained with the time-dependent EBE, over-estimating the electron-impact ionisation rate coefficients by a minimum of 3 orders of magnitude for times below 10^{-7}s. The previous differences are due to the instantaneous relaxation of the EEDF in the quasi-stationary approach.

Figure 3 shows the EEDFs obtained at 30 Td using the time-dependent solution for both, the rise time, ~10^{-7}s, and the fall time, ~1.5×10^{-6}s, (see figure 1) and adopting the quasi-stationary approach. Obviously, the latter is independent of the “history” of the EEDF, yielding the same results during both the rise and the fall times.

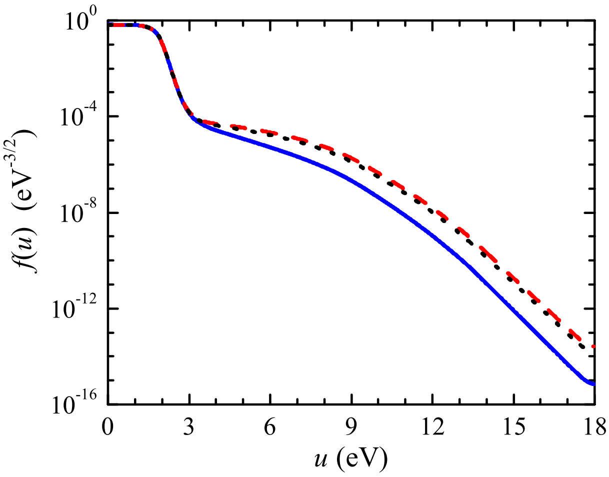

Fig. 3. EEDFs obtained at a reduced electric field of 30 Td, using time-dependent calculations during the pulse rise (solid blue) and the pulse fall (dashed red), and adopting the quasi-stationary approach (dotted black).

The EEDFs obtained with the quasi-stationary approximation, and thus the corresponding electron-impact rate coefficients, are clearly overestimated during the rise time and slightly underestimated during the fall time of the pulse. Therefore, the present results evidence the limitations of using the quasi-stationary approach to simulate pulses with durations below the μs timescale. Also, it was shown that the disagreements between this approximation and a full time-dependent description are noticeable even at longer times, of ~10μs.

Acknowledgments

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