Electron kinetics in fast-pulsed discharges

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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 represent a simple, yet powerful, tool to study and understand plasmas produced by fast-pulsed discharges. One of the main pieces of information that is 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 different instantaneous values of the reduced electric field, E/N.

Time-dependent EBE (two-term expansion)

Under the classical two-term expansion, and considering a space-independent exponential temporal growth for the electron density, the time-dependent EBE writes as follows:

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

Isotropic component equation

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

Anisotropic component equation

$$G_{\rm el}(u,t) = -\sum_k 2\frac{m_e}{M_k}\nu^{\rm el}_{k,c}(u)\,u^{3/2}\left[f(u,t) + \frac{k_B T g}{e}\frac{\partial f(u,t)}{\partial u}\right] \longrightarrow \text{Elastic collision operator}$$

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

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

The anisotropic component of the electron distribution function is assumed to be in steady-state because:

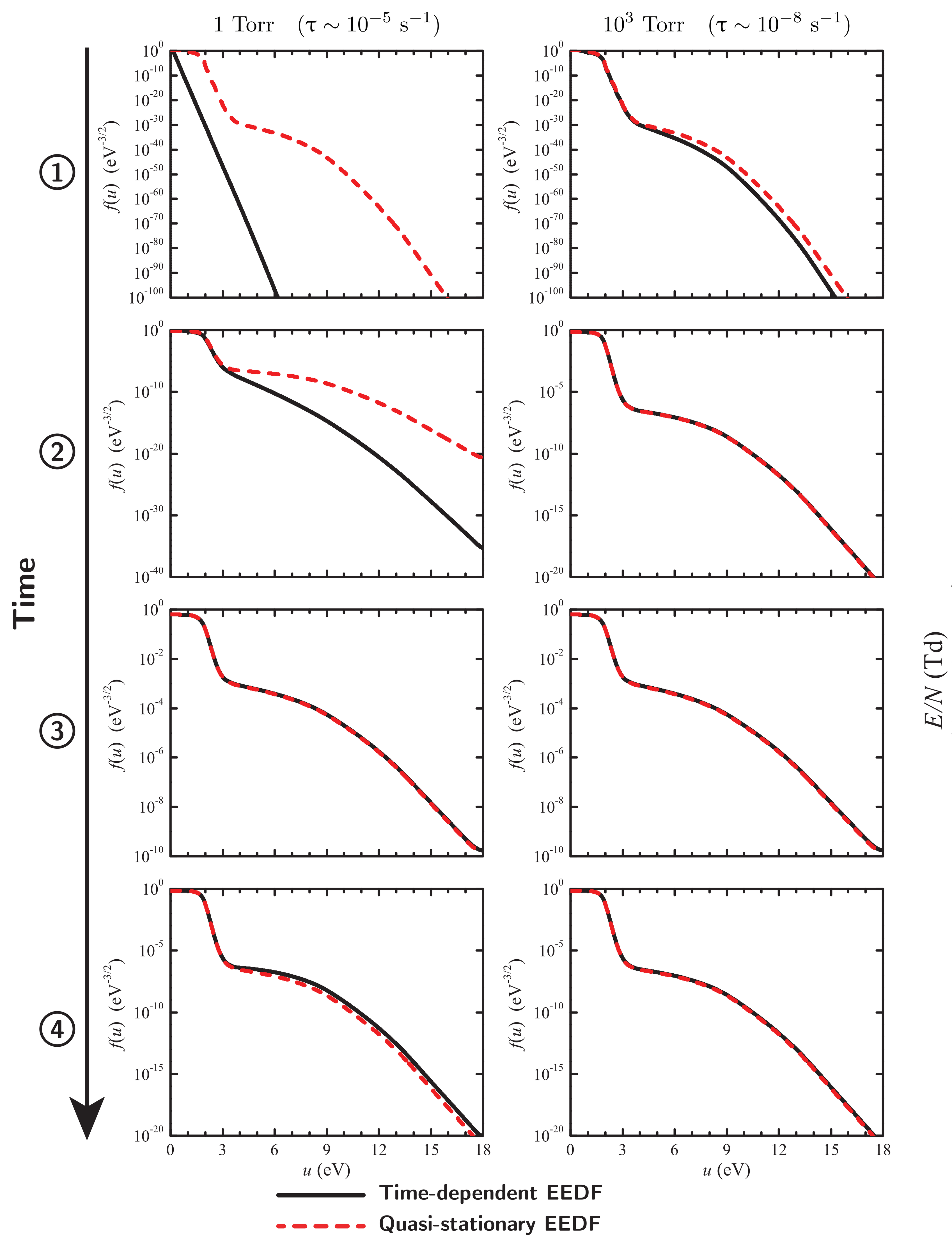
$$\underset{\text{Characteristic reaction time of the isotropic component of the EDF}}{\tau \sim \frac{1}{\sum_k \frac{m_e}{M_k}\nu^{\rm el}_{k,c}}} \gg \underset{\text{Characteristic reaction time of the isotropic component of the EDF}}{\frac{1}{\sum_k \nu^{\rm el}_{k,c}} \sim \tau_1}$$

In order to neglect the temporal derivative of the isotropic equation (*i.e.* quasi-stationary solution), the characteristic reaction time of the isotropic component of the EDF has to be much shorter than the characteristic time of the excitation.

$$\frac{10^{18}\ {\rm m^{-3}s^{-1}}}{N} \sim \tau \ll \tau_{\rm exc} \Leftrightarrow \text{Quasi-stationary solution}$$

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, for two different pressures 1 Torr and 10^3 Torr. The electron kinetics has been solved assuming either a quasi-stationary situation or solving the time-dependent EBE.



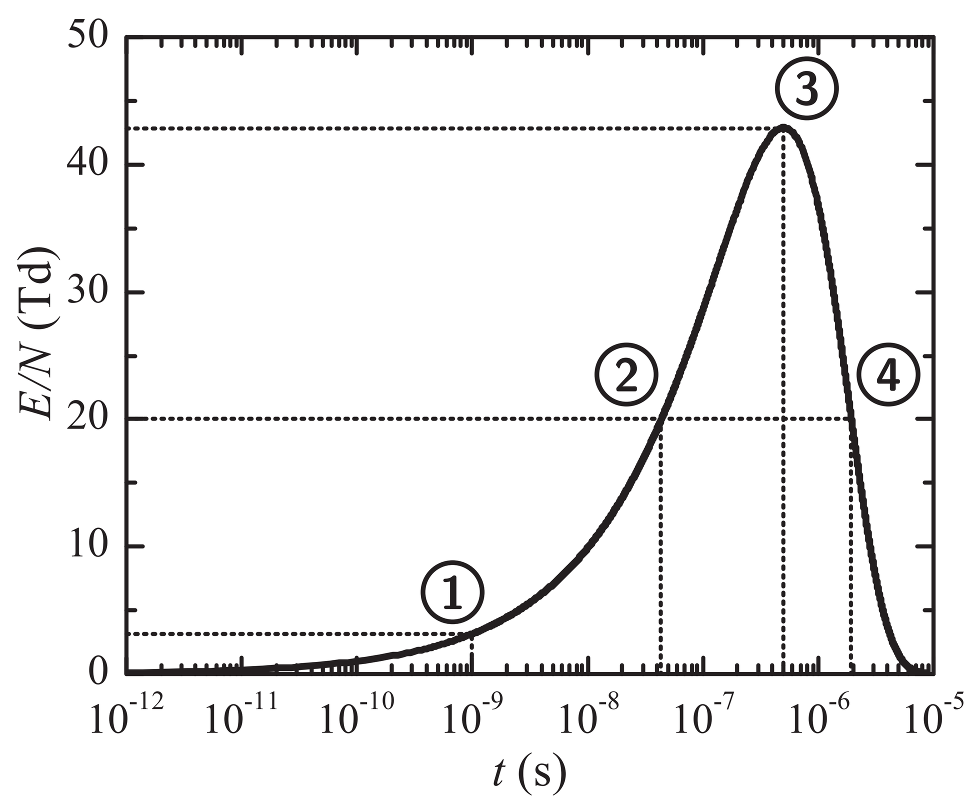
The implementation of the models is as follows:

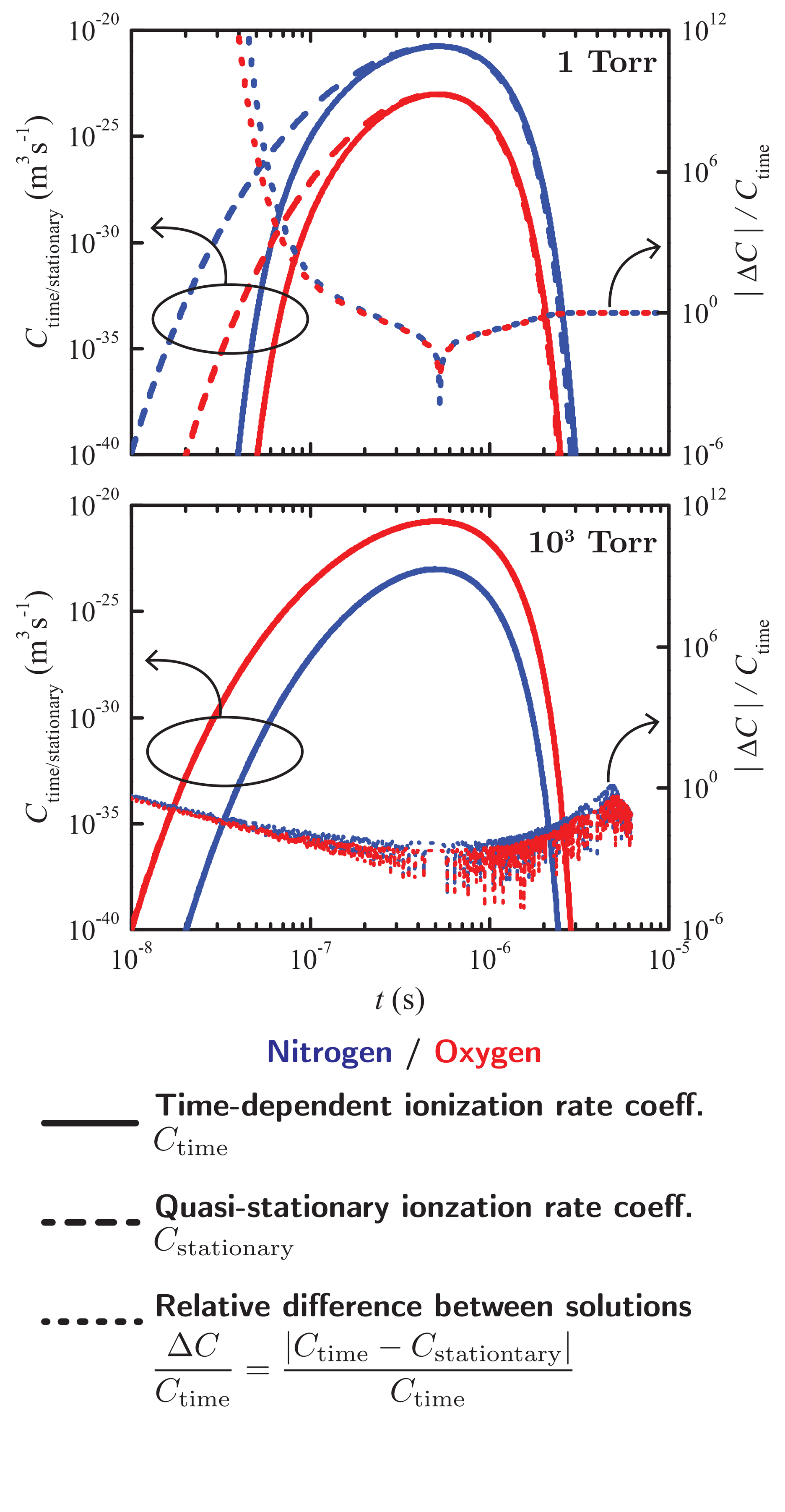
- Quasi-stationary solution: solution of the time-independent LoKI-B considering 1000 values of E/N logarithmically separated in the range 0-45 Td, then using linear interpolations to describe the time-dependent electron kinetics.
- Time-dependent solution: solution of the time-dependent LoKI-B directly using the time evolution of the electric field.

The electric field pulse is given by the following expression:

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

$$(\tau_{\rm exc} \sim 10^{-6})$$





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 for the cases of low and high pressures. The present results evidence the limitations of using the quasi-stationary approach in the μs timescale for low-pressure discharges. It was also shown that for high-pressure discharges the quasi-stationary approach is applicable in the μs timescale. However, it has to be noticed that in both cases the quasi-stationary solution fails in the ns timescale.

References

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