Are Local-Field and Local-Energy approximations appropriate for nanosecond discharges?

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Interest in nanosecond-pulsed discharges (NPDs) is rapidly growing due to their remarkable non-equilibrium properties. However, their potential comes with considerable complexity, and a detailed study of the fundamental processes in the discharge is necessary to determine the most efficient configuration for a specific application. NPDs are characterized by very high reduced electric fields, E/N, that can be as high as ~ 1000 Td, with rising times on the nanosecond timescale. These characteristics represent significant modeling challenges, particularly concerning electron kinetics and their coupling with heavy species.

Obtaining a comprehensive solution of electron kinetics in gas discharges that accounts for dependencies in space, velocity and time is often unfeasible. Therefore, the electron behavior is frequently studied under one of two assumptions [1,2]: the local-field approximation (LFA), which equates the solution of electron kinetics to the steady-state calculation with the local and instantaneous value of the reduced electric field (E/N); the local-energy approximation (LEA), which includes an equation for the local mean energy, with the rate coefficients and the electron power distribution among different collisional channels depending on the local value of mean energy.

In this work, we focus on time-locality to assess the impact of the LFA and LEA assumptions on the calculation of the temporal evolution of electron kinetics in nanosecond discharges. To do so, we consider an accurate Monte Carlo (MC) time-dependent formulation as a golden standard, implemented in LoKI-MC [3,4]. The study involves a nanosecond pulse mirroring typical conditions found in experiments, with a maximum *E/N* of 300 Td at 2.5 ns and vanishing after ~30 ns. Moreover, we assess electron relaxation in two background gases (air and argon) and two pressures (10 and 100 Torr).

Figure 1 illustrates the mean electron energy $\langle\varepsilon\rangle$ as a function of time in air at both pressures, comparing the rigorous time-dependent MC approach with the LFA and the LEA. At 10 Torr, the evolution of $\langle\varepsilon\rangle$ calculated by the LFA differs significantly from the rigorous approach. This discrepancy arises because at lower pressures electrons do not collide rapidly enough to adapt to fast *E/N* variations. After ~2 ns, the solutions begin to converge. However, around 20 ns, when the *E/N* has decayed to 25 Td, the LFA again deviates from the time-dependent solution. Notably, the LEA captures much better both the rise and decay of the energy. At 100 Torr, where electron collisions are significantly more frequent than at 10 Torr, the LFA is valid over a broader interval, yet the LEA still offers a better description than the LFA.

Figure 2 shows $\langle\varepsilon\rangle$ as a function of time in argon at both pressures. While the conclusions are similar, the failure of the LFA and the higher quality of the LEA are even more evident than in air, since energy relaxation is generally much weaker in argon.

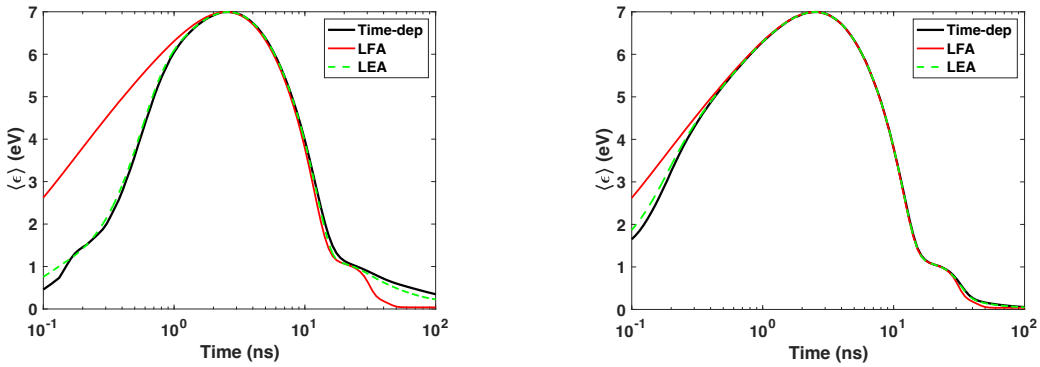

Figure 1: Temporal evolution of the mean electron energy in air at (a) 10 Torr and (b) 100 Torr.

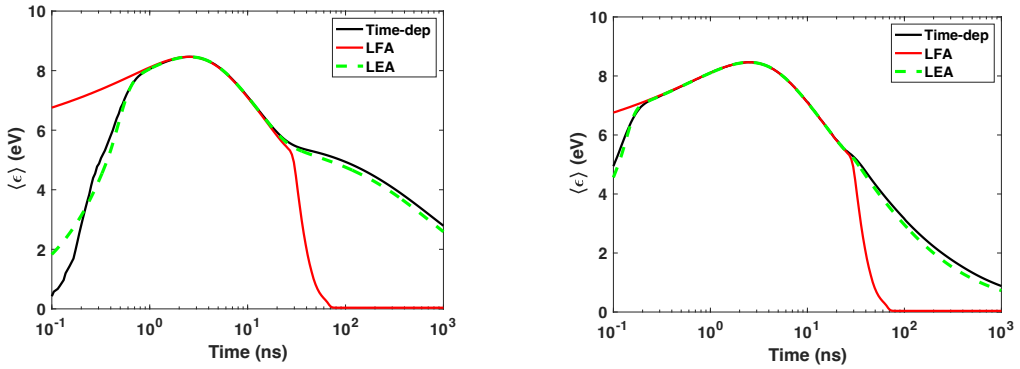

Figure 2: Temporal evolution of the mean electron energy in argon at (a) 10 Torr and (b) 100 Torr.

To evidence that these approximations can have an impact in the plasma chemistry, figure 3 illustrates the temporal evolution of the chemical kinetics in air at 10 Torr, using as input the different approaches for the electron kinetics. For the charged species depicted in figure 3a, the LFA significantly overestimates the decay of the ions. Additionally, figure 3b demonstrates that the neutral kinetics might also be affected, as the LFA cannot correctly capture the early rise of the excited states of N_2. Naturally, if we consider mixtures with rare gases, the differences would be greatly amplified.

In the conference, we will discuss in detail the physical reasons for the (in)success of the approximations, focusing on the comparison between the characteristic frequencies of relaxation and the time derivative of *E/N*. This discussion will also serve as a guideline on how modelers should check the validity of the time-locality approximations, even when a rigorous time-dependent solution is not available for benchmark.

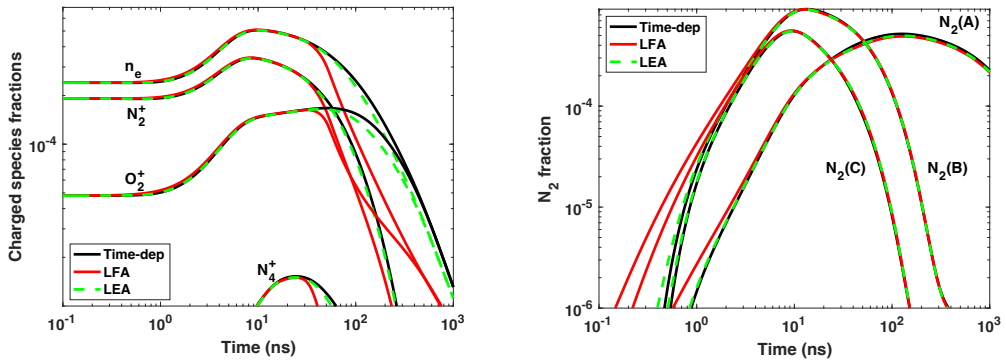

Figure 3: Temporal evolution of (a) charged species and (b) N_2 excited states, in air at 10 Torr.

IPFN activities were supported by the Portuguese FCT, under projects UIDB/50010/2020 (https://doi.org/10.54499/UIDB/50010/2020),UIDP/50010/2020(https://doi.org/10.54499/UIDP/50010/2020), LA/P/0061/2020 (https://doi.org/10.54499/LA/P/0061/2020) and PTDC/FISPLA/1616/2021 (https://doi.org/10.54499/PTDC/FIS-PLA/1616/2021).

[1] S. Dujko *et al.*, *J. Phys. D: Appl. Phys.* **46** (2013) 475202.

[2] G. K. Grubert *et al.*, *Phys. Rev. E* **80** (2009) 036405.

[3] T. C. Dias *et al.*, *Plasma Sources Sci. Technol.* **32** (2023) 095003.

[4] T. C. Dias *et al.*, *Comput. Phys. Commun.* **282** (2023) 108554.