MONTE CARLO CHEMICAL KINETICS IN LOW-TEMPERATURE PLASMAS

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Low temperature plasmas (LTP) are very important for various industrial and biological applications due to their non-equilibrium nature, which can enhance several chemical reactions. Nonetheless, these systems are extremely complex to study, because it is very difficult to diagnose experimentally the main processes that rule their behavior. Therefore, besides experimental efforts, it is important to model theoretically the physics of a LTP. If the model describes correctly the measured experimental quantities and their dependences with the discharge operating parameters, then we can infer the underlying physical picture. With this knowledge, industrial processes can be controlled and optimized.

Several LTP models adopt a deterministic description to couple the electron Boltzmann equation to a system of rate balance equations describing the heavy species kinetics. This strategy has been successful to study plasma chemistry in a variety of discharges. However, it fails for nanosecond discharges, subject of growing interest in the last years. These discharges operate with very high reduced electric fields (of the order of 100 Td and above) and in the nanosecond time scale. The most common method to solve the electron Boltzmann equation relies on a low-anisotropy approximation, which stands only for low reduced electric fields. Moreover, the deterministic approach is only valid for systems where the fluctuations and correlations are not relevant. In a nanosecond discharge, where the time scale of the discharge itself is the time scale of the electrons, the fluctuations and correlations may generate instabilities in the description on the heavy species chemistry. A simultaneous Monte Carlo description of both the electron and the heavy-species kinetics allow to properly describe these features.

In this work, we present a general Monte Carlo model for the heavy-species chemistry, which describes correctly the systems in the deterministic approach and goes further in situations where instabilities may be important. The modeling results are compared with well-established deterministic models. In the future, a similar Monte Carlo description will be applied to the electron kinetics, in order to have a fully coupled MC description of a LTP on the nanosecond time scale.

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