A Global Model For DBD Conversion Of CH_4/CO_2

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Non-thermal plasmas are being studied for conversion of CH_4 into other energy sources, either directly or through the production of Syngas intermediate. Of the different mixtures studied, CH_4/CO_2 is particularly interesting and has been studied in dielectric-barrier discharges (DBD) which provide interesting values of electron density and mean electron energy.

In the present work we focus on the complex kinetics associated with CH_4, CO_2 and its products, particularly in the description and coupling of the electron and chemical kinetics in the active phase of the discharge and in the post-discharge. For this purpose we developed a 0D kinetic model, allowing the study of the most important elementary processes and reactions occurring in the system. We specifically aim at a simplified global model for a DBD as a plug flow reactor. The time evolution of the system corresponds to the evolution of an elementary volume along the flow direction, averaged on the orthogonal directions to the flow.

At atmospheric pressure, DBD in CH_4 and CO_2 are filamentary, with conducting channels formed through streamer propagation in the gas gap. These microdischarges are simulated with a semi-empirical time-dependent electric field pulse, adjusted to reproduce the current measurements. A good description of the field pulses is essential to correctly simulate the non-homogeneous microdischarges in our global model.

The chemical kinetics is studied by solving the coupled continuity equations for each species. These include several neutrals, metastables, positive and negative ions and electrons. The electron Boltzmann equation is solved in the hydrodynamic regime with an expansion of the electron velocity distribution function (evdf) in density gradients using an iterative method based on the discrete ordinate S_n method [1]. The collision term includes elastic and 1st and 2nd kind inelastic collisions. Vibrational populations are considered for super-elastic and multi-step excitation and ionization. The calculated evdf is then used to obtain the rate coefficients of the electron collision reactions, in the local field approximation.

Our results show a significant dependence of the values of electron density and electrical characteristics, such as the current, on the magnitude and shape of the field pulse, which also influences the long-term chemistry. The main reactions and paths to the conversion of the reagents into more valuable products are discussed.

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[1] P. Segur, M. Yousfi, and M. C. Bordage, *J. Phys. D: Appl. Phys.*, **17**, 2199 (1984)