A DETAILED REACTION MECHANISM SET FOR VIBRATIONAL CHEMISTRY IN CO_2 PLASMAS

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Abstract. This contribution is devoted to the modelling of CO_2-containing discharges. The presented work is supported by a zero-dimensional chemistry model coupled with the homogenous electron Boltzmann equation which has been validated by isolating different aspects of the complex kinetics, namely through the: (i) study of the time-resolved evolution of the lower vibrationally excited CO_2 levels during the afterglow of CO_2 discharges (Silva 2018) (ii) investigation of the effect of electrons on the distribution of the lower vibrationally excited CO_2 levels obtained in pulsed and continuous glow discharges (Grofulovic 2018), (iii) investigation of the influence of N_2 on the CO_2 vibrational distribution function and dissociation yield in pulsed glow discharges (Terraz 2020), (iv) validation of the electron-impact dissociation cross sections of CO_2 (Morillo-Candas 2020) and (v) study of the gas heating in the afterglow of pulsed CO_2 glow discharges (Silva 2020). Herein we address different theories and scaling laws to describe the CO_2 decomposition and the vibrational excitation involving highly excited states. Special attention is devoted to the difference between state-to-state and single- or multi-temperature approximation methods. The influence of different reaction rate coefficients on important plasma parameters, namely the gas temperature, vibrational distribution functions and dissociation rates is analyzed in detail. In order to complement this study and validate our kinetic model, the simulation results are compared against experimental data obtained in pulsed DC glow discharges, with special interest on the understanding of the mechanisms leading to oxygen and CO production.

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