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Fast and accurate simulations of electrons in CO2 using Monte Carlo Flux LUCA VIALETTO, PEDRO VIEGAS, DIFFER - Dutch Institute for Fundamental Energy Research, SAVINO LONGO, University of Bari, PAOLA DIOMEDE, DIFFER - Dutch Institute for Fundamental Energy Research — Numerical models are fundamental to understand mechanisms underlying plasma-assisted activation of CO_2. Due to the complex chemical network and the presence of multiple time scales, those models require fast and accurate computational approaches. In this work, approximations that are usually employed in the study of electron kinetics in CO_2 are analyzed, together with strategies to overcome them. A fully native Monte Carlo Flux (MCF) code has been developed to calculate steady-state and time-dependent electron velocity distribution functions (EVDF). The MCF method is based on an highly efficient variance reduction technique and it has been extended to take into account the thermal velocity distribution function of the gas molecules and an accurate description of rotationally and vibrationally excited states.Deviations of rate coefficients up to 70% between MCF and two-term Boltzmann solvers are found, due to the anisotropy of the EVDF. Moreover, this extension provides a better agreement with measured transport coefficients at low reduced electric fields (E/N). A good agreement between experimental values of dissociation rate coefficients and MCF calculations is found at moderate E/N values after careful consideration and analysis of several cross sections data set.

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