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ELECTRON TRANSPORT COEFFICIENTS IN CO: SCANNING DRIFT TUBE MEASUREMENTS AND KINETIC COMPUTATIONS

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Abstract. In this work, we present scanning drift tube measurements and kinetic computations of electron swarm transport coefficients in CO, including drift velocity, longitudinal diffusion coefficient and ionization rate coefficient, as a function of the reduced electric field at room temperature. Kinetic computations are carried out based on a Monte Carlo (MC) simulation approach and by solving the electron Boltzmann equation. Using an MC technique, the ionization coefficient is computed from the spatial profile of the number of electrons in an idealized steady-state Townsend (SST) experiment. It is found that the measured and calculated transport coefficients agree generally very well.

1. INTRODUCTION

The knowledge of electron collisions and transport processes in CO is essential for understanding the fundamental electron-CO interactions in planetary atmospheres and interstellar media (Cambell et al. 2011). CO also offers a broad range of plasma-based technology applications, ranging from plasma etching (Omori et al. 1996) and plasma medicine (Carbone and Douat 2018) to gas lasers (Grigorian and Kochetov 2008) and syngas production (Cimerman et al. 2018). Experimental and

modelling studies on the activation of the CO_2 molecule (Pietanza et al. 2017), where the CO molecule is one of the most important resultant species, can also benefit from the related swarm-based studies.

In this work, as a part of our on-going investigations of electron transport in CO, we present scanning drift tube measurements of electron swarm transport coefficients and make comparisons with previous measurements. In addition, we test the completeness and consistency of Biagi's most recent cross-section set for electron scattering in CO (Biagi 2021) by comparing the measured electron swarm transport coefficients with those obtained by kinetic calculations and MC simulations. Finally, we investigate the spatial relaxation of electrons in an idealized SST setup in CO with the particular emphasis upon the calculation of the density-reduced effective Townsend ionization coefficient.

2. EXPERIMENTAL SYSTEM AND METHODS OF CALCULATIONS

Our measurements of the electron transport coefficients are performed with a 'scanning' drift tube apparatus. Similar measurements with this system have already been carried out for several gases (Vass et al. 2017, Pinhão et al. 2021). The system operates under time-of-flight (TOF) conditions, where the evolution of the initiated electron cloud is monitored through the detection of particles beyond a zone of variable drift length. The experimental system is unique because it allows the recording of 'swarm maps' which show the spatial and temporal development of electron clouds under TOF conditions. The derivation of the swarm transport coefficients of the electrons is based on fitting the swarm maps using the solution of the diffusion equation under hydrodynamic conditions. We observed a certain sensitivity of the detector system with respect to the pressure and the energy distribution of the electrons. A correction procedure was developed, which is based on the simulation of the electrons' motion in the experimental system, under the same conditions at which experimental recordings for the transport coefficients are made.

We apply two different methods to solve the electron Boltzmann equation. The first method includes a multi-term approach for the solution of this kinetic equation under spatially homogeneous (BE MT) and SST (BE SST) conditions. The second method is based on an expansion of the electron velocity distribution function with respect to spatial gradients of the electron density (BE DG). These two methods and the associated mathematical machinery are by now standard and for details the reader is referred to previous works (Vass et al. 2017, Pinhão et al. 2021).

In addition, we also employ an MC simulation technique. In our Monte Carlo simulations, we track many electrons (typically 10^6-10^7) simultaneously under TOF and SST conditions, respectively. The movement of a single electron is monitored until it collides with the background molecules of CO. The equation of the collision

probability is solved numerically by using the appropriate set of random numbers. The type of collision determines the scattering parameters after the collision, including the electron speed and direction of motion. Electron transport coefficients are determined after relaxation in the stationary state using formulae given in our earlier publications (Dujko et al. 2021).

3. RESULTS AND DISCUSSION

In figure 1 we show the variation of the drift velocity (a) and longitudinal characteristic energy (b) with the reduced electric field E/N. Panel (a) shows both families of the transport coefficients, the flux and the bulk ones, and panel (b) displays the bulk values of D_L/μ.

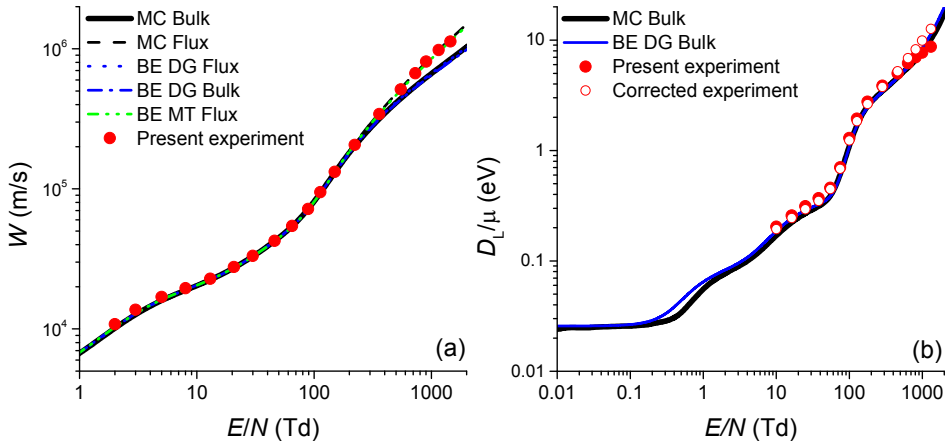

Figure 1: Comparison of the calculated flux and bulk drift velocities and the present experimental data (a), and comparison between the calculated bulk values of the longitudinal characteristic energy and the corrected and uncorrected experimental data (b).

The present experimental and calculated data for the bulk drift velocity (a) and D_L/μ (b) agree very well over the entire range of E/N considered in this work. This indicates that the experimental data in the scanning drift tube apparatus are the bulk transport coefficients. For $E/N \geq 130$ Td the bulk values are greater than the corresponding flux values for both the drift velocity and D_L/μ, which is a clear indication of the explicit effects of ionization processes on the transport coefficients.

In figure 2, we show the variation of the density-reduced effective Townsend ionization coefficient α_{eff}/N with E/N. The present experimental data for α_{eff}/N, are derived from the set of measured data $\{\nu_{eff}/N, W, ND_L\}$ where ν_{eff}/N is the density-

reduced effective ionization frequency, W is the bulk drift velocity and ND_L is the bulk longitudinal diffusion coefficient. The present modelling results include the MC and BE SST calculations under SST conditions (BE SST), while the MC and the BE DG results under hydrodynamic conditions (e.g., the MC Hydro and the BE DG Hydro) are derived from the set of the calculated coefficients $\{\nu_{eff}/N, W, ND_L\}$. For E/N < 300 Td, the agreement between experimental and modelling results is very good and lies within 5 %. For higher values of E/N the present experimental data agree very well with the modelling results (within 10 %), particularly with the MC SST results.

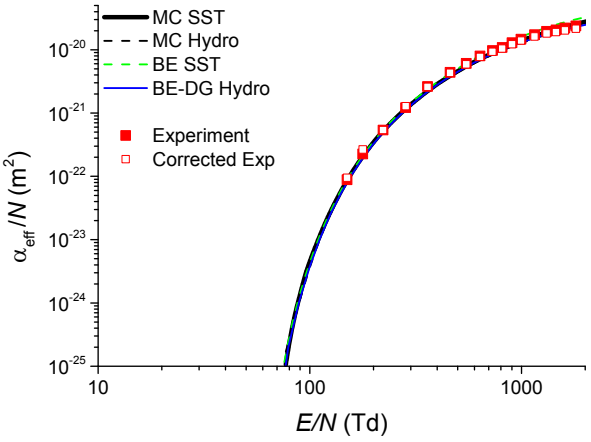

Figure 2: Variation of the density-reduced effective Townsend ionization coefficient with E/N.

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