

Kinetic mechanisms in vibrationally excited CO₂ plasmas

C. Fromentin^{(*)1}, T. Silva¹, T.C. Dias¹, V. Guerra¹, E. Baratte², O. Guaitella², A.S. Morriillo-Candas³, O. Biondo⁴

¹ *Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Universidade de Lisboa, Portugal*

² *Laboratoire de Physique des Plasmas (UMR 7648), CNRS, Univ. Paris Saclay, Sorbonne Université, École Polytechnique, France*

⁴ *Plasma Lab for Applications in Sustainability and Medicine – ANTwerp, Belgium*

^(*) chloe.fromentin@tecnico.ulisboa.pt

Recent measurements of the gas temperature, vibrational temperatures of CO₂ and CO, E/N, O(³P), CO(X¹Σ⁺) and CO₂(X¹Σ⁺_g) and O(³P) loss frequencies performed in low-pressure DC discharges provide an ideal set of constraints for validating numerical simulations from a 0D self-consistent kinetic model. The dominant elementary processes with impact on the overall coupled kinetics are highlighted with a special focus on the vibrational kinetics of CO₂ and CO.

Investigating the impact of CO on the vibrational temperature of the different CO₂ vibrational modes and on the plasma chemistry is relevant as it is a product of the dissociation. It will therefore be present in the discharge and vibrationally energy transfers between CO and CO₂ are known to be effective [1]. Hence, CO vibrations can promote CO₂ vibrational excitation and further molecular dissociation through the so-called ladder climbing mechanism. The system of election is a DC glow discharge, operating at pressures in the range p=1-5 Torr and discharge currents I=20 and 40 mA, in a Pyrex tube of radius R=1 cm, which is stable, axially homogenous, and easily accessible to a variety of diagnostics. A set of experimental data including, the gas temperature, vibrational temperatures of CO₂ and CO, reduced field E/N, densities of O(³P), CO(X¹Σ⁺) and CO₂(X¹Σ⁺_g) and O(³P) loss frequencies, was recently measured and provided by the Laboratoire de Physique des Plasmas. Our simulation results are obtained with the LoKI (LisOn Kinetics) simulation tool [2] solving a Boltzmann-chemistry 0D self-consistent kinetic model. The comparison of the model predictions with the experimental data will contribute to further develop the existing models [3-5] and to better control and enhance plasma-assisted CO₂ conversion.

The transfers between vibrationally excited CO and the asymmetric stretching mode (v₃) of CO₂ are very efficient and can promote the ladder climbing mechanism along this mode, with a potential positive effect on CO₂ dissociation. These CO molecules can transfer energy to the v₃ vibration because the energy difference between the first vibrational level of CO and the first asymmetric stretch vibrational level of CO₂ is only 25meV which is smaller than the average kinetic energy [1]. Moreover, due to the resonance effect of short-lived negative ions CO⁻, the observed cross sections of electron impact excitation of molecular vibrations of CO are rather large [6]. The process of vibrational transfer between CO and CO₂ and its effect on the overall kinetics will be discussed during the conference.

Acknowledgments: This work was partially supported by the European Union's Horizon 2020 research and innovation programme under grant agreement MSCA ITN 813393, and by Portuguese FCT-Fundação para a Ciência e a Tecnologia, under projects UIDB/50010/2020, UIDP/50010/2020 and PTDC/FIS-PLA/1616/2021.

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