Validation of complex plasma chemistries: CO_2 as a case study

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Abstract:
Low-temperature molecular plasmas are complex systems, where energetic electrons initiate a rich non-equilibrium chemistry by transferring their energy to the heavy-particles in a variety of collisional processes, that include excitation of vibration and electronic states, dissociation, and ionization. The presence of different particles, with specific properties and energies, makes these plasmas useful in a wealth of applications, ranging from aerospace to nanotechnologies. However, the different kinetics become strongly coupled and difficult to disentangle, so that it is often difficult to indentify the dominant phenomena and to optimize the plasma source for a particular application. Modelling emerges as a powerful tool, both to qualitatively interpret physical mechanisms and to quantitatively make predictions for real applications, ultimately leading to a better understanding of the relevant processes and input data. A key element is model *validation*, *i.e.*, the comparison of simulations with experimental results or observations.
In recent years, several laboratories in Portugal, France, The Netherlands, and Russia have engaged in a collective effort to systematically pursue a strategy for the development of kinetic models and validation of plasma chemistry schemes in molecular plasmas. CO_2 plasmas were chosen as a case-study, due to their importance in applications and the inherent coupling of electron, vibration, chemical, ion and surface kinetics [1]. The approach focuses on the design of experiments where specific aspects of the plasma kinetics can be isolated, providing the ideal testbed for validation of a particular aspects of the kinetics and the associated collisional data. Such step-by-step validation procedure has already allowed the validation of: complete and consistent cross section sets for CO_2 [2] and CO [3,4]; vibration-translation (V-T) and vibration-vibration (V-V) energy exchanges [5], and electron-vibration (e-V) input of vibrational energy [6] in low-excitation conditions; atomic oxygen recombination kinetics [7,8]; the electron impact dissociation cross section [9]; dynamics of gas heating in the afterglow [10]; back reaction mechanisms at low pressure [11,12]; chemical kinetics in vibrationally-cold plasmas [13]; and plasma chemistry in vibrationally excited plasmas [14,15]. The extension to other gases and mixtures will also be discussed at the conference.

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