Sensitivity and uncertainty analysis of a kinetic model for CO_2 non-equilibrium plasmas

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This work is dedicated to the systematic investigation of the influence that uncertain rate constants have on model predictions. The kinetic scheme examined here describes CO_2 plasmas with a very complex vibrational kinetics model. Uncertainty of the rate constants models arise from the experimental errors or the approximate theories. To rank the most influential rate constants we used the Morris method, that is a One-At-a-Time design for the sensitivity analysis (SA). The output parameters that were traced are the densities of some species, *i.e.* $CO_2(001)$ and $CO_2(010)$ and the vibrational temperatures $T_{1,2}$ and T_3. The results show that the dominant e-V reactions are also the ones with larger contribution to the uncertainty of the output.

1. Introduction

Modelling low-temperature plasmas usually involves very complex chemistry models described by data that are measured or calculated with some uncertainty. In order to make the simulations of experimentally difficult or inaccessible conditions more credible, the influence of the input uncertainty on the output must be studied [1].

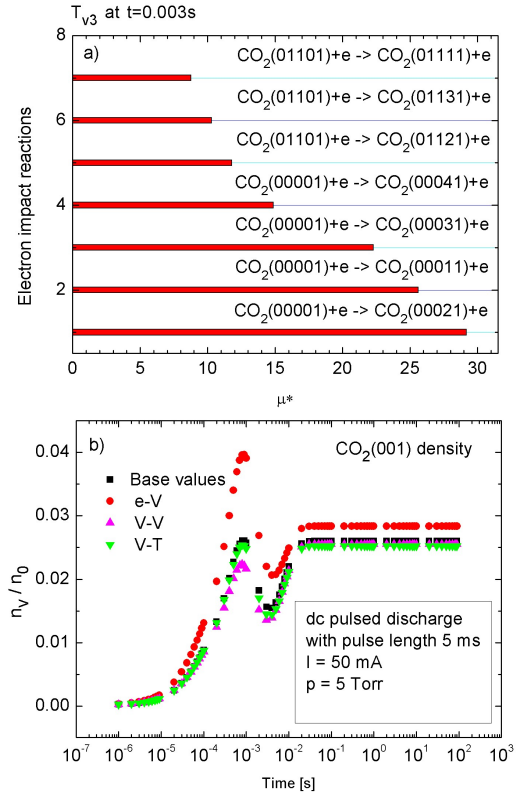

Figure 1 The result of SA, μ* [1] for the vibrational temperature T_{v3} a); and the simulation results using varied rate constants for e-V, V-V or V-T processes b).

A good example of such systems is CO_2 plasma. Recent interest in CO_2 conversion has set the goals for fundamental experimental research and plasma modelling. One particularity of these plasmas is the extended vibrational kinetics, which can comprise ~9000 vibrational levels in a full state-to-state description. In the present work, the SA was performed on a kinetic scheme describing a low excitation regime in CO_2, accounting for 72 individual vibrational levels and more than 1200 elementary processes. The operating conditions are well characterized experimentally, allowing the validation of the model presented in [2].

2. Results and discussion

The screening procedure used in this work, proposed by Morris [3], gives both the quantitative and the qualitative information on the influence of the input uncertainty. Figure 1a) shows that the e-V reactions contributing to the uncertainty of the T_{v3} are the ones populating the asymmetric levels from the ground state. Different simulation results for rate constants varied within the ascribed uncertainty are shown in figure 1b). The present analysis evaluates the level of model reliability, reveals the possible sources of model failure and therefore recommends directions for future improvement.

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References

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