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Plasma-based CO2 conversion: Better insights by modeling

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Plasma-based CO2 conversion is gaining increasing interest. To improve this application in terms of conversion, energy efficiency and product formation, a good insight in the underlying mechanisms is desirable. We try to obtain this by computer modeling. We use 0D chemical kinetics modelling to describe the plasma chemistry in three types of plasma reactors most commonly used for CO2 conversion, i.e., dielectric barrier discharges, microwave plasmas and gliding arc discharges.

We focus especially on the role of vibrationally excited CO2 levels, which are crucial for energy efficient CO2 conversion.

We have also studied the plasma chemistry in CO2/CH4 and CO2/H2O mixtures, for producing value-added chemicals, such as syngas and oxygenated compounds. A detailed chemical kinetics analysis allows to elucidate the different pathways leading to the observed results, and to propose solutions on how to further improve the formation of value-added products.

Finally, we also studied the plasma chemistry in CO2/N2, to investigate the effect of this important impurity in effluent gases. Several harmful NOx compounds are produced, and the reaction pathways for the formation of these compounds are again explained based on a kinetic analysis, which allows proposing solutions on how to prevent the formation of these harmful compounds.