PL0001

Plasma-based greenhouse gas conversion: Modeling the plasma chemistry and plasma reactor design to improve the application

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Plasma-based greenhouse gas conversion (mainly CO_2 and CH_4) 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 modelling, supported by experiments. We simulate both the plasma chemistry as well as the optimum reactor design, in the three types of plasma reactors most commonly used for gas conversion, i.e., dielectric barrier discharges (DBDs), gliding arc (GA) discharges and microwave (MW) plasmas. For the plasma reactor design, we use 2D or 3D computational fluid dynamics modelling. For the plasma chemistry, we make use of zero-dimensional chemical kinetics modeling, which solves continuity equations for the various plasma species, based on production and loss terms, as defined by the chemical reactions. We focus especially on the the role of vibrationally excited CO_2 levels, which are the key species for enhanced energy efficiency of the CO_2 conversion. Our model reveals the relative importance of various processes, responsible for the CO_2 conversion, in a range of different conditions, and this is linked to the energy efficiency in the various types of plasma reactors. We have also studied the plasma chemistry in CO_2/CH_4 and in CO_2/H_2O mixtures, with the purpose of producing value-added chemicals. The main products formed are a mixture of H_2 and CO, or syngas, with a tuneable H_2/CO ratio depending on the gas mixing ratio. The production of oxygenated compounds, such as methanol, formaldehyde, etc, is very limited, showing the need for combining with a catalyst. 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.

Keywords
CO2
plasma chemistry
plasma reactor design
chemical kinetics modeling
fluid dynamics modeling