Combined Plasma Chemistry and Plasma-Surface Interactions Modeling for CO_2 conversion by Gas Discharge Plasmas

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In recent years, there is a growing interest in the conversion of CO_2 into value-added chemicals or new fuels by means of plasma technology. To improve this application, especially in terms of energy efficiency, a good knowledge about the plasma processes is indispensable. We try to obtain this by computer modeling. This includes both modeling the plasma itself, as well as modeling the plasma-surface interactions.

We have developed zero-dimensional chemical kinetics models for describing the detailed plasma chemistry of pure CO_2 splitting [1,2], as well as the conversion of CO_2 in the presence of CH_4 (i.e., so-called dry reforming of methane) [3] or N_2. These models are applied to typical conditions of a dielectric barrier discharge (DBD) and a microwave discharge, which are most often used for these applications. Special attention is paid to the effect of vibrational levels of CO_2 on the conversion process [2].

Moreover, we have also developed two-dimensional fluid models for a packed bed DBD reactor, a microwave plasma and a gliding arc plasma. In a packed bed DBD, the discharge gap is filled with (dielectric) beads. This affects the electric field distribution and hence the electron temperature and density. It is already demonstrated in literature that such a packed bed DBD reactor gives rise to higher energy efficiencies in the conversion process, but the underlying mechanisms are not yet clear; hence the need for modeling. Furthermore, microwave and gliding arc plasmas are also very promising for energy efficient CO_2 conversion [4].

Finally, to improve the selectivity of the conversion process, the plasma is often combined with a catalyst in so-called plasma catalysis. Therefore, we have investigated the interaction of plasma species with a catalyst surface, by means of atomic scale molecular dynamics simulations [5-7].

In this presentation, we will briefly explain the models and show typical calculation results, that allow us to gain a better insight in the underlying physics and chemistry, in order to improve the applications.

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