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Plasma based CO_2 conversion into value added products: better insights from computer modelling

Weizong Wang[1,2] and Annemie Bogaerts[2]

[1]School of Astronautics, Beihang University

[2]Research group PLASMANT, Department of Chemistry, University of Antwerp

e-mail (speaker): wangweizong@gmail.com

Successfully converting the greenhouse gas CO_2 gases into value-added chemicals and fuels would be interesting from both an economic and ecological perspective. This would lead to the successful generation of an artificial closed carbon loop, which fits into the 'cradle-to-cradle' concept, i.e., upcycling waste material into new feedstock [1]. Atmospheric non-equilibrium plasmas offer unique perspectives, because of their capacity to induce chemical reactions within gases with a limited energy cost at mild conditions as well as their advantages of easy operation, quick and efficient reaction process [2]. However, more fundamental research is crucially needed, to better understand the underlying mechanisms, in order to improve the conversion and energy efficiency of plasma technology. For this reason, we perform extensive computer modelling of gliding arc (GA) and dielectric barrier discharge (DBD) plasma based CO_2 conversion. For gliding arc plasma, we present fluid modelling of gliding arc-based CO_2 conversion with a detailed non-equilibrium plasma chemistry set [3]-[6]. Based on the model, a chemical kinetics analysis is performed, which allows investigating the different pathways for CO_2 loss and formation as well as the role of vibrational states on CO_2 conversion (see Fig.1). These investigations of the CO_2 plasma chemistry allow us to propose solutions on how to further improve the CO_2 conversion by using gliding arc technology. The plasma chemistry for a DBD plasma is described with a comprehensive zero-dimensional chemical kinetics model, combining the knowledge gathered in this field so far, and supported with extensive experimental data [7]. This set can be used for chemical kinetics plasma modelling for all possible combinations of CO_2, CH_4, N_2, O_2 and H_2O, to investigate the bigger picture of the underlying plasmachemical pathways for these mixtures in a DBD plasma. Moreover, detailed uncertainty analysis and sensitivity studies, which reveal the impact of the uncertainties of the used rate coefficients and cross sections on the model predictions, are performed in the modelling of plasma based CO_2 conversion [8]-[9].

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Fig. 1 Energy efficient CO_2 conversion by gliding arc plasma via the ladder climbing process of vibrational excitation