

Self-consistent 1D modelling of the CO₂ conversion in microwave discharges

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Splitting of the atmospheric CO₂ into CO and O₂ together with water electrolysis are the basic processes required to transfer the intermittent electricity produced by the wind and solar power plants into storable chemical fuels. An up to 80 % energy efficiency of the CO₂ splitting in microwave (2.4 GHz) induced plasmas was reported back in 1970s-1980s [1, 2]. To facilitate the theoretical understanding and, thus, optimization of the process, recently a very detailed model of the CO₂ plasma chemistry has been compiled [3, 4, 5]. The model explicitly describes 72 heavy species, including vibrationally excited states, and takes into account more than 5000 reactions. With this reaction set, however, the maximum calculated efficiency of only around 30 % was obtained [4]. This result seem to contradict not only with the experimental values, but also with theoretical calculations reported in the past.

In the present paper the energy efficiency of the process is investigated on the basis of a simple 1D model of the plasma flow. The electron density and temperature (average energy), as well as the translational-rotational temperature of heavy particles are calculated self-consistently. For the chemical kinetics the reaction set published in [5] is revised and implemented by translating it into Fortran code. Analysis in the relevant range of discharge parameters will be presented. Conditions of achieving the highest reported efficiency in the model will be discussed.

References

- [1] V. D. Rusanov, A. A. Fridman, G. V. Sholin *Sov. Phys. Usp.* **24** 447 (1981).
- [2] A. Fridman *Plasma Chemistry*, Cambridge: Cambridge University Press, 2008
- [3] T. Kozak, A. Bogaerts *Plasma Sources Sci. Technol* **23** 045004 (2014).
- [4] T. Kozak, A. Bogaerts *Plasma Sources Sci. Technol* **24** 015024 (2015).
- [5] P. Koelman et al. *Plasma Proceses and Polymers* **14** 1600155 (2017),
<https://plasimo.phys.tue.nl/resources/>