Keep-in-Touch meeting

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Plasma Modeling of atomic oxygen in the effluent of CO_2 microwave discharges

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Microwave (MW) discharges provide a promising route for energy-efficient CO_2 dissociation, the limiting step for sustainable fuel production and in situ resource utilization on Mars. Understanding both the active plasma and the post-discharge region is essential for optimizing efficiency and gaining deeper insight into the underlying mechanisms. This study models the kinetics of a 2.45 GHz MW CO_2 plasma under varied conditions: pressures of 120-500 Pa, absorbed powers of 600-1200 W, and flow rates of 74-370 sccm, focusing on atomic oxygen $O(^3P)$ dynamics in the post-discharge region. A pseudo-1D approach is developed through sequential simulations using the LoKI-B Boltzmann solver and the LoKI-C chemistry solver, extended to include CO_2 and CO vibrational states, as well as the electronically excited $O(^1S)$ state.

The model is compared against experimental data from TALIF measurements showing good agreement with temperature and conversion. A key insight is the observed $O(^3P)$ concentration peak in the post-discharge which was reproduced by the current model, highlighting the effect of thermal contraction. Additionally, surface recombination at the reactor walls plays a dominant role in $O(^3P)$ depletion. By incorporating complex chemistry sets, even in space resolved problems, the search for possible pathways of experimentally observed phenomena is broadened, but action needs to be taken in order to keep computational time reasonably low with a large number of reactions.