

Insight into contraction dynamics in CO₂ microwave discharges through comparisons between simulations and experiments

L. Vialetto¹, P. Viegas^{1,2}, A. van de Steeg¹, G. van Rooij^{1,3}, M. C. M. van de Sanden^{1,5},
S. Longo⁴, J. van Dijk⁵, P. Diomedè³

¹ *DIFFER - Dutch Institute for Fundamental Energy Research, The Netherlands*

² *Department of Physical Electronics, Faculty of Science, Masaryk University, Czech Republic*

³ *Faculty of Science and Engineering, Maastricht University, The Netherlands*

⁴ *Dipartimento di Chimica, Università degli Studi di Bari, Bari, Italy*

⁵ *Department of Applied Physics, Eindhoven University of Technology, The Netherlands*

Microwave (MW) plasma reactors are very promising for efficient CO₂ dissociation for the production of carbon-neutral fuels and chemicals. They are a crucial component of a future energy grid based on electricity. The optimal conditions for these MW reactors have shown a strong correlation with pressure and discharge contraction dynamics. Contraction mechanisms have been studied experimentally in relation to the skin-depth of wave absorption, the ionization degree of the plasma core, the gas temperature and the heat capacity of the plasma. However, it is experimentally difficult to assess most discharge parameters, particularly since the plasmas under study have high temperatures (between 3000 K and 7000 K), their composition is highly variable (main species CO₂, CO, O₂, O and C) and they are strongly reactive. As such, simulations are required to assess discharge contraction mechanisms. Given the importance of contraction dynamics for the reactor performance, this understanding is key for reactor optimization. A fully native 1-D radial fluid model, including neutral, electron and ion kinetics and gas temperature, has been developed to simulate a CO₂ MW discharge operated at DIFFER. The model is coupled to a Monte Carlo Flux code for the electron kinetics. Model results are validated against spatially-resolved measurements of the main neutral species and electron number density, gas and electron temperature, obtained by advanced laser scattering diagnostics at DIFFER. As pressure increases, the inhomogeneous gas heating causes significant gradients in neutral and charged species mole fractions profiles. Moreover, the transition from diffuse to contracted plasma is accompanied by a change in the dominant charged species, leading to two different ionization mechanisms that dominate the diffuse and contracted regime, respectively. These processes facilitate the increase in the peak electron number density with pressure that induces radial plasma contraction.