Self-consistent 2D fluid modelling of a microwave excited plasma in argon

M. Baeva(*)[1], A. Bösel[1], J. Ehlbeck[1], D. Loffhagen [1]

[1] *Leibniz Institute for Plasma Science and Technology, INP Greifswald, Felix-Hausdorff-Strasse 2, 17489 Greifswald, Germany*
(*) baeva@inp-greifswald.de

A two-dimensional model of microwave induced plasma in argon at atmospheric pressure describing self-consistently the gas flow and heat transfer, the in-coupling of the microwave energy into the plasma, and the reaction kinetics is presented. The balance of the charged particles is essentially controlled by the kinetics of the molecular ions. A contraction of the discharge is observed at conditions that are typical for analytical applications (flow rate of 200 ml/min, power dissipation of 20 W). The plasma is far from thermodynamic equilibrium with gas temperatures of above 2000 K and electron temperatures of about 1 eV. The maximum electron density value is about 4×10^{21} m^{-3}. Comparison with experimental data is presented which demonstrates a good agreement.

The plasma is induced by coaxially fed microwaves under gas flow conditions. The mass, momentum, and energy balance equations for the neutral gas along with the energy balance for the electrons and the transport of excited argon atoms, atomic and molecular ions are solved to obtain the gas flow parameters as well as the spatial distributions of the gas temperature, the electron temperature, the species densities, and the electromagnetic field in the entire computational domain (Fig. 1). The kinetic scheme accounts for elastic scattering, processes of excitation/deexcitation in collisions with electrons, direct and stepwise ionization of argon atoms, chemo-ionization, production of molecular ions due to the process of ion conversion, three-body and dissociative recombination due to electron and atom impact [1]. The set of partial differential equations is solved numerically using the commercial package COMSOL Multiphysics [2] based on finite element methods. The thermodynamic and transport properties of the fluid such as heat capacity are taken in the form of look-up tables as functions of the gas temperature [3].

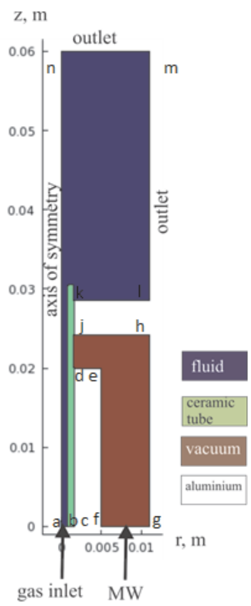

Fig. 1: Sketch of the computational domain. abklmn - fluid region, cbkb - ceramic tube, cdef - inner conductor, defghj - vacuum, hjlk - end part, outer conductor.

Calculations have been performed at atmospheric pressure for given gas flow rate and gas temperature (300 K) at the inlet surface ”ab”, and microwave power input at port ”fg”. Typical operating conditions for analytical applications are gas flow rates of 200-400 ml/min and absorbed microwave power of about 20 W. The spatial distributions of the charged particles Ar^+ and Ar_2^+, and of the excited argon atoms are shown in Fig. 3. The plasma column extends over a length that exceeds by a factor of about 3 to 4 the length of the excitation area, corresponding to the propagating microwave field. The atomic ions (Fig. 3a) are distributed mainly around the axis, while the distribution of their density along the axis of symmetry is asymmetric and peaked around z=0.0175 mm. There it reaches a value of about 4×10^{21} m^{-3}. The distribution is bell-shaped in the radial direction with density decreasing by an order of magnitude within a distance of 0.4 mm. Until about half-way in the tube radius, quasi-neutrality is essentially preserved by the atomic ions. Beyond, the molecular ion density (Fig. 3b) grows and becomes larger than the atomic ion density, reaching its maximum value of about 8×10^{19} m^{-3}.

This behavior can be explained with the strong non-linear dependence of the rate coefficients for dissociative recombination, electron impact dissociation of the molecular ions, and ion conversion (Cut at axial position z=0.025 m in Fig. 3). Above gas temperatures of about 1200 K, the molecular ion density

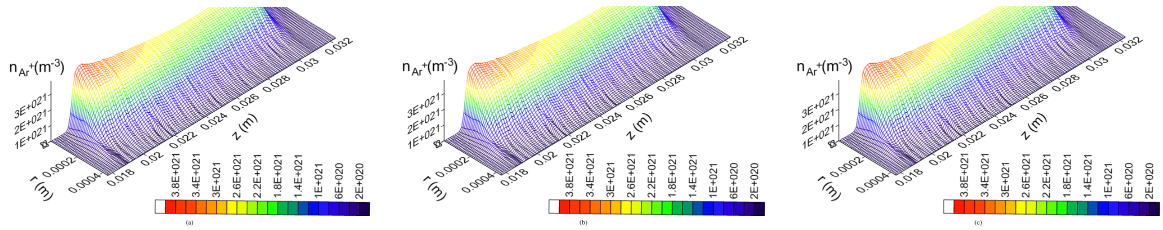

Fig. 2: Spatial distribution of the density of atomic ion (a), molecular ions (b), and excited atoms (c).

is significantly lower than the atomic ion density due to the electron impact dissociation of Ar_2^+ and the dissociative recombination of the molecular ion in collisions with electrons. The excited atoms produced by the latter process contribute additionally to the production of atomic ions due to chemo- ionization. Towards the tube wall, however, the gas temperature decreases and the molecular ion density increases as a result of the process of ion conversion and the larger neutral atom density. For temperatures of about 1200 K, the molecular and atomic ion densities become almost equal, however, near the walls, where the temperature gradients are steep, the molecular ion density becomes the dominant ionic species. Similarly, for positions characterized by temperatures below 1200 K, i.e. near the edges of the plasma column, the molecular ion density exceeds the atomic ion density. Optical emission spectroscopy was applied in order to measure the average electron density and gas temperature. The electron density was determined from the Stark broadening of the H_β-line at 486.1 nm. The line broadening of H_β due to the linear Stark effect can be related to the electron density according to [4]. Hydrogen atoms were provided in the discharge by introducing water vapor into the carrier gas in such a small amount that the line emission of Ar does not change. The experimentally observed Stark broadening was determined by unfolding the recorded line profile from the Doppler, the instrumental broadening, and the van der Waals broadening. Fig. 4 presents the electron density obtained as a function of the radial position r at z=0.02 m and the axial position z. The maximum values agree within 40 %. In axial direction downstream the gas flow, the experimental values are lower by about a factor of six. This is the region close to the upper end of the tube and outside, where the deviations from axial symmetry in the experiment become considerable. The gas temperature has been determined from the OH emission spectra from the transition OH($A^2\Sigma^+$, v=0)→OH($X^2\Pi^+$, v'=0) at 306.3 nm. The results obtained for gas flow rates of 200 and 400 ml/min are presented in Fig. 5 together with the corresponding modelling results. The comparison demonstrates a good quantitative and the qualitative agreement.

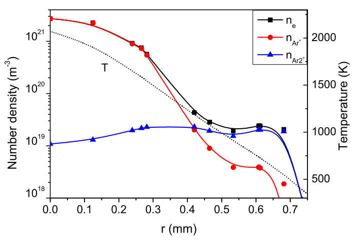

Fig. 3: Radial distribution of the charged particle densities and the gas temperature (dashed curve).

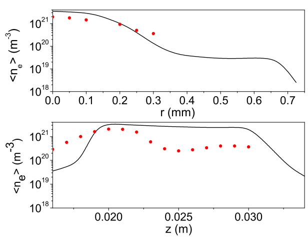

Fig. 4: Comparison of experimental and calculated averaged electron density along the z-axis.

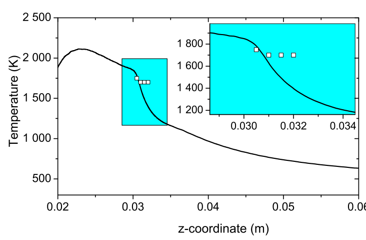

Fig. 5: Comparison of measured (symbols) and calculated (line) gas temperature along the z-axis.

References

[1] Y. Kabouzi, D. B. Graves,E. Castanos-Martinez, M. Moisan, *Phys. Rev. E* **75** (2007) 016402.
[2] COMSOL 4.1, www.comsol.com.
[3] B. Pateyron and G. Delluc and N. Calv, *Mecanique et Industries* **6** (2005) 651.
[4] H. R. Griem, Spectral line broadening by plasmas, (1974) Academic Press, Inc., New York.