2D self-consistent modelling of an argon microwave plasma over a wide range of pressure

A. Berthelot[1], St. Kolev[1,2] and A. Bogaerts[1]

[1] Research Group PLASMANT, Department of Chemistry, University of Antwerp, BE-2610 Antwerpen-Wilrijk, Belgium
[2] Faculty of Physics, Sofia University, 5 James Bourchier Boulevard, BG-1164 Sofia, Bulgaria

Abstract: A 2D axisymmetric argon plasma fluid model is presented for a microwave plasma. The effect of the pressure on the plasma parameters is studied over a wide range of pressures going from 10 mbar to atmospheric pressure.

Keywords: microwave discharges, argon plasmas, fluid plasma models

1. Introduction

Over the last decades, many studies focused on the description of surface-wave plasmas produced by microwave discharges [1] both from a theoretical and an experimental point of view. These discharges have a wide range of applications, such as gas conversion, plasma medicine, material processing and surface treatment [2] as they offer relative simplicity and low running costs. They can be operated over a wide range of pressure (from few mTorr to several atmospheres), using different frequencies and various geometries [3]. Among these different geometries, the so-called surfaguide discharges offer the possibility to create low-temperatures plasmas using a broad range of operating frequencies, determined by the geometry of the waveguide and they are able to handle high power coupling between the plasma and the microwave source [3].

A theoretical model for these discharges is presented in [4] at low pressure. More recently, a self-consistent 2D model was proposed in [5] at atmospheric pressure. Recently, microwave discharges have been applied to CO_2 conversion and the pressure has been shown to be a key parameter to obtain better energy efficiency, which is crucial in this domain [6].

The goal of this study is to get a better understanding of the effect of the pressure on microwave discharges. The presented model is a self-consistent 2D fluid plasma model operated over a wide range of pressure conditions: from 10 mbar to atmospheric pressure.

2. Model description

The model is a time-dependent model implemented in the commercial software COMSOL Multiphysics ® (www.comsol.com). It solves equations to determine each species density (including the electrons), the electron energy, the gas temperature and velocity, the plasma potential and the electromagnetic fields. The model considers the following heavy species: Ar atoms, Ar^+ ions, Ar_2^+ molecular ions, $Ar(4s)$, i.e., all 4s levels considered as a single lumped excitation level, $Ar(4p)$, i.e., all 4p levels and Ar_2^* which includes $Ar_2(^1\Sigma_u^+)$ and $Ar_2(^3\Sigma_u^+)$ excited molecules. The set of reaction between the different species as well as the transport parameters used are presented in [7]. The EEDF is pre-calculated using Bolsig+ [8] and is used to calculate the rate coefficients of electron impact collisions for different pressure regimes.

The frequency considered is 2.45 GHz and a sketch of the 2D-axisymmetric computational domain is shown in Fig. 1. The computational domain is based on the setup used in [9].

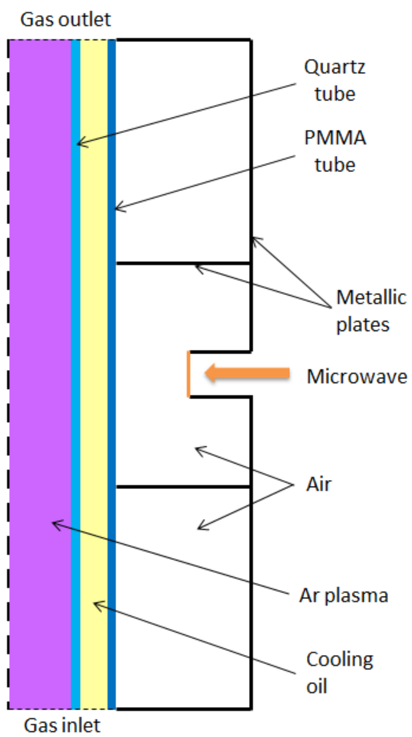

Fig. 1. Sketch of the computational domain.

By comparing the EM field distribution in a 3D geometry and in a 2D-axisymmetric geometry, we have made sure that a 2D-axisymmetric model could accurately reproduce the EM field created in this configuration.

3. Results and discussion

First, the model was developed for a pressure of 1000 Pa. Fig. 2 shows the distribution of the electron density and the electron temperature in the plasma at a pressure of 1000 Pa, a flow of 500 sccm and two different electromagnetic powers: 50 W and 100 W.

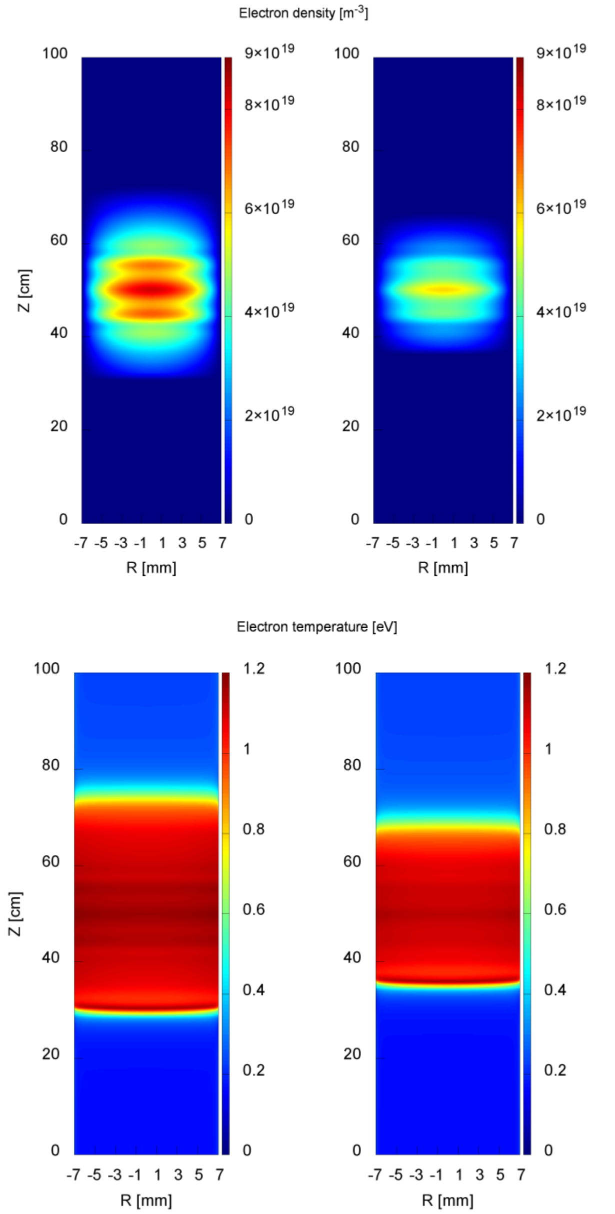

Fig. 2. Electron density in m^{-3} (top) and electron temperature in eV (bottom) at 1000 Pa and with a gas flow of 500 sccm. The left panel shows the results at 100 W and the right panel at 50 W.

It is found that the electron density reaches a maximum value in front of the waveguide for both power inputs. Moreover, the electron density profile exhibits two secondary maxima that are both located 6cm, i.e., half a wavelength, from the main peak. The maximum electron density is found to be 8.3×10^{19} m^{-3} in the 100 W case with a 44 cm long plasma and 6×10^{19} m^{-3} in the 50 W case with a 33cm long plasma.

The electron temperature profile is almost flat in the plasma with values between 1 and 1.1 eV in both cases.

Fig. 3 shows the gas temperature T_g for the same conditions. It is found that the heavy particle temperature profile resembles the electron density profile. The maximum value of T_g is 1250 K with 100 W and 1050 K with 50 W. Note that T_g drops to almost 300 K close to the quartz tube since the outer surface of the quartz tube is assumed to be cooled at 300 K.

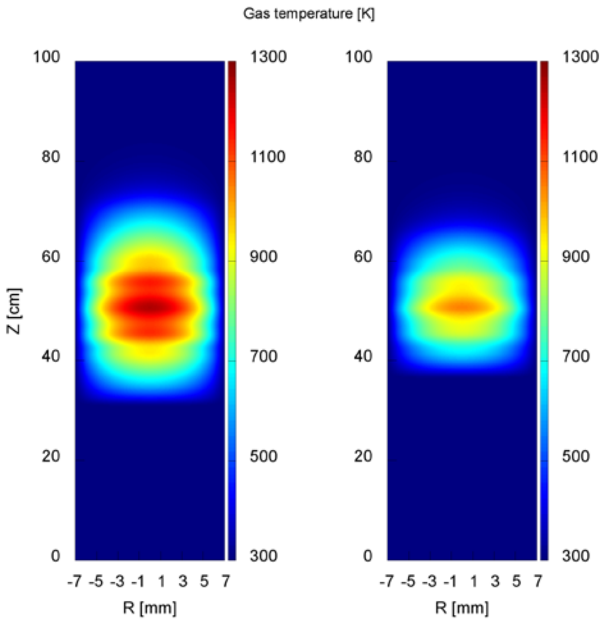

Fig. 3. Gas temperature (K) at 1000 Pa and with a gas flow of 500 sccm. The left panel shows the results at 100 W and the right panel at 50 W.

Axially, omitting the two secondary maxima, the electron density decreases linearly from the maximum value in the centre of the tube to the end of the plasma, which is consistent with literature [10]. Note that these two secondary maxima are due to an additional resonance of the EM field caused by the two horizontal metallic plates shown in Fig. 1.

Fig. 4 shows the preliminary results obtained at atmospheric pressure in the same configuration with a power of 100 W. The axial scale is different to show the plasma in more detail. It is found that the plasma has a ring-shape and that the maximum electron density is close to the quartz tube. The plasma is also contracted axially and its size is decreased by a factor of 10. The electron temperature in the plasma is still approximately 1 eV and the gas temperature has a maximum value of 1500 K. Note that at atmospheric pressure, an additional background power density of 10^5 $W.m^{-3}$ is added to avoid strong density gradients that would result in numerical instabilities. It artificially creates an electron density of 10^{16} m^{-3} and is also responsible for the background electron temperature of 0.8 eV outside the plasma. This artificial background power deposition has no effect on the results in the plasma since it is very low compared to the microwave power deposition that reaches 10^8 W.m^{-3} in the plasma.

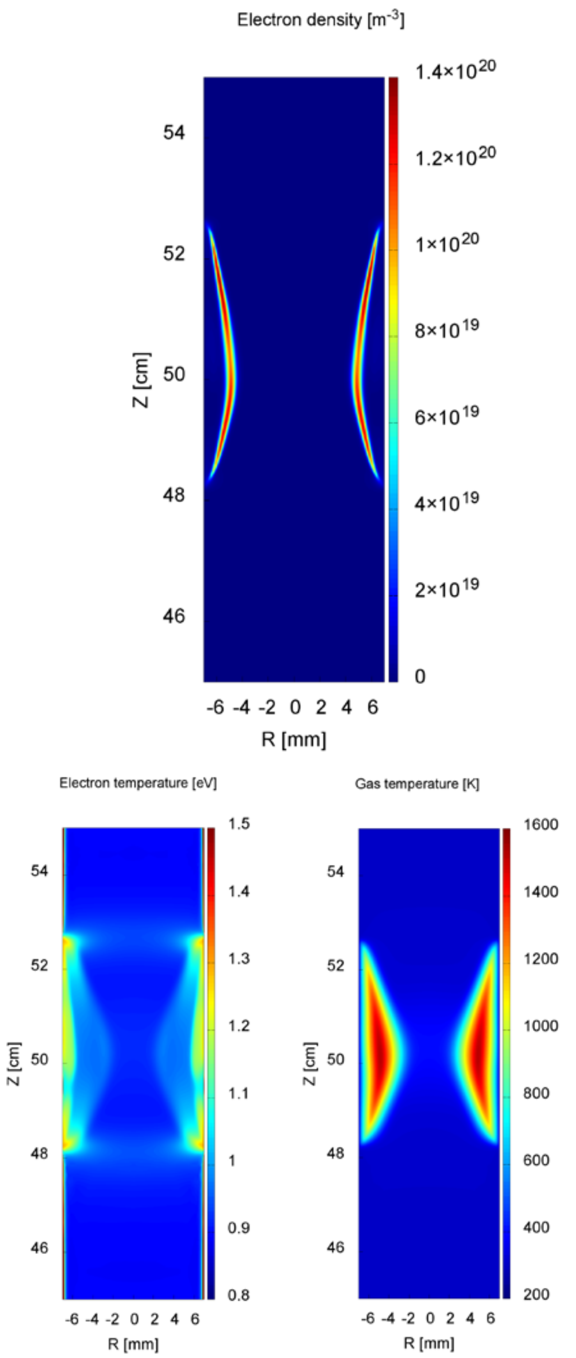

Fig. 4. Electron density in m^{-3} (top), electron temperature in eV (left, bottom) and gas temperature (K) (right, bottom) at atmospheric pressure with a power of 100 W and a flow of 500 sccm.

4. Conclusion

Microwave argon discharges are modelled using Comsol Multiphysics ® at different pressures. A preliminary comparison of the model results at different pressures shows an axial and a radial contraction of the plasma that becomes ring-shaped when the pressure increases.

Results at low pressure appear to be in good agreement with previous research conducted on similar setups. A comparison with the experiments will be performed in the near future to benchmark the results of the model at low pressure. At atmospheric pressure, a benchmarking of the model results will be done by comparing the results with literature [5].

Intermediate pressures will also be studied to see the transition between the different regimes of the discharge in argon.

Subsequently, a reduced CO_2 set of chemistry will be made from the set of [11] using the Principal Component Analysis (PCA) method developed by [12] to study the different pressure regimes of a CO_2 microwave plasma. This will give insights on the effect of pressure on the efficiency of CO_2 dissociation and especially on the behaviour of the vibrational excitation in a CO_2 discharge.

5. Acknowledgments

This research was carried out in the framework of the network on Physical Chemistry of Plasma-Surface Interactions - Interuniversity Attraction Poles, phase VII (PSI-IAP7) supported by the Belgian Science Policy Office (BELSPO) and it was supported by the European Marie Curie RAPID project within the 7th programme.

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