

A Numerical Model of the Plasmaline[®] Microwave Plasma Source

Christian Hunyar, Eberhard R auchle, Lukas Alberts, Rudolf Emmerich, Matthias Graf,
Mathias Kaiser and Klaus-Dieter Nauenburg

Fraunhofer-Institut Chemische Technologie (ICT), Department of Polymer Engineering/MW and
Plasma, Pfinztal (Berghausen), Germany

The Plasmaline[®], a linearly extended microwave (2.45 GHz) plasma source, is well suited to generate large-scale ($> 1 \text{ m}^2$) dense plasmas for technical use in the low-pressure range. In this paper, we present a numerical model of microwave Argon plasma that solves the coupled system of Maxwell's equations, continuity equations for electrons and metastable states and the electron heat equation. The solutions are self-consistently calculated with the COMSOL Multiphysics finite element software in case of axial symmetry. This model can successfully predict the transient and spatial development of the Plasmaline[®]'s plasma parameters and field distribution. The simulations are in good qualitative agreement with experimental results.

1. Introduction

The Plasmaline[®] device can be used to produce linearly extended plasmas up to several meters; in an array arrangement, large area plasmas, up to several square meters, can be obtained. Since a direct access to the plasma is possible, the Plasmaline[®] device is well suited for plasma treatment of large surfaces. A schematic view of the setup is shown in Fig. 1.

For this work the electrodynamics of the propagating electromagnetic fields and particle transport equations for the production and spatial distribution of different species, e.g., electrons, ions, metastables combined with the thermodynamics of the heat equation for the electron temperature were calculated self-consistently using the *COMSOL Multiphysics* code specialized for the Plasmaline[®] geometry. The microwaves (MWs) propagate along an inner conductor and are produced by magnetrons at one or both ends. The inner conductor is located within a non conducting dielectric tube, e.g., quartz glass or ceramics filled with a dielectric medium or a non ionized gas, e.g., air at normal pressure. Plasma is produced outside the tube in a gas atmosphere at reduced pressure and is accessible for technical applications. The MWs propagate mainly in the region between the inner conductor and the surrounding dielectric tube. The dimension of this region determines the axial damping of the waves. At high microwave power a tubular plasma more dense than the critical density is formed outside the dielectric tube. It acts as the outer conductor of a coaxial line. Argon (Ar) discharges are considered here because the basic phenomena and basic data for Ar are widely known.

2. Theory

As the electromagnetic field oscillates significantly faster than the change of the dielectric properties of the plasma, a time harmonic approximation of Maxwell's equations can be used. It results in the following equation for the electric field $\vec{E}(\vec{r})e^{i\omega t}$ [4]:

$$\nabla \times \nabla \times \vec{E}(\vec{r}) - \omega^2 \varepsilon(\vec{r}, \omega) \varepsilon_0 \mu_0 \vec{E}(\vec{r}) = 0 \quad (1)$$

where ω is the angular frequency, \vec{r} is the space coordinate, ε_0 and μ_0 are the electric and

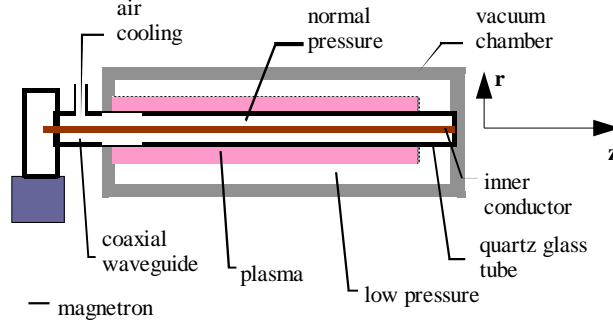


Fig.1 Schematic view of a Plasmaline[®] plasma source

magnetic constants respectively, and $\varepsilon(\vec{r}, \omega)$ is the relative dielectric function containing the dielectric properties of the medium. For plasma in the cold low pressure approximation [5]

$$\varepsilon(\vec{r}, \omega) = 1 - \frac{\omega_p(\vec{r})^2}{\omega^2 + \nu(\vec{r})^2} \left(1 + i \frac{\nu(\vec{r})}{\omega} \right) \quad (2)$$

The plasma frequency ω_p depends on the local electron density $n_e(\vec{r})$:

$$\omega_p(\vec{r})^2 = \frac{n_e(\vec{r})e^2}{m_e \varepsilon_0} \quad (3)$$

where e is the electron charge and m_e the electron mass and $\nu(\vec{r})$ is the effective electron collision frequency for momentum transfer for collisions of electrons [6], [7].

Three different predominant species of the reactions occurring in this system are considered: neutral Ar atoms (density N), electrons (n_e) (and Ar^+ ions (n_i)) and metastable excited Ar^* atoms (n_*). For low pressure discharges (under several 100 Pa) non-equilibrium conditions occur so charge neutrality between electrons and ions can be assumed. At the same time, the degree of ionization is low which results in an approximately constant density of neutral Ar ions. Additionally, a homogeneous temperature of the heavy particles (Ar^+ , Ar^* and Ar) can be assumed. The electron density is determined by the continuity equation for this species in the plasma:

$$\frac{\partial n_e}{\partial t} + \nabla \Gamma(n_e, T_e) = R_2 + R_3 + R_6 \quad (4)$$

where R_2, R_3, R_6 [2] are the rates of the reactions which increase n_e . The electron flux $\Gamma(n_e, T_e)$ (with T_e being the electron temperature) is also dependent on the ambipolar field in the plasma and can therefore be approximated to:

$$\Gamma(n_e, T_e) \approx -\frac{e}{m_{\text{Ar}} \nu_{iN}} \nabla(n_e T_e) \quad (5)$$

where ν_{iN} is the collision frequency between neutrals and ions [2] and m_{Ar} the mass of an Ar atom. Assuming a Maxwell distribution of velocities in the plasma, which is also appropriate in

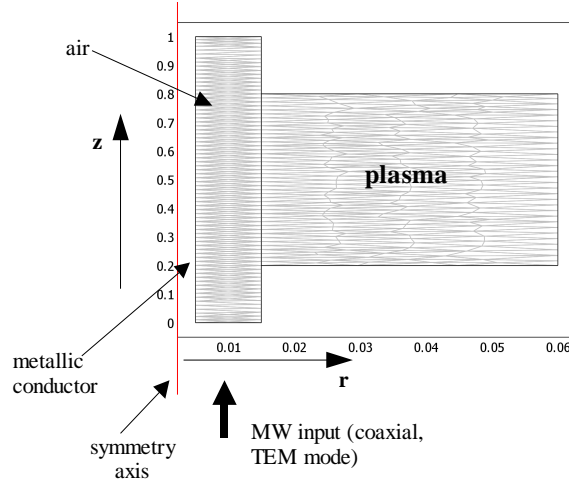


Fig. 2: Scaled geometry model of the Plasmaline[®] plasma source (dimensions in m)

our case, the reaction rates R_i for the reactions are dependent on the product of the densities (n_j) of the reactants and a temperature dependent reaction constant:

$$R_i = \left(\prod_{j=1}^{N_{\text{reactants}}} n_j \right) \cdot K_i(T_e) \quad (6)$$

The reaction constants are usually of a form [1], [2] $K_i(T_e) = \alpha_{ij} T_e^{\alpha_{2j}} e^{-\alpha_{3j}/T_e}$ with α_{ij} values from literature. A continuity equation similar to (4) can be found for the metastable Ar^* :

$$\frac{\partial n_*}{\partial t} + \nabla(-k_B T_* \nabla n_*) = R_1 - R_3 - R_4 - R_5 - 2R_6 - R_7 - R_8 \quad (7)$$

with the appropriate reaction rates for the metastable production and loss and the temperature of the metastables (T_*) approximately the temperature of the neutrals.

In addition to the continuity equations, the heat equation for the electrons has also to be implemented in the model to attain a self-consistent transient solution (T_e in eV):

$$\frac{\partial}{\partial t} \left(n_e \frac{3}{2} e T_e \right) = -\nabla Q_e + W_{\text{abs}} + W_{\text{coll}} \quad (8)$$

where the electron heat flux is

$$Q_e = \frac{5}{2} \Gamma(n_e, T_e) e T_e - \frac{5}{2} \frac{n_e e T_e}{m_e \nu_{eN}} \nabla(n_e T_e) \quad (9)$$

and the local power density caused by the microwaves

$$W_{\text{abs}}(\vec{r}, t) = 1/2 \omega \varepsilon(\omega, \vec{r}, t) \vec{E}(\vec{r}, t) \vec{E}^*(\vec{r}, t) \quad (10)$$

with the energy loss over reactions

$$W_{\text{coll}} = e(11.56R_1 + 14.3R_{1a} + 15.7R_2 + 4.14R_3 + 11.56R_4) + \Delta_{\text{elast}} R_9 \quad (11)$$

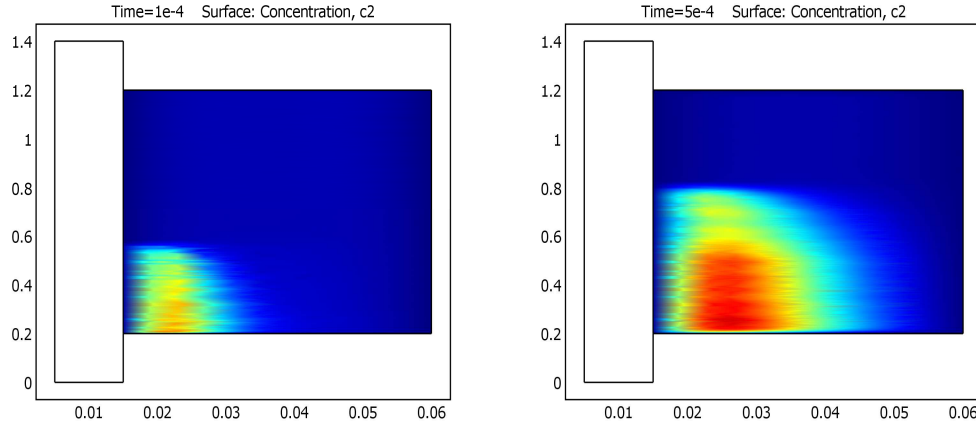


Fig. 3. Electron density n_e in the Plasmaline[®] simulation model for 800 W power input in Ar after 1.0 and $5.0 \cdot 10^{-4}$ s (values in 1 m^{-3}).

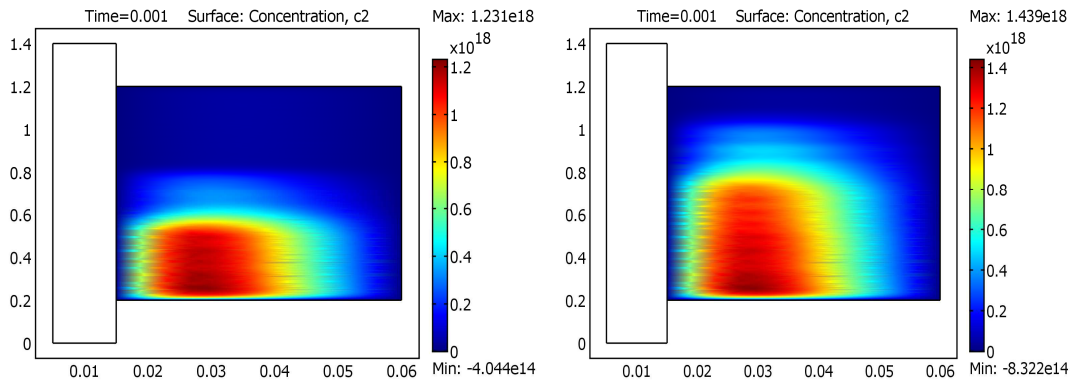


Fig. 4. n_e for 800 W (left) and for 1600 W (right) power input after $10 \cdot 10^{-4}$ s.

and the energy loss for one elastic collision $\Delta_{\text{elast}} = 3m_e / m_{Ar} eT_e$.

This system of PDEs was transferred in a Finite Element Method model for *COMSOL Multiphysics* and self-consistently solved. Fig. 2 shows the basic geometrical and physical model that was used for the simulations. As the system has a rotational symmetry, the according calculation modes were used and a 2.5D model was simulated.

3. Numerical Results

The simulation results shown in this section were all performed in the geometry with 1 m length of the plasma chamber and the outer chamber radius of 0.06 m. The pressure of the simulated Ar gas was 200 Pa.

3.1 Electron Density

Fig. 3 shows the electron density n_e for a simulation run with 800 W MW power input from the bottom port of the model at two simulation times. It can be seen that the plasma density forms a column parallel to the quartz glass tube but in a certain distance which grows over the process

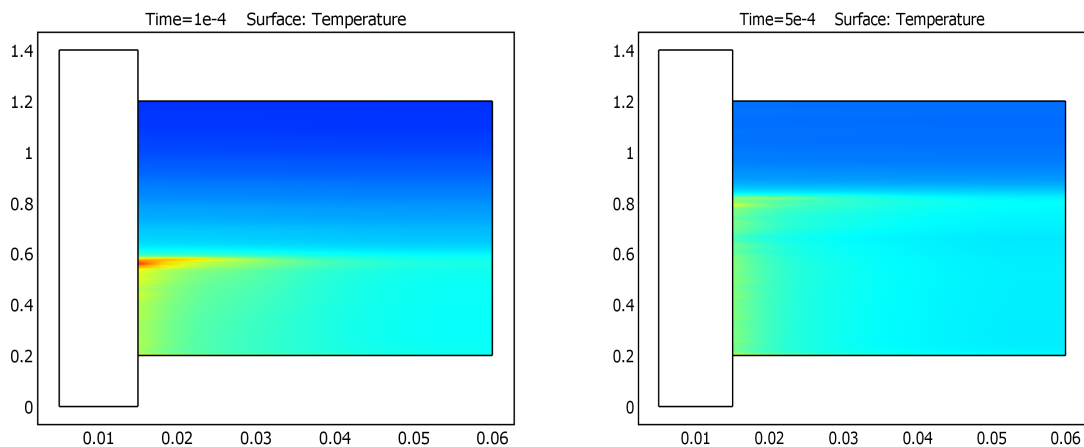


Fig. 5. Electron temperature T_e in Ar for 800 W power input after 1.0 and $5.0 \cdot 10^{-4}$ s (values in eV).

time until it reaches a certain extent and density that depends on the input MW power. Fig. 4 shows that the power level decides the length of the plasma column.

3.2 Electron Temperature

Fig. 5 shows the corresponding electron temperature T_e of the process mentioned in the last subsection. It can be seen that after a first strong rise of the temperature at the edge of the plasma column, which causes the production of new electrons there and with this the growth of the column, the temperature follows the top of the column until this reaches its maximum extent. Then the temperature gradients start to even out in the radial direction and the temperature sinks to lower values. The density of the metastable states mostly follows the temperature distribution.

3.3 Pulsed Power Input

Fig. 6 shows the result of a simulated pulsed operation of a Plasmaline[®]. A much faster rise of the temperature than the electron density can be observed after the power is turned on. Then the production of electrons increases and the temperature drops again quickly. This delayed reaction can also – on a higher plasma density level – be observed in the second pulse. This is a behavior which corresponds well with experimental observations.

4. Conclusions and Outlook

The numerical model employed in this paper to investigate the propagation of surface waves in a Plasmaline[®] plasma source did show good agreement with experimental results. It could be verified that depending on the applied microwave power long (> 1 m) plasma columns can be generated. Published physical parameters for low pressure microwave Argon discharges are used so the discharge for a given geometry can be calculated with only two input parameters: gas pressure and microwave power. According to published experimental results the electron temperature in the simulation develops faster than the electron density. This could be verified in the simulation and leads us to the conclusion that numerical simulation is a valuable guideline and tool for the design of plasma sources for Ar and other surface wave discharges. Further simulations with an expanded model in full 3D are in the process of being made (also for other plasma sources) together with experimental verification of the simulation results.

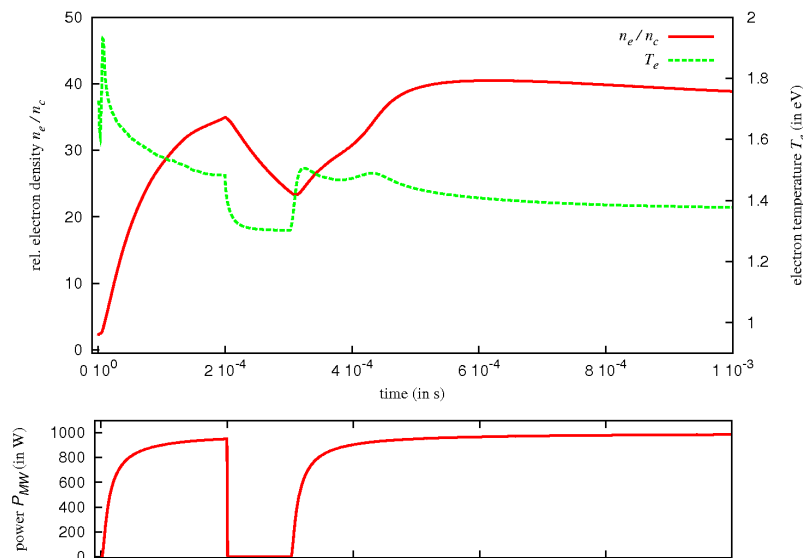


Fig. 6. T_e and n_e for two pulses (first short then long) with 1 kW maximum power input.

References

- [1] D. P. Lymberopolous and D. J. Economou, Fluid simulations of glow discharges: Effect of metastable atoms in argon, *J. Appl. Phys.*, vol. 73, pp. 3668-3679, 1992.
- [2] R. A. Stewart, P. Vitello, D. B. Graves, E. F. Jaeger and L. A. Berry, Plasma uniformity in high-density inductively coupled plasma tools, *Plasma Sources Sci. Tech.*, vol. 4, pp. 36-46, 1995.
- [3] H. Kousaka and K. Ono, Fine structure of the electromagnetic fields formed by backward surface waves in an azimuthally symmetric surface wave-excited plasma source, *Plasma Sources Sci. Tech.*, vol. 12, pp. 273-386, 2003.
- [4] J. D. Jackson, *Classical Electrodynamics*, Wiley, N.Y., 1998.
- [5] S. R. Seshadri, *Fundamentals of Plasmaphysics*, Elsevier, N.Y., 1973.
- [6] U. Kortshagen, A. Shivarova, E. Tatarova and D. Zamfirov, Electron energy distribution function in a microwave discharge created by propagating surface waves, *J. Phys. D*, vol. 27, pp. 301-311, 1994.
- [7] E. Castaños Martinez, Y. Kabouzi, K. Makasheva and M. Moisan, Modeling of microwave-sustained plasmas at atmospheric pressure with application to discharge contraction, *Phys. Rev. E*, vol. 70, 066405, 2004.