COMSOL Multiphysics Simulations of the Electric Field and Gas Flow in a Microwave Axial Injection Torch

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Abstract

The electric field and the gas flow in the reactor chamber of a microwave axial injection torch were simulated. Based on the simulations, the optimal design and configuration of the device for plasma ignition were found. The simulations were carried out using COMSOL Multiphysics and are a preliminary, yet necessary, step to a plasma model, currently in progress.

1 Introduction

The atmospheric pressure microwave plasma torch design described by Zajíčková et al. [4] has been used at the Masaryk University in Brno for various PECVD processes. The original intention was to synthesise carbon nanotubes (CNTs) and multiwalled CNTs. CNTs are widely used in the field of material engineering and also in the emerging field of nanoelectronics. At the Masaryk University, CNTs have been grown at the atmospheric pressure at quite high growth rate, directly on the Si substrate (without a SiO_x barrier layer). The detailed description of the nanotube deposition can be found in [5].

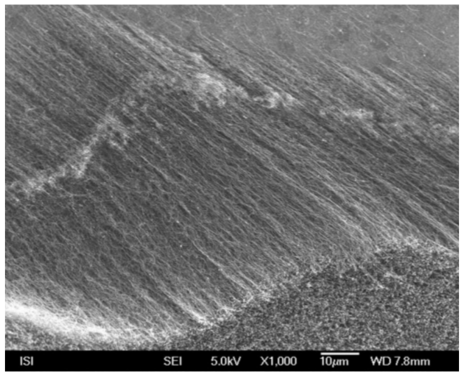


Figure 1: Top view of CNTs deposited in plasma AIT [5]

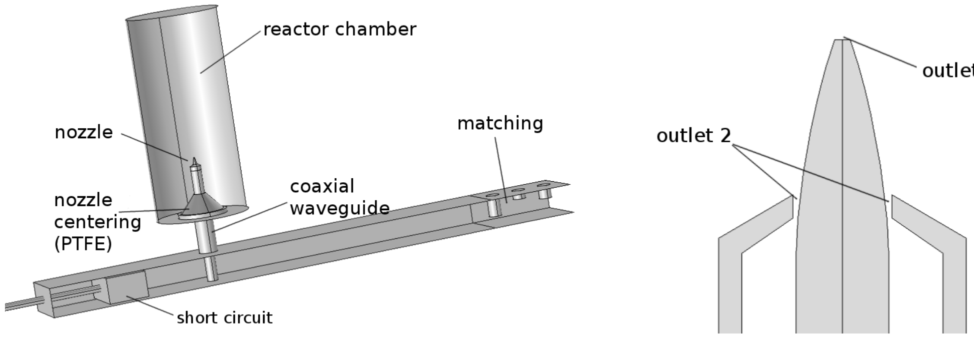
Another, quite recent, application of the plasma torch is synthesis of biocompatible and chemically stable maghemite ($\gamma - Fe_2O_3$) nanoparticles with applications e.g. in ferrofluids, high-density magnetic recording or magnetic resonance imaging [3].

The subject of this work is to simulate the electric field and gas flow in the torch. The presented simulations are the first step towards the complete description of the conditions and processes in the reactor. Their main aim was to find an optimal configuration for plasma ignition (as specified below). The simulations led to a few modifications of the design. These modifications have been tested and their suitability is discussed. RF and CFD modules in COMSOL Multiphysics were used for the simulations.

2 Methodology and model

The simulation described in this work is the first step towards a complete description of the physical and chemical processes in the plasma torch. In this first phase, the conditions in the reactor before the ignition of the plasma are described. Whether the plasma will at the given pressure be ignited or not depends on the electric field and the gas composition in the reactor chamber.

Once the optimal conditions for the ignition are found, one of simplified plasma models, e.g. [2] and eventually a full chemical model can be implemented.



(a) The simulated axial injection torch (b) Detail of the nozzle (cross-section)

Figure 2: The geometry of the simulated torch

2.1 Geometry

The experimental setup (see fig. 2) consists of a cylindrical quartz reactor chamber, 300 mm in length and 75 mm in diameter. The microwave power is supplied to the reactor chamber through a coaxial waveguide of outer diameter 14 mm. The inner conductor of the waveguide has the diameter of 16 mm and serves as a gas supply pipe to the reactor chamber.

The coaxial waveguide is coupled to a waveguide containing a short circuit. The microwave power is fed to the waveguide through a triple stub matching unit. The distance of the stubs is $\frac{\lambda}{4}$, $\lambda = 17.5$ cm. The waveguide is made of aluminum.

The inner conductor is ended with a nozzle (fig. 2(b)). The depositions are usually carried out in a mixture of gases. Previous experiments have shown that supplying all gasses only through the central channel results in clogging the nozzle. Therefore, the gases are supplied to the reactor chamber through 2 outlets, the inner channel and the outer coaxial outlet.

The reactor chamber is enclosed by a casing with walls covered with microwave absorbing material (not shown in the figure).

2.2 Electromagnetic field

The model solves Maxwell equations on the computational domain shown in figure 2(a). GMRES solver allowing relative error of order 10^{-5} was chosen for the simulations. MW power supplied to the device is usually around 200W at 2.45 GHz so these values have been used in the simulations. Rectangular port boundary condition was used for the input port. The main goal is to minimize the reflected power and thus achieve the highest electric field above the nozzle. At atmospheric pressure, the breakdown electric field required for argon/hydrogen plasma ignition is roughly $E_B = 200$kV/m.

For the metal parts, the impedance boundary condition defined as

$$\sqrt{\frac{\mu_0\mu_r}{\epsilon}}\mathbf{n} \times \mathbf{H} - (\mathbf{n} \cdot \mathbf{E})\,\mathbf{n} = (\mathbf{n} \cdot \mathbf{E_s})\,\mathbf{n} - \mathbf{E_s} \tag{1}$$

was initially used ($\mathbf{E_s}$ denotes the source field). However, first simulations have shown that the ressistive losses do not exceed 1% of the input power and for this reason the impedance boundary condition was replaced by a simpler perfect conductor boundary condition. This boundary condition sets the tangential component of $\mathbf{E}$ to zero

$$\mathbf{n} \times \mathbf{E} = \mathbf{0} \tag{2}$$

As previously mentioned, the reactor chamber is enclosed by metal casing with MW absorbing material on the walls. The absorption was simulated by Perfectly Matched Layers in COMSOL.

The matching was simulated separately from the rest of the model (the waveguide and the reactor chamber) and the two models were linked through scattering matrices.

2.3 Hydrodynamic module

The Reynolds number for typical conditions is approx. 4000. Therefore, gas flow in the chamber was considered turbulent. Transport of Concentrated Species was used to determine the concentration of Hydrogen in Argon. The gas mixing simulations were performed in 2D axial symmetry.

The diffusion coefficient for hydrogen/argon mixture was calculated using the Chapman-Enskog relation [1]

$$D = \frac{1.86 \cdot 10^{-3} \cdot T^{3/2} \sqrt{M_{H_2}^{-1} + M_{Ar}^{-1}}}{p \sigma_{12}^2 \Omega} \quad [\mathrm{cm}^2/\mathrm{s}] \tag{3}$$

where M_{H_2} and M_{Ar} are the molar masses of the gasses, T is the absolute temperature p is the pressure in atmospheres. σ_{12} is the average of H_2 and Ar collision diameters in Ångström (tabulated in [1]). The so-called temperature-dependent collision integral Ω is a function of temperature and Lenard-Jones potential ratio and is also tabulated [1].

The temperature of the gasses during deposition has not been measured yet but it is estimated to be of the order of $10^2 - 10^3$ K. In this region Ω can be approximated by an exponential function (with less than 2% error) as

$$\Omega(T) = 0.44 \cdot e^{-2.13 \cdot 10^{-3} T} + 0.646 \tag{4}$$

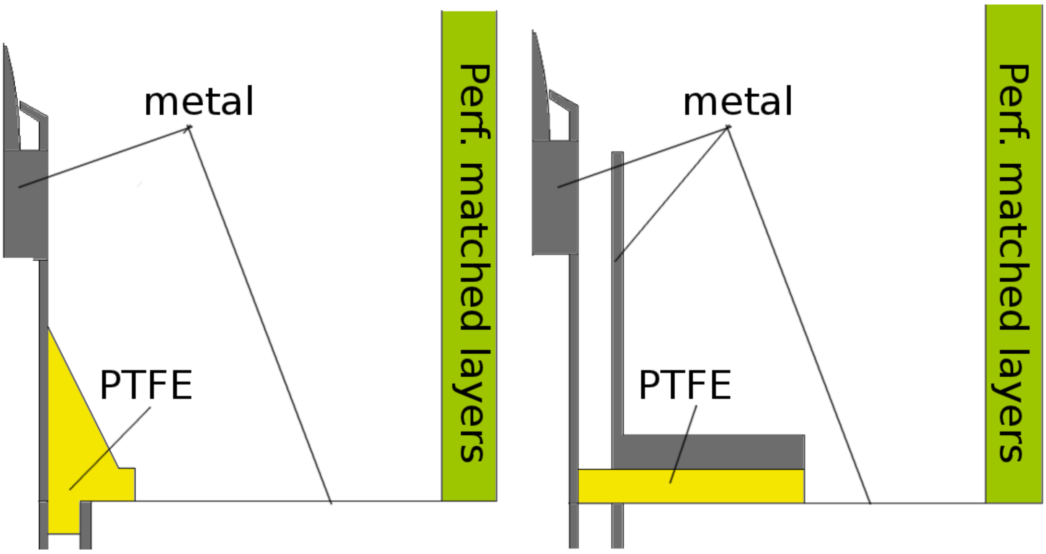
which for the argon-hydrogen diffusion coefficient gives

$$D = 3.02 \cdot 10^{-4} \cdot \frac{T^{3/2}}{e^{-2.13 \cdot 10^{-3} T} + 1.47} \quad [\mathrm{cm}^2/\mathrm{s}] \tag{5}$$

3 Results

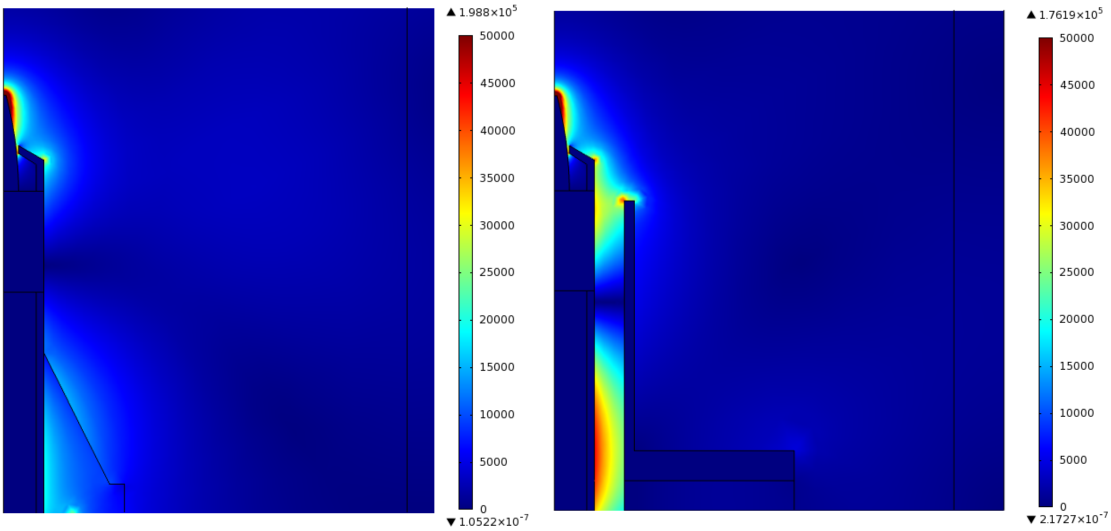
3.1 Electric field

Two configurations of the reactor chamber were proposed (fig. 3). These configurations were tested and it has been found out that configuration no. 1 is more suitable because the electric field above the gas inlet is slightly higher (fig. 4). The scale of figure 4 was reduced in order to show more detail. The absolute electric field maximum (of order 10^5 V/m) occupies a small area above the tip of the nozzle.



(a) Geometry no. 1 (b) Geometry no. 2

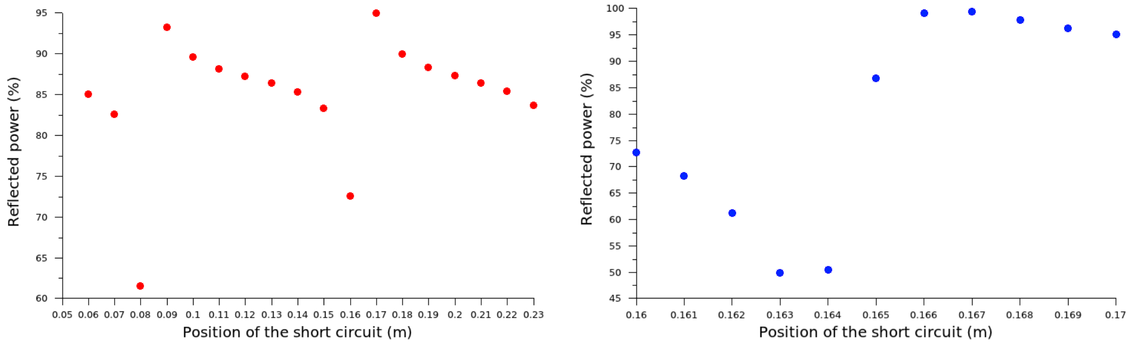
Figure 3: Two proposed geometries of the reactor chamber



(a) Geometry no. 1 (b) Geometry no. 2

Figure 4: Comparison of the electric field norm (V/m) in the two geometries.

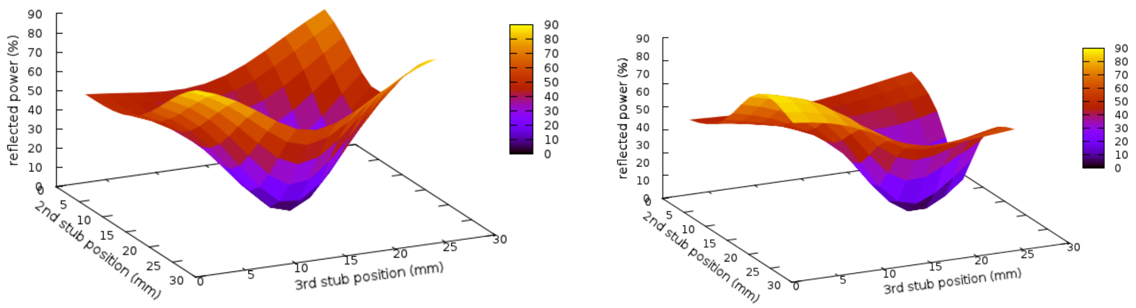
In subsequent simulations, only geometry no. 1 was considered. Firstly, the dependency of reflected power on the position of the short circuit was simulated (fig. 5). The minimum of the reflected power was found for $L_p = 16.3$ cm. For this setting, a little under 50% of the input power is reflected. This is of course unacceptable for operation and it has to be compensated with the triple stub matching unit.



(a) 5-23 cm, 1 cm step (b) 16-17 cm, 0.1 cm step

Figure 5: The reflected power with respect to the position of the short circuit

A parametric sweep was run over the positions of all the three stubs and several minima of the reflected power were found. Figure 6 shows the dependency of reflected power on the position of two stubs with the third in constant position. Stubs are numbered 1 to 3, where stub 3 is the one nearest to the input port. Some of the optimal values are mentioned in table 1. As it is usually possible to measure the reflected power with error not smaller than 1%, there is no point in attempting to further minimize the calculated reflected power.



(a) $s1 = 0.2$ cm (b) $s1 = 1.4$ cm

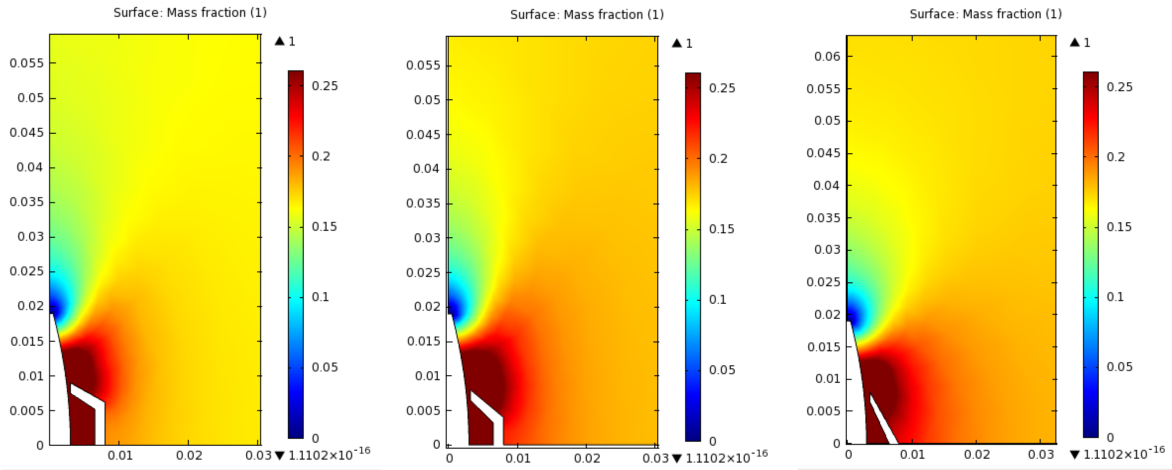
Figure 6: The dependency of the reflected power on the position of stubs 2 and 3 with stub 1 in constant position $s1$

1^{st} stub position (cm)	0.2	1.0	1.4
2^{nd} stub position (cm)	1.4	1.6	1.4
3^{rd} stub position (cm)	1.6	1.9	2.2
calculated reflected power	1.5%	0.5%	1%

Table 1: Positions of the stubs in the matching unit for which the reflected power would be minimal ($L_p = 16.3$ cm).

3.2 Hydrodynamic module

Only a basic evaluation of the gas flow and gas mixing was performed at this phase. Figure 7 shows hydrogen mass fraction in the chamber for different designs of the nozzle. The original design is shown in figure 7(a). For this geometry, the desired H_2 mass fraction (in this particular case around 0.166) is achieved quite far from the tip of the nozzle. This can be modified by moving the outer outlet downwards as figures 7(b) and 7(c) show.



(a) Original nozzle (b) Proposed design 1 (c) Proposed design 2

Figure 7: Gas mixing in the reactor chamber

4 Conclusion

The results obtained by these simulations helped find the optimal configuration for the ignition of the plasma in the torch. This included choosing the proper geometry and finding optimal configuration of the short circuit and the three stub matching. In addition, gas flow in the reactor chamber was simulated. The influence of the shape of the nozzle on the gas mixing was examined and discussed. The results will be very useful in subsequent simulations when plasma is added to both the electric field and gas flow models.

References

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