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Numerical simulations of a microwave plasma torch at atmospheric pressure

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Abstract: Physical processes taking place in an atmospheric microwave plasma torch have been investigated by setting up numerical models with COMSOL Multiphysics. The simulation of cold gas flows in the plasma torch led to an optimisation of the gas management. Furthermore, the plasma itself could be modelled by taking its electrical conductivity, drift diffusion equations and a set of reaction mechanisms into account.

Keywords: atmospheric plasma torch, numerical simulation, plasma simulation

1. Introduction

Atmospheric microwave plasma devices have the advantage of being applicable without any complex and expensive vacuum system. Using microwaves for the power supply also helps to avoid geometrical restrictions and allows one to obtain a free-standing plasma for various applications. These range from the conversion of waste gases to the deposition of coatings. For a better understanding and an optimisation of an atmospheric microwave plasma torch this work focusses on a stepwise description of the physical processes by numerical simulations using COMSOL Multiphysics. Individual models of the cold gas flow, the plasma described by the Drude theory and a preliminary model containing a set of reaction mechanisms can then be coupled in order to describe and predict the plasma processes.

2. Experimental Setup

The setup of the microwave plasma torch is shown in Fig. 1. A microwave with a frequency of 915 MHz and a power of 5 kW is guided through a wave guide into a resonator geometry. That consists of a cylindrical shaped wide-band resonator and a narrow-band coaxial resonator.

There are two different gas inlets available for the gas supply: a tangential and an axial one. The axial inlet serves as well as the inner conductor of the coaxial resonator. The gas is led through a quartz tube which is centred in the resonator geometry. High electric fields can here ignite and sustain the plasma.

3. Theory of Gas Flow Simulations

For the numerical simulation of gas flows the Navier-Stokes equations are solved. One of them is also known as the continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \qquad (1)$$

which describes the temporal and spatial development of the fluid density ρ. Furthermore, the conservation of momentum has to be considered:

$$\rho \frac{\partial \vec{v}}{\partial t} + \rho(\vec{v} \cdot \nabla)\vec{v} = \nabla \cdot (-p\mathrm{I} + \tau) + \vec{F} \qquad (2)$$

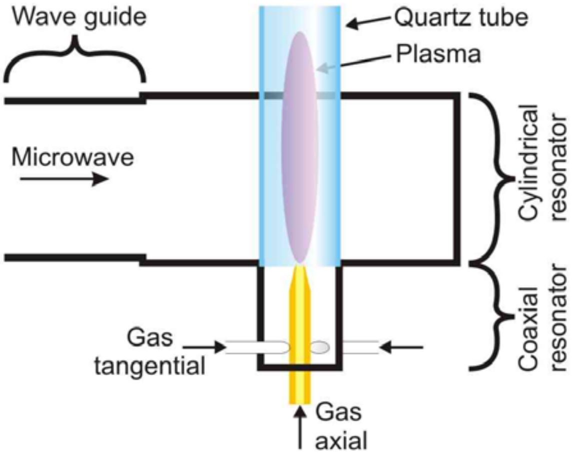

Fig. 1. Setup of the atmospheric microwave plasma torch. Microwaves (915 MHz, 5 kW) are used to ignite the plasma in the centre of the resonator geometry. Gas is fed in through axial and tangential inlets.

Temporal and spatial changes of the velocity $\vec{v}$ are caused by forces on the right hand side of the equation. These can in turn be induced by gradients of the pressure p, inner stress of the fluid τ or external forces $\vec{F}$ which include for example the gravitation.

4. Theory of Plasma Simulation

A plasma is characterised by an electric conductivity σ and a permittivity ε. Exposure to an external alternating electromagnetic field cause a frequency dependence of these two parameters as shown in equations (3) and (4):

$$\sigma(\omega) = \frac{e^2 n_e}{m_e(\nu + i\omega)} \qquad (3)$$

$$\varepsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2\left(1 - \frac{i\nu}{\omega}\right)} \qquad (4)$$

e indicates the elementary electric charge, n_e the electron density and m_e the electron mass. ν is the collision frequency for collisions between electrons and neutral particles. It depends on the density of the neutral species, the mean electron velocity and the collision cross section. ω is the frequency of the external electromagnetic field and ω_p the plasma frequency.

To calculate the distribution of the electric field the wave equation is solved:

$$\nabla \times \left(\frac{1}{\mu_r} \nabla \times \vec{E}\right) - k_0^2 \left(\varepsilon_r - \frac{i\sigma}{\omega\varepsilon_0}\right) \vec{E} = 0 \qquad (5)$$

The electrostatic field in the plasma caused by the separation of electrons and ions can be computed with the Poisson equation

$$\nabla \cdot \vec{E} = \frac{\varrho}{\varepsilon_0} \qquad (6)$$

where ϱ is the space charge density.

To describe the behaviour of electrons, ions and neutral species in the plasma continuity equations have to be solved as described in [1]. As an example the equation describing the temporal and spatial change of the electron density n_e is given here:

$$\frac{\partial n_e}{\partial t} + \nabla \cdot \vec{\Gamma}_e = S_e \qquad (7)$$

$\vec{\Gamma}_e$ is the electron flux caused by the electron diffusivity and the static electric field. On the right hand side of the equation the source term S_e contains rate coefficients for ionisation and recombination processes.

The reaction mechanisms of collisions which were considered in the simulation are listed in Table 1.

Table 1. Reaction mechanisms of collisions considered in the plasma model.

Reaction	Description	Rate coefficient [1]
$e + Ar \rightarrow e + Ar$	Elastic collision	$3.78 \cdot 10^{10}$
$e + Ar \rightarrow e + Ar^*$	Excitation	$1.09 \cdot 10^{8}$
$e + Ar^* \rightarrow e + Ar$	Superelastic collision	$4.62 \cdot 10^{8}$
$e + Ar \rightarrow 2e + Ar^+$	Ionisation	$4.31 \cdot 10^{7}$
$e + Ar^* \rightarrow 2e + Ar^+$	Ionisation	$1.71 \cdot 10^{10}$
$Ar^* + Ar^* \rightarrow e + Ar + Ar^+$	Penning ionisation	$3.73 \cdot 10^{8}$
$Ar^* + Ar \rightarrow Ar + Ar$	Quenching	1807

5. Results and Discussion of the Gas Flow Simulations

Since the gas temperature of the plasma reaches values up to 7000 K, which is known from optical emission spectroscopy measurements, the gas management has to be adapted in a way that the quartz tube, which contains the hot plasma, gets protected. In order to do that a tangential gas supply in addition to an axial one has been set up as shown in Fig. 2.

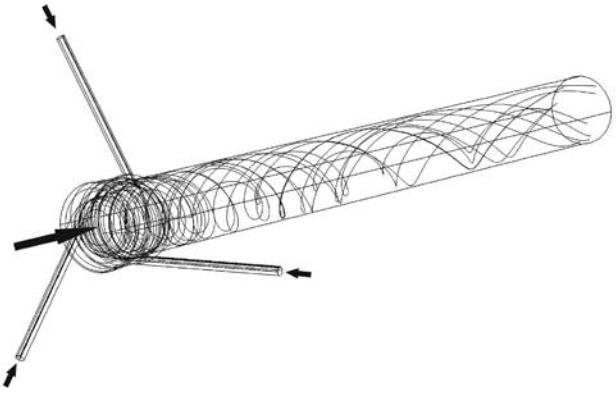

Fig. 2. Arrangement of an axial and three tangential gas supplies. The tangential ones cause a rotational gas flow which helps to envelop the hot plasma.

The simulation of the cold gas flow in Fig. 2 with a total flow of 50 slm (standard litre per minute) demonstrates how the tangential gas inlet leads to a rotational gas flow. This will help to envelop the hot plasma in the centre of the tube.

In Figs. 3 and 4 it becomes obvious that high flow velocities at the wall of the quartz tube come along with a high pressure in these areas which induces a steep pressure gradient towards the centre of the tube. Therefore, the gas in this central area is flowing backwards towards the gas inlets. As the diagrams show, the additional axial gas supply can help to prevent this effect. These findings have to be considered in further studies on the stability of the plasma.

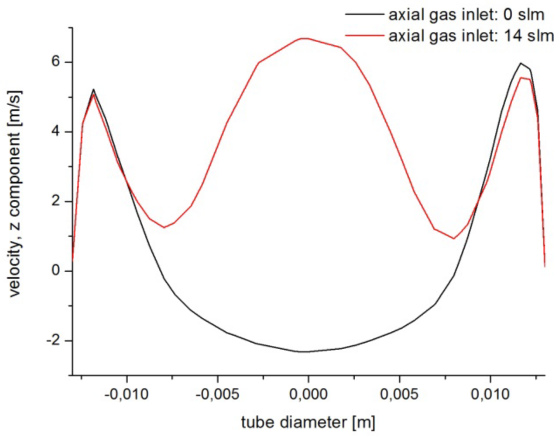

Fig. 3. Velocity plotted against the tube radius. Distance to tangential gas inlets: 2 cm. High velocities at the wall of the tube come along with negative velocities in the centre. An additional axial gas inlet helps to supress this backflow.

It could also be shown that the extent of the rotational area in the tube depends on the inlet velocity of the gas

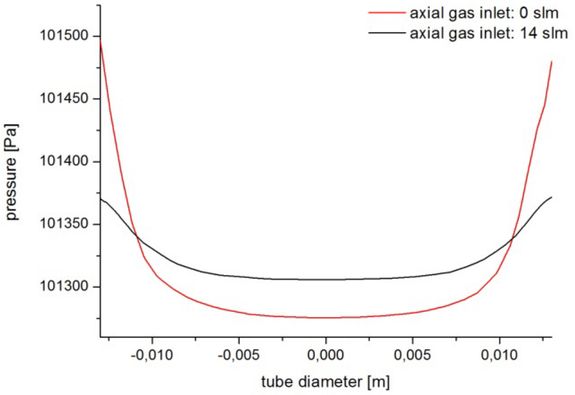

Fig. 4. Pressure plotted against the tube radius. Distance to tangential gas inlets: 2 cm. High flow velocities on the wall of the tube cause a pressure drop in the centre. An additional axial gas inlet weakens the effect.

and can therefore be regulated by adjusting the gas flow rate. In order to avoid the utilisation of a high amount of gas for sustaining the rotational gas flow the diameter of the gas inlets can be reduced.

6. Results and Discussion of the Plasma Simulation

As a first step towards the simulation of the plasma its interaction with the electromagnetic field of the microwave was investigated. To do so the frequency dependent conductivity of the plasma, as explained in section 4, is defined in the centre of the resonator geometry where the plasma is operated in the quartz tube (Fig. 5).

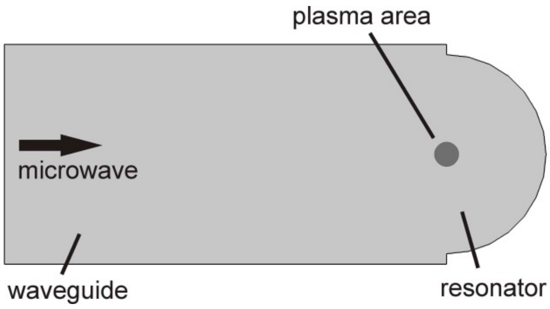

Fig. 5. Geometry used for the modelling of the plasma. In the centre of the resonator a plasma area is defined. A waveguide for the heating with microwaves is connected to the resonator.

Fig. 6 shows the normalised electric field strength in the centre of the conductive plasma area plotted against the electron density. Not until the density reaches the cut off density of $1.04 \cdot 10^{16}$ 1/m^3 the electric field gets expelled from the plasma area. The absence of a sharp cut off comes from the fact that a considerable collision frequency between electrons and heavy particles has to be taken into account when atmospheric conditions are assumed. Collisions disrupt the phase relation between electron oscillation and electromagnetic wave and therefore also the opposing field. For this reason the wave can be transmitted in the case of higher electron densities as well.

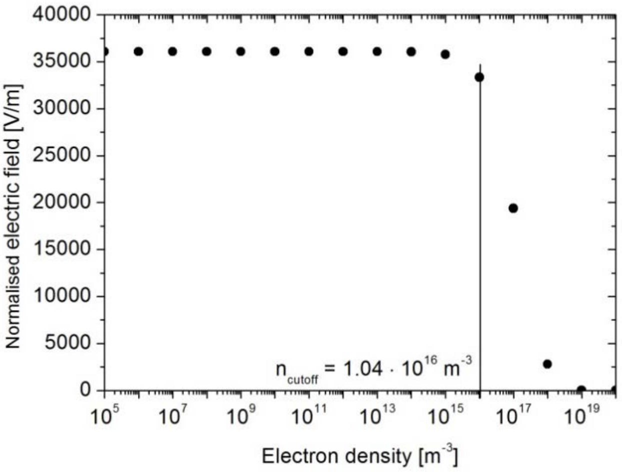

Fig. 6. Normalised electric field in the centre of the plasma area plotted against the electron density. Since collisions are considered no sharp cut off can be observed.

Until now the electron density has been assumed as a constant value defined in an area considered as plasma. In a next step the development of the electron density is modelled by using the equations introduced in section 4 and a set of reactions caused by collisions as shown in Table 1. Due to stability reasons of the numerical simulation an initial electron density of $1 \cdot 10^{13}$ 1/m^3 has been assumed. It could be shown that with increasing time electrons gain energy from the microwave field and collisions with neutral particles cause a rising electron density which reaches a maximum of $1 \cdot 10^{19}$ 1/m^3 in the centre of the plasma area (Fig. 7). This value is already in the range of experimentally determined values.

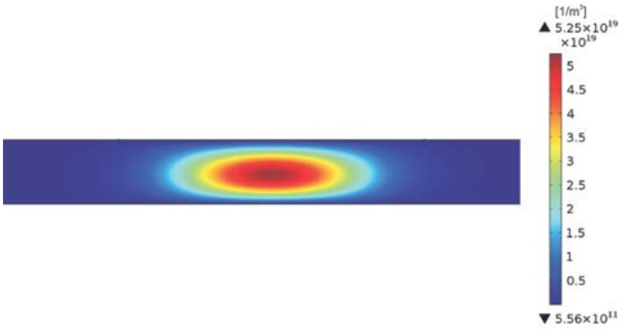

Fig. 7. Electron density in the plasma area. A maximum density of 1·1019 1/m3 is reached in the centre.

7. Conclusion

To investigate an atmospheric microwave plasma torch numerical simulation models have been developed. Modelling the cold gas flow led to a better understanding of the behaviour of the flows and to an optimisation of the gas management. The simulation of the interaction between a conductive plasma and the electromagnetic field of a microwave showed how this field gets transmitted or reflected depending on a predefined plasma density. A further model described the development of the electron density distribution in a simple argon plasma. In future an enhanced model can be developed in which a complete set of reaction mechanisms is considered.

8. Acknowledgements

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9. References

[1] M. Lieberman. *Principles of plasma discharges and materials processing.* (New York: Wiley) (1994)