Numerical modeling of a plasma jet discharge: on the fluid dynamics and argon/humid air plasma chemistry.

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Abstract: We present some results of a 2-dimensional (2D) fluid model, taking into account the fluid dynamics and plasma formation of an atmospheric pressure RF driven plasma jet device. The discharge is created inside the discharge tube, through which pure argon flows into the surrounding, quasi stationary, humid air. A chemistry set of 130 reactions was applied, to describe the generation of 28 relevant different species. 2D profiles of the convective flow, together with the mixing of the surrounding air into the argon stream are shown. Finally, results of electron, \( \text{N}_2^+ \) and \( \text{O}_2^- \) densities are discussed in respect to (biomedical) applications.

Keywords: modeling, plasma jet, argon, humid air, biomedicine

1. Introduction

The plasma jet devices within our interest can be used for biomedical applications, such as sterilization [1], dermatology [2], blood coagulation [3], chronic wound healing [4], dental treatment [5], cancer treatment [6], etc. The technology of low temperature atmospheric plasmas (LTAP’s) looks very promising but a lot of questions remain on the plasma chemistry. Moreover, a lot of experience with different techniques, time and money is needed in experiments to measure the huge amount of different species densities and other quantities. And even then it is unsure whether the right information at the correct location can be obtained at all.

Figure 1. RF plasma jet device developed by P. Bruggeman and co-workers at the Eindhoven University of Technology.

In this work results will be presented on an existing experimental plasma jet device (Figure 1), developed by P. Bruggeman and co-workers at the Eindhoven University of Technology. The feed gas of the device can be either helium or argon, which is running through a dielectric tube. Coaxially inserted in this tube, a needle electrode serves as a first electrode. At a distance of 5 mm, a metal plate functions as a grounded electrode. A hole in this plate allows free propagation of the jet. By applying a voltage to the needle electrode a noble gas discharge is created, which flows out of the tube into the surrounding humid air. By dissociation and recombination processes, biomedically active species \( \text{O}_2^- \), \( \text{H}_2\text{O}^- \), \( \text{NO} \), \( \text{OH} \), \( \text{NO}_3^- \), etc. are created.

The complexity of biomedical devices and living tissue present a great challenge for modelers, to provide much needed complimentary data to experimental work. The use of numerous totally different devices and operating conditions, importance of temperature effects for the application, very complex chemistry (both humid air and noble gases), plasma bullet formation, etc. are the main reasons. To simulate this, highly developed models are required and calculation time is always an issue.

2. Description of the model

In this study, the 2-dimensional (2D) plasma hydrodynamics model nonPDPSIM was used for the
investigation of some plasma jet processes. This model was developed by M. Kushner and co-workers. The model will be only briefly described here but more information can be found in [7] and previous work of the authors.

As mentioned above, many different processes occur in these kind of discharges and several modules need to be used, which are given schematically in Figure 2. Simulations are performed using a time-slicing technique where updates of charged particle transport and electric field are obtained using an implicit Newton’s method. Subsequently, neutral particle densities and electron temperature ($T_e$) are updated. With lower frequency, modules of processes which occur on a much coarser timescales are called, e.g. fluid dynamics.

The fundamental equations necessary to describe charged particle transport are the continuity equations for electrons and ions, Poisson’s equation for the electric potential in the gas phase region and finally the continuity equation for charges on surfaces and in materials. To solve these equations, the fluxes of the charged species need to be obtained. For reasons of calculation time and stability of the model, these fluxes are formulated using the Scharfetter-Gummel method.

The necessary electron impact rates and transport coefficients for electrons are obtained by calling a Boltzmann solver, which solves Boltzmann’s equation for a two-term spherical harmonic expansion of the electron energy distribution. Over a range of E/N values, a look-up table is constructed for the transport coefficients as a function of the average electron energy, assuming local field approximation. To obtain a more accurate value for the average electron energy the electron energy conservation equation is implicitly solved.

For the update of the neutral particle densities, the continuity equation is implicitly solved. The flux of neutral particles is determined by diffusion, but optionally also by convection. In this case, the bulk neutral fluid flow needs to be known, so the fluid dynamics module needs to be called. This module is based on solving the Navier-Stokes equations, i.e. mass, momentum and energy conservation equation for neutral fluid velocity and gas temperature ($T_g$). It is very important that there are continuous updates of these variables, because of the time-slicing technique.

The experimental geometry is transferred into a numerical grid with an external mesh generator, which is capable to construct a nonstructured mesh consisting of triangular cells. In this way we can vary the resolution over the geometry, from very small cells ( ~ 10 µm ) at regions with high electric field gradients and/or large density gradients, to much larger cells at remote regions to reduce the calculation time. The mesh consists of nearly 8000 nodes, with high resolution around the needle electrode tip (Figure 3).

To study LTAP’s we first developed an extensive reaction set of more than 700 reactions, which is suitable to describe the complex chemistry of a noble gas plasma flowing into the surrounding gas consisting of humid air. However, in this study we use a reduced chemistry set of 130 reactions at maximum and only 28 species at most. Amongst them are bioactive species such as N, O, O$_2$, OH, HO$_2$, NO, O$_3$. 

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**Figure 2.** Working scheme of the nonPDPSIM code, with the different modules that are being used.

**Figure 3.** Part of the simulated plasma jet geometry with a high mesh resolution at the end of the needle electrode tip.
3. Results and discussion

We have performed calculations for a peak voltage of 600 V applied to the needle electrode, at an RF frequency of 13.56 MHz. The initial values for pressure and gas temperature are 760 Torr and 300K. Argon is fed through the dielectric tube, along the needle electrode, with a flow speed of 1.5 slm. We assume that the surrounding humid air consists of 99% nitrogen-oxygen mixture (with 80/20 molar fractions) and 1% water, which represents normal humid air.

Figure 4. The 2D steady state convective flow field and the densities of the water component of the surrounding, quasi stationary humid air. The left border of the figure is the symmetry axis of the plasma jet device.

An essential characteristic in these kind of microplasmas is the mixing between the surrounding humid air and the argon plasma flowing out of the device, where convection plays a major role. In Figure 4, the direction of the steady state convection flow of the neutral particles is shown. The mass efflux through the pump, is the same as the mass influx through the nozzles and as a result the outflow develops by itself in such a way that the plasma jet doesn’t ‘feel’ the presence of the pump. The absolute values of the flow vectors in the plasma jet itself along the symmetry axis of the device, are at least three orders of magnitude larger than for the outer regions, so the surrounding humid air can be considered stationary. Nevertheless it is clear from the figure that water (and also oxygen and nitrogen) is drawn into the plasma jet, along its entire length. This results in a density gradient of these air components in the argon gas stream. In the center of the jet, at an axial distance of 2 mm out of the tube, the water content is still only 0.01% mass ratio of the total gas mixture, but at 7 mm it is already 0.2% and at the pump even 0.35%.

Figure 5. Time-averaged 2D profile of the electron density, only the relevant part of the geometry is shown.

The implementation of the fluid dynamics has a strong effect on the plasma fluid part of the code. From the time-averaged electron density, given in Figure 5, an important conclusion can be made: the distribution of electrons is determined by the convection of the heavy particles rather than diffusion of electrons, because the density decreases much faster in the radial than in the axial direction. This asymmetry can be explained by the fact that energetic species and anions are carried with the flow along the plasma jet and generate new electrons through heavy particle collision processes like electron detachment, Penning ionization, etc. Furthermore, it can be seen that electrons are mainly generated at the tip of the needle electrode, for
which both bulk ionization and secondary electron emission processes are responsible. The calculated absolute values of the electron density, with a maximum just next to the thin sheath at the needle electrode of $2.5 \times 10^{13}$ cm$^{-3}$, will be validated in the future by comparison with experimental results.

Finally, to demonstrate that charges (and energy) created in the argon plasma are efficiently transferred to the diffusing air components, the profiles of $N_2^+$ and $O_2^-$ are shown in Figure 6. Indeed, it can be seen that both species reach a rather high density, with a maximum in the order of $10^{11}$. In contrast to the electrons, these heavy particles are still present after the hole in the grounded counter electrode. This is a very important conclusion for the applications, since it is known that ions like $N_2^+$, but especially the bioactive species like $O_2^-$, have a strong effect on cells and tissue.

4. Acknowledgments

W. Van Gaens is indebted to the Institute for the Promotion of Innovation by Science and Technology in Flanders (IWT Flanders) for financial support. The authors would like to thank P. Bruggeman and co-workers at the Eindhoven University of Technology for providing experimental data and M. Kushner and co-workers for providing the nonPDPSIM code and useful advice. Finally, the computer facility CalcUA, provided by the University of Antwerp is acknowledged.

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