Numerical modelling of an atmosperic pressure plasma reactor using control volume methods and unstructured grids

M. Zakari [1,2], H. Caquineau [1,2(*)], P. Ségur [1,2] , F. Bras [1,2], N. Gherardi [1,2], N. Naudé [1,2], P. Descamps [3]

[1] *Université de Toulouse ; UPS, INPT ; LAPLACE (Laboratoire Plasma et Conversion d'Energie) ; 118 route de Narbonne, F-31062 Toulouse cedex 9, France*
[2] *CNRS, LAPLACE, F-31062, Toulouse, France*
[2] *Dow Corning S. A., Rue Jules Bordet, B7180 Seneffe, Belgium*
[(*)] hubert.caquineau@laplace.univ-tlse.fr

A numerical code based on control volume methods and unstructured grids has been developed and used to calculate discharge propagation in a specific plasma reactor in He-N_2 mixtures at atmospheric pressure. First results show that a surface discharge very quickly occurs along the reactor glass tube and propagates at almost constant velocity.

At the present time, numerical modelling of plasma discharge plays a very important role in understanding the processes occuring in industrial plasma reactors. However, even if most of the complex physical and chemical mecanisms are usually embedded inside the best available numerical codes, few of them [1] are able to accurately describe the full complicated structure of industrial reactors. The reason is that, in many cases, as conventional cartesian structured grids are used, it is difficult to locate grid points on the reactor walls especially if they are curved.

In order to overcome this drawback, we developped a code based on unstructured grids methods. Contrary to most other unstructured codes [2], [3] this one uses the control volume method and is, for the moment, limited to a two dimensional axisymetric geometry.

The numerical model is based on the continuity equations for electrons, ions and neutral particles. They are coupled to the Poisson equation. Calculations are made in a mixture of helium-nitrogen (100 ppm nitrogen) at the atmospheric pressure. Swarm parameters needed for the calculations (electron and ion mobility, diffusion coefficients, ionisation and excitation coefficients) are obtained from a numerical solution of the Boltzmann equation using a multiterm code developed by Segur et al. [4]. Furthermore classical local field approximation is employed.

Our numerical method uses vertex-centered control volumes in which dual control volumes are made by joining centroid of triangles or quadrangles with the midpoints of the opposite side [5]. The electric field at every node is calculated with a weighted least square root method based on the knowledge of the value of the electric potential at the nodes surrounding the centre node. Numerical discretization of continuity equations are explicit or implicit, depending of the type of problem investigated. Numerical solution of linear systems are made by using Super LU and Pardiso direct solvers (Poisson equation) and by using iterative Sparskit library with preconditioning developed by Y. Saad (transport equations) [6].

Upwind schemes are used for the moment and higher order methods (MUSCL) will be introduced in a near future. Photoionisation is included in the code but not photoelectric effect. The meshing of the computational area is made with SALOME an open source software freely available at http://www.salome-platform.org/.

A simple chemistry has been added including four different ionic species (i. e. He^+, He_2^+, N_2^+, N_4^+), three different neutral excited species ($He(2^3S)$, $He(2^3P)$, He_2) and fifteen different reactions.

The geometry of the reactor investigated in this work is given in figure 1. It is essentially a vertical tube made of glass, located above a horizontal glass grounded plate. At the top of the tube a metallic point, on which the voltage is applied, is centred on the main axis. In this figure, metal electrodes are in black and dielectric in orange. A sinusoidal voltage of 18 kHz frequency is applied to the point electrode with an amplitude of 12 kV. The filling gas is located inside the white regions of the figure. Note that the length of the reactor is around 5 cm and its radial extension around 0.5 cm.

Calculations have been initiated with a Gaussian electron and ion seed located at the top of the points with a maximum value of 10^{13} cm^{-3} together with a background of electrons and ions of 10^{8} cm^{-3} uniformly distributed inside the gas gap. We may note that a 150 000 nodes mesh is used.

Figure 2 shows at five different times the spatial distribution of the reduced electric field module (in Townsend units) obtained with a positive point. Figure a shows the initial distribution of the electric field corresponding to the initial distribution of electrons and ions. Figure b, c, d and e give the structure of the propagation of the electric field at 56, 116, 176 and 236 ns. At the beginning of the propagation, a first filamentary discharge located on the symetry axis of the reactor propagates as a cathode directed streamer. An advancing front of the order of 50 Townsend appears followed by a region of low electric field. For times higher than 56 ns, as the width of the advancing front increases, the extension of the discharge is constrained by the dielectric tube : a surface discharge occurs along the wall of the glass tube. In spite of the appearance of a surface discharge, the propagation velocity of the discharge front remains almost constant as it is controled by the seed of charged particles in front of the discharge.

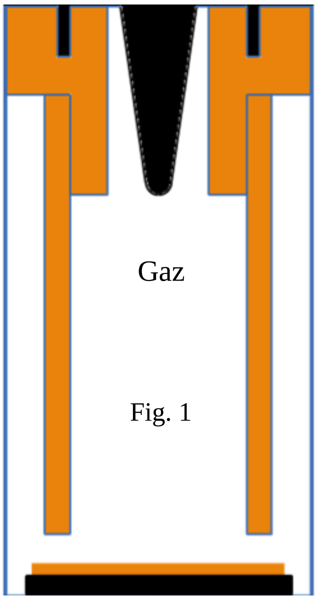

Fig. 1

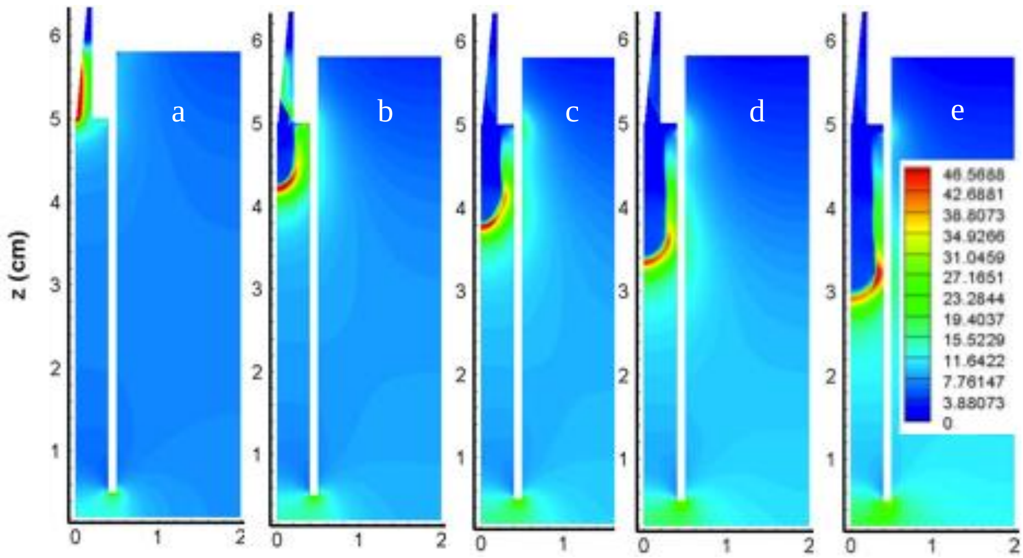

Fig. 2: Spatial distribution of reduced electric field (Townsend) at different times t. Figure a: t=0, Figure b: t=56 ns, Figure c: t=116 ns, Figure d: t=176 ns, Figure e: t=236 ns.

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