Surface Dielectric Barrier Discharge Plasma MATLAB Simulaion

C.Piferi, R.Barni and C.Riccardi

Università degli Studi di Milano-Bicocca, Milano, Italy

c.piferi@campus.unimib.it

Abstract

Dielectric barrier discharge and surface dielectric barrier discharge plasma are a developing field of research. We are interested in knowing the species produced during these plasma discharges. We developed a MATLAB code which simulates the plasma discharge and calculates the produced species according to the reaction rates and the electron temperature. In order to do that, we selected different series of chemical species interesting in and the reaction rates involved between them. We are using this code to simulate atmospheric pressure plasma generated in air with a percentage of pentane.

Experimental Device

The program simulates a single microdischarge of atmospheric plasma produced in air with a less then 1% of pentane. We can set the duration of the microdischarge and the repetition time of the same. The microdischarge shape is a semi-cylinder laying on a surface. We can divide the simulation process in three different parts. The first one, that is of the order of ns, represents a ionization wave during the plasma formation; the second one, of the order of μs, dominates by the chemical kinetic occurring at room temperature since there are no more energetic electrons are involved; the last one describes the diffusion of the molecules between the nearly regions close to the plasma region. In order to model the microdischarge we simulate the ionization wave triggered by an increased of the electronic temperature. For the whole duration of the microdischarge we consider the electrons having a Maxwellian distribution function.

Model

Discharge parameters

- Flow temperature and pressure;
- electron temperature;
- plasma density;
- pentane concentration;
- microdischarge dimensions;
- repetition frequency of the microdischage (HV frequency).

Species involved

- Electrons;
- pentane (C_5H_{12});
- CH_x;
- C_2H_x;
- C_3H_x;
- C_4H_x;
- C_5H_x;
- C_6H_x;
- atomic oxygen;
- atomic hydrogen;
- molecular hydrogen;
- air (all the other species).

Reactions

In our code we considered only two body like reactions that can produce one or more products. The reaction rate are evaluated from the Arrhenius experimental formula

$$K = A\,T^b \exp\left(-\frac{E_a}{T}\right)$$

We do not consider the ionic dynamics. The reaction we considered are

- ionization and neutralizaion of the electrons;
- dissociation reactions due to the interaction of a species with an electron;
- oxidation reactions;
- reactions between species;
- wall reactions and diffusion of the species form the outside to the inside and the opposite.

Continuity density differential equation

The whole simulation is based on the resolution of the continuity density differential equations

$$\frac{\mathrm{d}n_k}{\mathrm{d}t} = \sum_{i\leq j}^{N} K_{i+j\to k} n_i n_j - \sum_{i,j=1}^{N} K_{i+k\to j} n_i n_k - \frac{D_k}{\Lambda_k^2} n_k$$

since we assumed only two body reaction and we are interested in study density of species (n_k), and where N is the number of the considered species. The first term in the right side is the sum of all the two body reaction that contribute to the formation of the k-th species of the sistem. The second term is the sum of all the reaction that involes the k-th species in the reagents. The last term is the diffusive one, where we assumed that $-D\nabla^2 n \sim -\frac{D}{\Lambda^2} n$; the Λ^2 are parameters that depends on the system geometry and are discussed by P.J. Chantry. We assumed that the diffusion to the outside can happen through the lateral surface of the semi-cylinder and to the dielectric surface.

Code

To resolve the differential equation for all the N species involved in the simulation we used the ode (ordinary differential equation) solver `ode23s` MATLAB function. `ode23s` is based on a modified Rosenbrock formula of order 2. The simulation starts with a microdischarge.

The initial conditions are the starting density ($n_{k,0}$) of the Air, C_5H_{12} and electrons; the other density are placed to zero. The electrons temperature is in the order on the eV. The ode solver returns the density shape of the species for the entire microdischarge duration.

→ Final density →

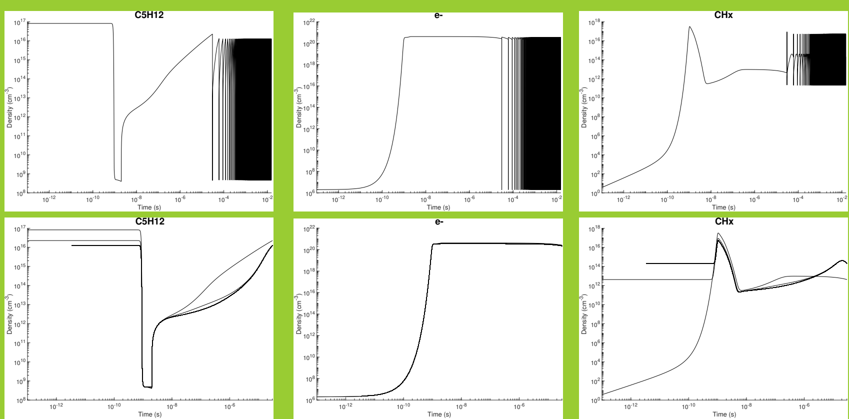
Repeats the ode solver call assuming the room temperature for the electrons. This part of the simulation ends after an HV period.

→ Final density $n_e = n_{e,0}$ →

Repeats the ode solver call assuming energetic electrons of the order on the eV. The ode solver returns the density shape of the species for the entire microdischarge duration.

→ Final denisty → (back to the room-temperature step)

Simulation Output



- Repetition frequency 33 kHz;
- microdischarge duration 2 ns;
- energetic electron temperature 5 eV;
- starting electron density 2x10^6 cm^{-3};
- starting air (molecular oxygen) density 2.5x10^{19} cm^{-3};
- starting C_5H_{12} density 8.3x10^{16} cm^{-3};
- room temperature 25 meV; microdischarge radius 100 μm;
- microdischarge length 0.5 cm;
- number of repetition 500.

In the first line there are the density plots in log-log scale. We can see that the C_5H_{12} decreases quickly during the discharge and then, due to the diffusion to the outside it increases. On the opposite the CH_x increases during the discharge and then decreases for the kinetical reactions and the diffusion. The electron density, instead, grows during the discharge, slowly decreases during the diffusion and then, due to a code setting, returns to 2x10^6 cm^{-3}. Plotting the density using the relative time (second line plots), that is t=0 when the microdischarge starts, we can see that all the density inside of the microdischarge reach a plateau after some repetition, that is important for the next implementation of the code when we will investigate the behavior of the outflow.

Future Implementation

This code needs some implementation in order to improve the simulations output. First of all it is important to set good starting parameters (duration of microdischarge, electron density, etc.). It is also important to include other species like nitrogen and ozone. After that we would like to use the code to compare the simulation with the laboratory device output. When we will reach a good accordance between the simulation and the experiment we could use the simulation to have a preview of the outcome saving time and money discarding the worst configurations.

References

[1] Kogelschatz, U. : 2003, *Plasma Chemistry and Plasma Processing*, **23**, 1.
[2] Corke, T. C., Enloe, C. L., Wilkinson S. P. : 2010, *Annu. Rev. Fluid Mech.*, **42**, 505.
[3] Barni, R., Esena, P., Riccardi, C. : 2005, *J. Appl. Phys.*, **97**, 073301.
[4] Li, J., Dhali, S.K. : 1997, *J. Appl. Phys.*, **82**, 4205.
[5] Chantry, P.J. : 1987, *J. Appl. Phy.*, **62**, 1141.
[6] NIST Chemical Kinetics Database : https://kinetics.nist.gov/kinetics/index.jsp.
[7] GAPHYOR Database : https://www-amdis.iaea.org/w/index.php/GAPHYOR_LPGP
[8] Kinema Database : https://kinema.com/
[9] Shampine, L. F., Reichelt, M. W. : 1997, *SIAM Journal on Scientific Computing*, **18**, 1.