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SURFACE DIELECTRIC BARRIER DISCHARGE PLASMA MATLAB SIMULATION

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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.

1. INTRODUCTION

Surface Dielectric Barrier Discharges (SDBD) are a particular configuration of electrodes that could be used for atmospheric pressure non-equilibrium plasma treatments. The presence of an insulating material between the electrodes prevents the transition of the electrical discharge towards arcing, with the formation of a non-thermal plasma at, or near, the atmospheric pressure. The flat geometry implied by SDBD increases the contact area between the discharge region and the device active parts, which is beneficial for the exposure of materials to the plasma. We developed our MATLAB simulation starting from a plasma device composed by an exposed metal electrode glued onto a dielectric surface. Such a configuration allows the formation of a thin plasma layer above the insulating surface. Any material placed there will be in contact with the plasma gas phase and it will receive a large flow of activated and reactive species. This could be used to apply plasma processes to materials at atmospheric pressure without a damaging heat load, because plasma is generated near the room temperature. Besides surface treatments, SDBD were developed and applied also to aerodynamics, by using asymmetrical electrode layouts. Our simulation investigates the SDBD discharge made in air with a small percentage of pentane (C_5H_{12}). We will outline how the code works, the approximations we have done, some results and future implementations.

2. MODEL

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.

2. 1. APPROXIMATIONS

To develop the code we need to choose the discharge parameters and the species and the reactions involved in the simulation.

The discharge parameters are: the flow temperature and pressure; the electron temperature; the plasma density; the pentane concentration; the microdischarge dimensions; the repetition frequency of the microdischage, also called as HV frequency.

This is a preliminary work so we are using a little number of involved species and reaction. The first species involved is the electron one. We negletted the nitrogen dynamics and we named as Air the species that involes the molecular oxygen dynamics. We are interested in the pentane decomposition, so we concentrated on the hydrocarbons species, that we divided in class as CH_x, C_2H_x, C_3H_x, C_4H_x, C_5H_x, C_6H_x. However, we consider the pentane as a specific species and not in the class C_5H_x. The other species involved are the atomic oxygen (O), the atomic hydrogen (H) and the molecular hydrogen (H_2).

In our code we considered only two body reaction that can produce one or more products. The reaction involved are selected from the NIST Chemical Kinetics Database, GAPHYOR Database and Kinema Database. The reaction rate are evaluated from the Arrhenius experimental formula

$$K = A\ T^b \exp\left(-\frac{E_a}{T}\right) \tag{1}$$

where all the parameters are obtained from the same databases. The reaction we considered are the ionization and neutralizaion of the electrons, the dissociation reaction due to the interaction of a species with an electron, the oxidation reaction and the reaction between species. The latter is composed by hydrogen switch, extraction or acquisition of one or more atomic or molecular hydrogen, and acquisition of C_nH_x. For example we can have $H+C_nH_x \rightarrow C_nH_x+H_2$, $H+C_nH_x \rightarrow C_nH_x$ or $H_2+C_nH_x \rightarrow C_nH_x+H$. After that we also considered the wall reaction and the diffusion of the species form the outside to the inside and the opposite. We do not consider the ionic dynamics.

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

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

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 of (2) 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.

2. 2. CODE

The code needs to resolve the differential equation for all the N species involved in the simulation. To do that we used the ode (ordinary differential equation) solver `ode23s` MATLAB function. `ode23s` is based on a modified Rosenbrock formula of order 2. It is a single-step solver, it is efficient at solving problems that permit crude tolerances or problems with solutions that change rapidly, as can happens in our system. The `ode23s` solver evaluates the Jacobian during each step of the integration, so supplying it with the Jacobian matrix is critical to its reliability and efficiency.

We run the simulation in two different stages: in the first one we simulate the plasma discharges, with energetic electrons of the order on the eV, and in the other, due to the chemical kinetic and the diffusion, setting the electron temperature as room temperature. We can outline the code as follows: 1. The simulation starts with a microdischarge. The initial conditions are the starting density ($n_{k,0}$) of the Air, C_5H_{12} and electrons, while the other density are placed to zero. The ode solver returns the density shape of the species for the entire microdischarge duration. 2. Starting from the final density of the previous step, we repeat the ode solver call assuming the room temperature for the electrons. This part of the simulation ends after an HV period. We repeat steps 1 and 2 for the desired number of times, taking care that when we repeat the discharge (point 1) the starting density are the final density of the previous step, except for the electrons that is set as $n_{e,0}$.

3. SIMULATION

We show now the density profile inside the discharge volume of the C_5H_{12}, the electrons and the CH_x (Fig.1). We chose to report this four species in order to show the different trends. The simulation parameters are: 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 Fig.1 we plot the density 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 (Fig.2), 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.

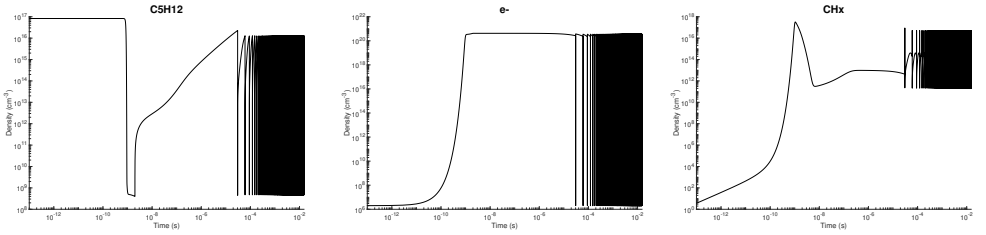

Figure 1: Pentane (left), electrons (center) and CH_x (right) density profile.

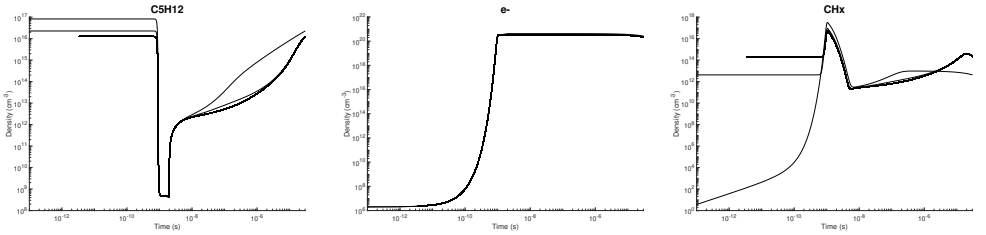

Figure 2: Pentane (left), electrons (center) and CH_x (right) density profile using relative time.

4. FUTURE IMPLEMENTATIONS

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.

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