Simple modelisation of ozone generation by positive corona discharge

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Ozone molecule has unique oxidizing properties that are in the base of its many industrial applications, such as air cleaners, water purification, odor control, gas treatment, etc. [1-4]. Therefore, many studies have been devoted to unveil the mechanisms of generation of ozone in electrical discharges [5-7], and to increase the efficiency of ozone production. In this work, we present a numerical study of ozone production by positive DC corona discharge. The electrical discharge occurs between a wire and a coaxial cylinder, and pure oxygen is feed into the discharge cell (Fig. 1). As it is well known, the corona discharge is initiated when the electric field near the wire is sufficiently high to ionize the gaseous species. The minimum electric field is a function of the wire radius, the surface roughness of the wire, air temperature, and pressure [8].

Corona discharge has been simulated by using a hydrodynamics model that combines the physical processes in the corona discharge with the chemistry of ozone formation and destruction in the oxygen stream. Basically, it consists in a set of continuity equations, coupled with Poisson's equation. The continuity equations govern the transport and the gain/loss balance of every species due to the chemical reactions induced by the electrical discharge. The current-voltage characteristic (CV) measured in experiments is used as input data to the numerical simulation.

Fig. 2 presents the radial distribution of charged species and the electric field for a positive DC corona discharge from the wire (anode) to the cylinder (cathode) at room temperature ($T = 300$ K) and atmospheric pressure. The anode and cathode radius are 0.00625 cm and 1.35 cm, respectively, the applied voltage is 8 kV, and the gas flow rate is 100 cm^3/min.

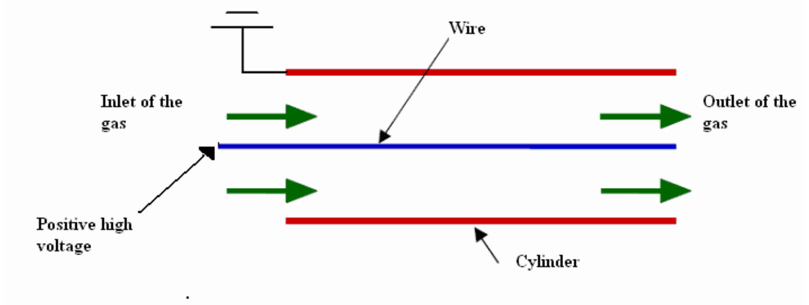

Fig.1. Schematic diagram of the positive corona discharge cell.

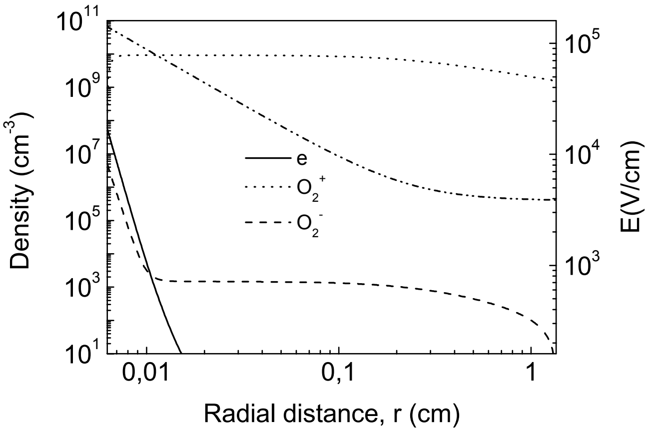

Fig. 2. Radial distribution of charged species (left axis) and electric field (right axis) in a positive corona discharge, for V = 8 kV and Q = 100 cm^3/min.

The distribution of species is the result of the competition between ionization and electron attachment. Near the wire, the electric field is very high, so ionization prevails over attachment and new electrons are produced. A few millimeters away from the wire, the ionization rate equals the attachment rate. All newly produced electrons attach to oxygen molecules to form negative ions,

$$e + O_2 + M \rightarrow O_2^- + M \quad (M = O_3, O_2, \text{etc.}).$$

Theses negative ions move then towards the discharge wire. Outside the ionization region, the electric field strength is insufficient to produce electrons. Therefore, positive ions drift into this volume towards the grounded cylinder. The plasma is in a non-equilibrium state and has a low degree of ionization.

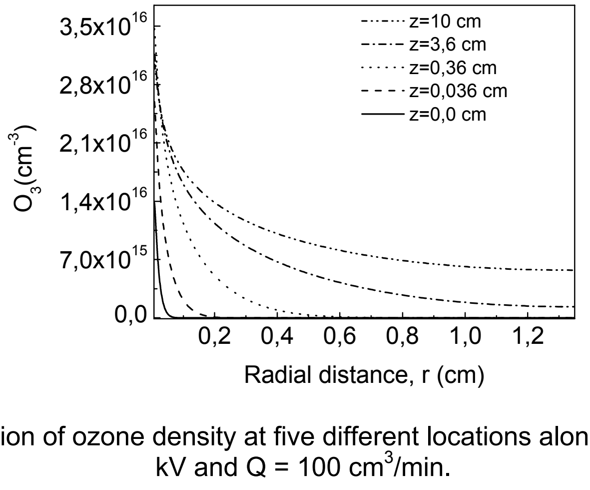

Fig. 3. Radial distribution of ozone density at five different locations along the cylinder, for V = 8 kV and Q = 100 cm^3/min.

The radial variation of the ozone density is represented in Fig. 3. As expected, ozone concentration increases progressively as the oxygen flow advances along the cylinder. Just after the entry of the oxygen gas into the discharge tube (z = 0.0 cm), the radial distribution of ozone is highly inhomogeneous. In that location, the density of ozone has a maximum in the vicinity of the wire, where the active region of the corona discharge is located, and then sharply declines. This decline reveals that ozone diffusion has not had enough time to act in the radial direction. A crude estimate of the diffusion time of ozone gives t_d ~ 5 s, which is much shorter than elapsed time of flow. As oxygen gas advances along the cylinder, ozone diffuses towards the cathode and its concentration becomes more uniform. Finally, Fig. 4 shows the axial distribution of ozone at a constant radial distance and for two different values of the applied voltage. After a certain entrance length, ozone density is observed to increase linearly along the axial direction for low applied voltages.

The predictions of the numerical simulation are compared with the experimental measurements in Fig. 5. In that figure, the averaged ozone density has been plotted as function of the applied voltage. The results of the simulation are in qualitative agreement with the experimental measured data. The numerical simulation tends to overestimate the ozone density, as the predicted ozone concentration is 50% higher than the actual measured concentration.

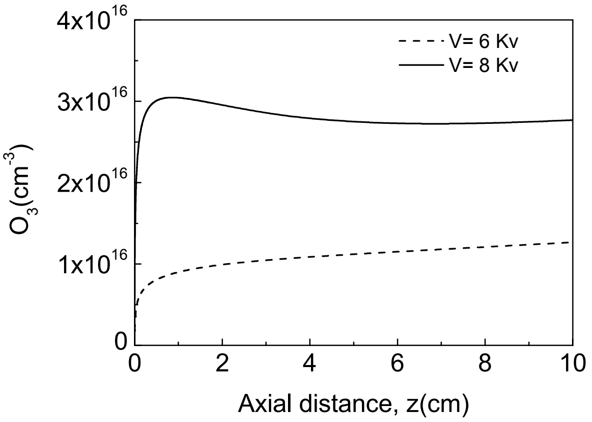

Fig. 4. Axial variation of ozone density in the vicinity of the wire (r = 0.01668 cm) for two different applied voltages and Q = 100 cm^3/min.

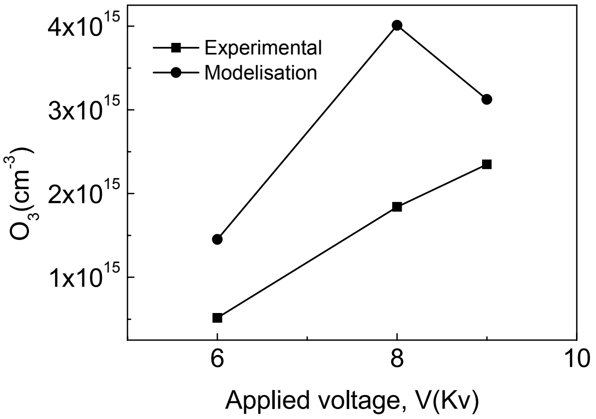

Fig. 5. Experimental and numerical results of ozone density as a function the applied voltage for Q = 100 cm^3/min.

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