# Numerical modeling of ozone production in direct current corona discharge

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## Abstract

Ozone has many industrial uses, including treatment of municipal water, wastewater, cooling towers, industrial process water, effluent water treatment, food processing, through to water fit for consumption and marine life. In this paper, we study the ozone production by negative electric corona discharge, witch involves passing the feed of gas, air rich, through an electrical discharge. This is done by applying a high voltage between two electrodes separated. The electrical charge between two surfaces creates a sequence of dissociation and subsequent collisions of oxygen with electrons creating ozone. So to describe this phenomenon we use (1D) numerical model for the charged particles. The electron number density and electric field are determined from solution of the one-dimensional coupled continuity equations of charge carriers and Poisson's equation. Simulation result show the variation of the electrical field, charged particles density, and ozone ($O_3$) particle density.
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## 1. Introduction

The importance of the ozone molecule it's due to its strong oxidant properties [1], it's used for air cleaners, water purification, gas treatment..., etc. [2–4]. That signifies that the efficiency of ozone production is very important parameter. In this paper we study the ozone production by electric negative corona discharge [5]. Many studies has been devoted to understand the mechanism generation of ozone in corona discharge [6–8].

In corona discharge, ozone is generated when an electrical discharge occurs between two conductors separated by discharge gap (wire and cylinder) Fig. 1, and feed with oxygen flowing between the electrodes. The corona discharge is initiated when the electric field near the wire is sufficient 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 [9]. The free electrons produced in the initial ionization process are accelerated away from the wire in the imposed electric field. Inelastic collisions of electrons and neutral gas molecules produce more.

Secondary electrons to sustain the discharge may be produced by photoemission from the discharge electrode, bombardment of the discharge surface by positive ions, or photoionization in the gas. At atmospheric pressure, the most significant mechanism for the generation of secondary electrons is photoemission from the discharge electrode surface. The yield of photoelectrons depends on the wavelength of photons as well as the work function of the discharge electrode material. The negative corona discharges may depend on the electrode material as well as the condition of the surface. Free electrons attach to electronegative gas molecules ($O_2$) to form negative ions. Recombination with positive ions is neglected. Consequently, ionization competes primarily with electron attachment. Near the discharge electrode, ionization prevails over attachment and new electrons are pro-

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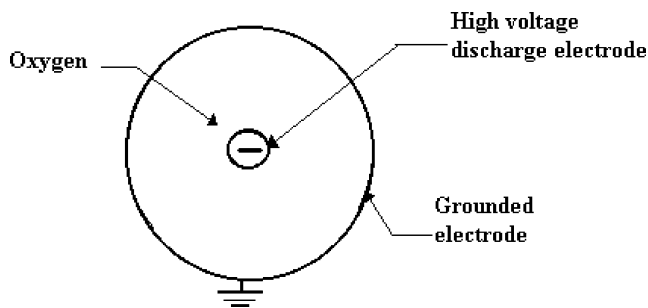 *E-mail address:* y_yanallah@univ-tiaret.dz (K. Yanallah).

Fig. 1. Corona discharge in wire cylinder electrode geometry.

duced. The radius at which the rate of ionization balances the rate of the electron attachment defines the ionization boundary [6].

## 2. Calculation details

In order to take into account the roles played by the main species, we consider only the charged and neutral species.

### 2.1. Charged species

On the basis of hydrodynamics, the densities of charged species, such as electron and ions, are calculated respectively from the following equations of continuity;

$$\frac{1}{r}\frac{d}{dr}[rq_e n_e \mu_e E] = (\alpha - \beta)q_e n_e \mu_e E \tag{1}$$

$$\frac{1}{r}\frac{d}{dr}[rq_p n_p \mu_p E] = \alpha q_e n_e \mu_e E \tag{2}$$

$$\frac{1}{r}\frac{d}{dr}[rq_n n_n \mu_n E] = \beta q_e n_e \mu_e E \tag{3}$$

$$\nabla^2 V = -\frac{e(n_p - n_n - n_e)}{\varepsilon_0} \tag{4}$$

Here, $r$ is the radial coordinate. $n_e$, $n_p$, and $n_n$ are respectively the densities of electron, positive ion $O_2^+$, and negative ion $O_2^-$. The symbols $\alpha$, $\beta$, and $\mu$ denote respectively the ionisation, attachment, and mobility coefficients. This coefficients were calculate by the BOLSIG Code [10].

Where $\varepsilon_0$ is dielectric constant $e$ is the elementary charge and $V$ the electric potential. The electric field $E$, is computed using

$$\vec{E} = -\vec{\nabla}V \tag{5}$$

The mean free path of oxygen molecules is about 100 nm at atmospheric pressure so the local approximation is always valid. So it is assumed that the ionisation, and attachment coefficients of the gas are function of $E/N$, where $E$ is the local electric field and $N$ is the neutral gas number density.

The exchange of energy between charged and neutral particles, cause a macroscopic movement of the gas (electric wind). This effect can be neglected, both for charged and neutral species [11]. The discharge is assumed to have axial symmetry. Diffusion is neglected for charged species,

compared with electrical drift. For the value of current taken in this work, we suppose that the temperature is homogeneous in the volume of the reactor.

The boundary conditions for the Eqs. (1)–(3) are: the density of positive ions on the anode surface is $n_p(R) = 0$ ($R$ is the outer electrode radius) and the density of the negative ions on the cathode surface is $n_n(r_0) = 0$ ($r_0$ is the inner electrode radius). The boundary condition on the cathode for the electron density is calculated from the current density, that is determined experimentally [12]:

$$I = 2\pi r_0 e \sum_i \mu_i n_i E \tag{6}$$

The finite difference method used to solve the equation system.

### 2.2. Neutral species

The chemical kinetics of an oxygen discharge involves a large number of reaction, about 200 reactions have been used, and in some models there was used only four [13]. In this study we use the model of four reactions [1]. The concentration of molecular oxygen is assumed to be constant [13]. The $O_3$ is mainly produced from the dissociation of $O_2$ by collision with the electrons (R1), followed by three bodies reaction (R2). The destruction of $O_3$ is described by the reactions (R3) and (R4).

$$e + O_2 \xrightarrow{K_1} e + O + O \tag{R1}$$

$$O + O_2 + O_2 \xrightarrow{K_3} O_3 + O_2 \tag{R2}$$

$$O + O_3 \xrightarrow{K_4} O_2 + O_2 \tag{R3}$$

$$O_2 + O_3 \xrightarrow{K_5} O + O_2 + O_2 \tag{R4}$$

$$K_1 = 2.10^{-9} \text{cm}^3 \text{s}^{-1}$$

$$K_3 = 6.9 \times 10^{-34} \left(\frac{300}{T}\right)^{1.25} \text{cm}^6 \text{s}^{-1}$$

$$K_4 = 1.8 \times 10^{-11} \exp(-2300/T) \quad \text{cm}^3 \text{s}^{-1}$$

$$K_5 = 7.3 \times 10^{-10} \exp(-11400/T) \quad \text{cm}^3 \text{s}^{-1}$$

Here $T$ is the temperature ($K$), $K_i$ the rate reaction are taken from [1].

According to this model of four reaction, to calculate the oxygen and ozone density, we must know the electronic density witch is determined from the solution of Eqs. (1)–(4). So the neutral particles densities ($O$, $O_3$) that take part in chemical reactions into the inter space electrode are given by the following equations:

$$\frac{1}{r}\frac{d}{dr}\left[rD_i \frac{d(N_i)}{dr}\right] = S_{p_i} - S_{d_i} \tag{7}$$

where $N_i$ is the concentrations of neutral particles of type $i$, $S_p$ is the term of particle formation, and $S_d$ is the term of particle destruction, and $D_i$ is the diffusion coefficient.