Numerical modeling of negative corona discharge in pure carbon dioxide

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1. Introduction

Corona discharge is present in many industrial processes, such as in the treatment of polymer films, the production of ozone or the decomposition of gaseous pollutants [1]. In this paper, our attention will be focused on the use of wire-to-cylinder negative corona discharge for the decomposition of carbon dioxide. As it is well known, CO_2 is a green house gas that contributes to the global warming of Earth atmosphere. In addition, this gas is the major constituent of Martian atmosphere [2]. Therefore, the study of its decomposition by means of electrical discharges and its transformation in other compounds has a double interest: it can help to the development of new technologies aiming to the reduction CO₂ emissions, and it can provide important clues on the presence of trace gases in the Martian atmosphere (like ozone) that are essential for live supporting.

2. Numerical model

Corona discharge is modeled as a stationary and homogeneous discharge in the axial and azimuthal directions [3]. On the basis of a hydrodynamic model, the electrical discharge is simulated using a set of continuity equations that describe the generation and destruction of charged and neutral species due to the chemical reactions at each point of the inter-electrode gap. This set of equations is coupled to Poisson's equation and the heat equation. The chemical model includes 21 species (e, O⁺, O₂⁺, O₃⁺, CO₂⁺, O⁻, O₂⁻, O₃⁻, CO₃⁻, CO₄⁻, O, O₂ O₃, O(¹D), O₂(¹ Δ_g), O(¹ Σ_g^+), O₂^{*}, O₃^{*}, CO, C and C₂O) and a total number of 47 reactions. The selection of reactions was based on the study of Soria and al. [4] and Mikoviny and al. [5].

3. Results

The numerical results presented in this section were obtained for 1 atm and 298 K. The axial gas flow rate through the cylinder was taken as $Q = 100 \text{ cm}^3/\text{min}$ and



Fig. 1: Radial distribution of electrons and negative ions at exit of the cylinder.

the applied voltage was set to V = 6 kV.

The radial distributions of electrons and negative ions at the outlet of cylinder are presented in Fig. 1. The structure of the electrical discharge is very similar to that in pure oxygen, which has been previously studied [3, 4]. The inter-electrode space is divided into three regions: active, ionization and drift region. In the drift region, the principal charge carrier is CO_3^- , and in lesser degree CO_4^- and O_3^- .

Carbon dioxide is decomposed by the impact of energetic electron provided by the electrical discharge,

$$e + CO_2 \rightarrow CO + O + e.$$
 (R1)

Molecular oxygen, which is necessary for the production of ozone, is generated according to process,

$$O + O + CO_2 \rightarrow O_2 + CO_2. \tag{R2}$$

Other radicals and excited species are also formed in the active region and then diffuse toward the outer electrode (see Fig. 2). Most of these radicals are also produced by direct electron impact dissociation and excitation of CO_2 and O_2 . Finally, ozone is mainly generated via a three-body reaction of O and O_2 , with CO_2 acting as the third body partner,

$$O + O_2 + CO_2 \rightarrow O_3 + CO_2. \tag{R2}$$

References

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Fig. 2: Radial distribution of neutral species at exit of the cylinder.