Chemical kinetic numerical of analysis of NO_x removal by negative corona discharge

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***Abstract*— This study presents a chemical kinetic analysis of different species involved in nitrogen-oxygen mixed gas treated by stationary negative corona discharge at atmospheric pressure. We take account 16 different chemical species reacting following 120 selected chemicals reactions. The mathematical model used consists of a system of equations that takes into account the variation of the density and the chemical kinetics of the environment. The reaction rate coefficients are taken from the literature. We analyse especially, the temporal evolution (10^{-9} – 10^{-3} s) of NO, NO_2, NO_3 and N_2O_5 species under different values of electrical field. The results show that the evolution of these nitrous oxides is substantially affected by the application of the electrical discharge. This allows us the important role played by the negative corona discharge in NO_x removing.**

Keywords— Nitrogen oxide, NO_x reduction, rate reaction, reduced electric field

I. INTRODUCTION

Negative corona has been studied for a long time and many papers have been published on this subject [1-4]. Many of them give qualitative results but relatively little has been done in the way of quantitative explanation and modeling. Partly, the reason for this is the inherent complexity of the chemical reactions that occurs in a corona discharge and the coupling with the electric field, gas velocity and gas temperature [5].

There are many industrial applications where the electric corona discharge is used. For example electrostatic precipitation, generation of ozone, decomposition of toxic gases, powder coating and many others [6-7].

Numerical simulation of this process can lead to a better understanding of the phenomena involved and can be used in the optimization of corona devices.

The chemical reactivity of the neutral gas mixture enables transformation of the toxic molecule into harmless particles (such as N_2 O or N) or to create acids (such as the nitric acid) inside the plasma [8-9].

This study takes into account twenty different chemical species participating in one hundred and seventy selected chemical reactions. The reaction rate coefficients are taken from the literature, and the density is analyzed by the continuity equation without the diffusion term.

The aim of the present simulation is to complete these studies by analysing various plasma species under different reduced electric fields in the range of 70-300 Td. In particular we analyze the time evolution of depopulation (10^{-9} - 10^{-3} s) of NO_x. We have found that the depopulation rate of NO and NO_2 is substantially affected by the rise of reduced electric field This allows us to ascertain the important role played by the reduced electric field.

II. MATHEMATICAL MODEL

The mathematical model consists of a system of equations that takes into account the variation of the density and the chemical kinetics of the environment. We developed a zero order numerical code to resolve the transport equations for neutral and charged particles. The algorithm is based on the time integration of the system of equations under consideration the variation of the density and the chemical kinetics of the environment.

The chemical kinetics equation systems can be described by an ordinary differential equation system which has the following form :

$$\frac{dN_i}{dt} = \sum_{j=1}^{j_{max}} Q_{ij} \quad (1)$$

where :

$$Q_{ij} = (G_{ij} - L_{ij}) \quad (2)$$

N_i represent the vector of all species densities i considered in the plasma and Q_{ij} the source term vector depending on the reaction coefficients and corresponding to the contributions

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from different processes. G_{ij} and L_{ij} represent respectively the gain and loss of species i due to the chemical reactions j. The solution of such a system requires the knowledge of the initial concentrations.

The total density N of the gas is given by the ideal gas law:

$$P = N K_{\beta} T \quad (3)$$

where P represents the pressure, k_B Boltzmann constant and T the absolute temperature.

The reactivity of the gas is taken into account in the source term Q_{ij} of the density conservation Eq. (1).

$$G_{ij} = \sum_{\alpha} K_{\alpha}(T)\,(n_i\, n_j)_{\alpha} \quad (4)$$

$$L_{ij} = \sum_{\beta} K_{\beta}(T)\,(n_i\, n_j)_{\beta} \quad (5)$$

$K_{\alpha}(T)$ and $K_{\beta}(T)$ are the coefficients of the chemical reaction number α or β and $(n_i\, n_j)$ is the product of densities of species i and j interacting in response to the reaction α or β. These coefficients satisfies Arrhenius formula:

$$K_{\alpha}(T) = A.\, exp\,(-\theta_{\alpha}/T) \quad (6)$$

$$K_{\beta}(T) = B.\, exp\,(-\theta_{\beta}/T) \quad (7)$$

where A and B are the constants factor and θ_{α} and θ_{β} are the activation energy of the reaction and T the absolute temperature of the species involved in the warm rain that has left the chemical reaction .

III. RESULTS AND DISCUSSIONS

We consider synthetic air at atmospheric pressure and room temperature. Our study deals with twenty chemical species among neutral species. These different species react following selected chemical reactions. The main plasma reactions included in the kinetic model and their rate constants [10,11].

Fig. 1 shows the time evolution of the density of NO for various values of reduced electric field. We remark that the reduction is faster with increasing reduced electric field, and is very important until $t = 10^{-6}$ s. In the beginning, the NO generation is not significant because the N radical generated reacts mostly with NO_x.

Fig. 2 shows the time evolution of NO_2 density at various values of reduced electric field. We observe, in the beginning from 10^{-9} to 10^{-7} s, a little rise of the density followed by a significant reduction especially for three values of the reduced electric field.

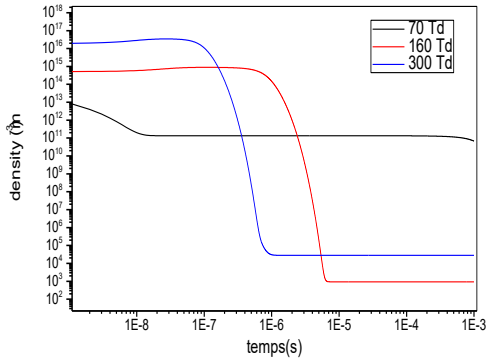

Fig.1: Temporal evolution of NO density in mixture N_2/O_2 at atmospheric pressure for the different reduced electric field.

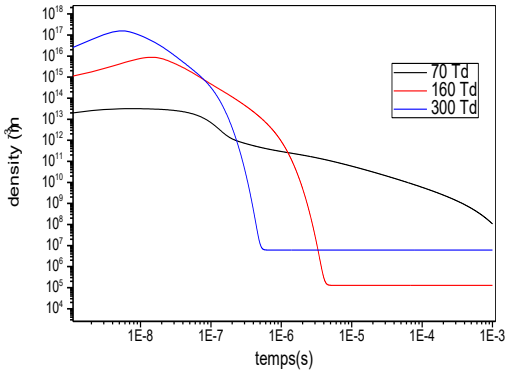

Fig. 2: Temporal evolution of NO_2 density in mixture N_2/O_2 at atmospheric pressure for the different reduced electric field.

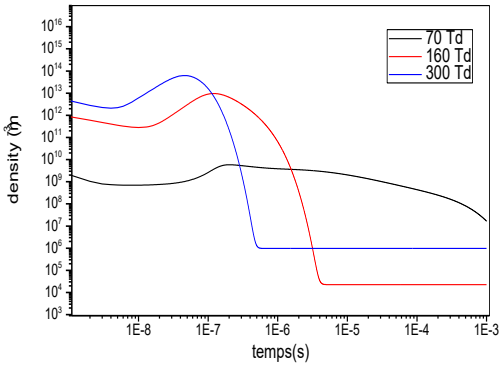

Fig.3: Temporal evolution of NO_3 density in mixture N_2/O_2 at atmospheric pressure for the different reduced electric field.

We remark, in Fig 3, that the evolution of NO_3 density is almost similar to NO_2, while the NO_3 creation takes place from 10^{-7} s for all reduced electric field values.

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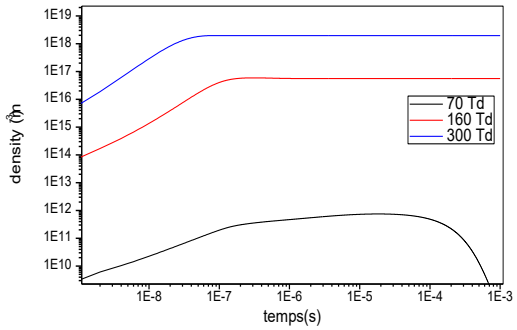

Fig. 4: Temporal evolution of N_2O_5 density in mixture N_2/O_2 at atmospheric pressure for the different reduced electric field.

In Fig 4, we shows the the temporal evolution of N_2O_5 density in mixture N_2/O_2 at atmospheric pressure for the different reduced electric field. The creation is observed for all reduced electric field values excepted for 70 Td from 10^{-4} to 10^{-3} s.

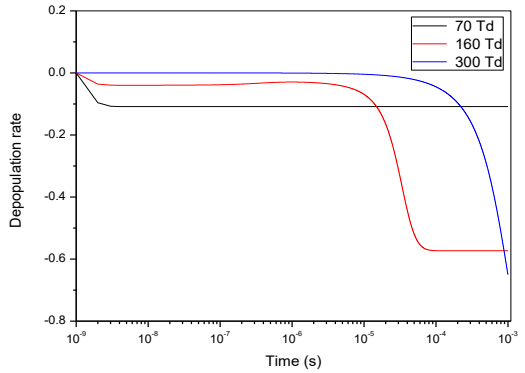

Fig.5: Temporal evolution of depopulation rate of NO in mixture N_2/O_2 at atmospheric pressure for the different reduced electric field.

Fig 5 displays the temporal evolution of depopulation rate of NO in mixture N_2/O_2 at atmospheric pressure for the different reduced electric field. We note that only for 70 Td there is a reduction whereas we have a creation for all other values due to the responsible reactions.

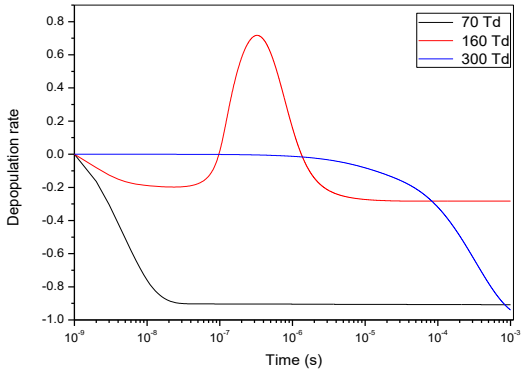

Fig. 6: Temporal evolution of depopulation rate of NO_2 in mixture N_2/O_2 at atmospheric pressure for the different reduced electric field.

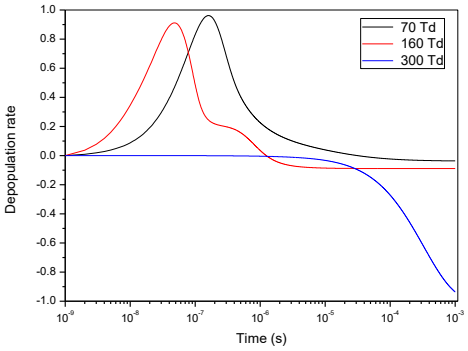

Fig. 7: Temporal evolution of depopulation rate of NO_3 in mixture N_2/O_2 at atmospheric pressure for the different reduced electric field.

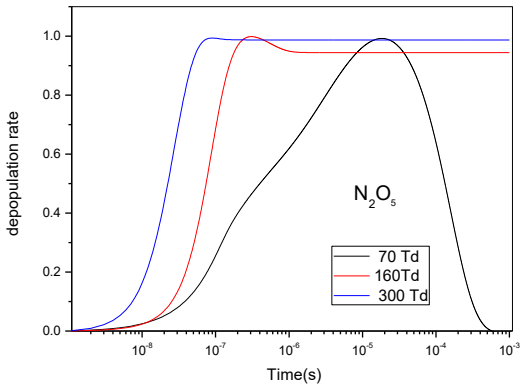

Fig. 8: Temporal evolution of depopulation rate of N_2O_5 in mixture N_2/O_2 at atmospheric pressure for the different reduced electric field

IV. CONCLUSION

This simulation must consider various effects induced by the passage of a corona discharge in a mixed gas. For the sake

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of simplification, we assume that the gas has no convective movement gradients and the pressure remains constant.

In the literature, it has generally been emphasized that certain radicals influence the NO or NO_2 removal. In this work, the results obtained show the significant role played by the high reduced electric field.

The time evolution of the NO_x density show two types of evolution, which depends strongly on the increase of reduced electric field, the reduction of dominant species in the mixture N_2/O_2 such as NO.

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