NUMERICAL ANALYSIS OF NO_X REMOVAL IN POLLUTED AT ATMOSPHERIC PRESSURE AND AMBIENT TEMPERATURE

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Abstract

The aim of this work is to analyse the time evolution of the NO_x species involved in a corona discharge used for NO pollution control in polluted air at atmospheric pressure and ambient temperature. The model takesin to account 20 chemical species (electrons, molecules N_2, O_2, H_2O, CO_2, OH, HNO_3, CO, O_3, atoms N, O, H, nitric oxides NO, NO_2, NO_3, N_2O_5, negative ions (O^-,O^-_2,O^-_3) and metastable specie N(^{2}D), in the mixture of a specific flue gas (N_2: 76%, O_2: 6%, H_2O: 6% and CO_2: 12%, and a few ppm of NO). These chemical species react following 100 selected chemical reactions. The density is analyzed by the continuity equation without diffusion term. We analyze the time evolution (10^{-9}-10^{-3} s) of the density and the rate coefficient of certain reactions, under different reduced electric fields in the range of 50-300 Td .The obtained results show the contribution of N, O, OH radicals and N(2D) in reduction of NO and NO_2. So, the NO removal efficiency reached 90% under 300 Td.

Introduction

Nowadays, gas discharge plasmas and their applications in physics, chemistry, biology, and environmental programs are being widely studied. They can be used for reforming the poisonous pollutants, such as NO_x, So_x et CO_x … These studies are based on the numerical equations for the reduction of NO_x gases in reactors.

The common thermal and catalytic techniques used for many years to remove the NO_x and SO_x present in industrial flue gas or emitted by the vehicles will not permit us to respect the new emission limits which become more and more severe to protect the environment. These effects can also have a direct impact on the targeted applications such as electron beam processes which were particularly studied for treatment of gaseous effluents polluted by nitrogen oxides, sulphur and/or ozone production, medical applications and surface treatment [1].

Basic formulas

The basic formulas used in the present paper consist of a mathematical system of equations that take into account the variation of the density and the chemical kinetics of the environment.

$$\frac{dN_i}{dt} = \sum_{j=1}^{j_{\max}} Q_{ij} \quad \text{where } j = 1, \dots, j_{\max} \qquad \text{where} \qquad Q_{ij} = \left(G_{ij} - L_{ij}\right)$$

Where 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 from different processes. G_{ij} and L_{ij} represent respectively the gain and loss of species i due to the chemical reactions j. The algorithm is based on the time integration of the system of equations under consideration.

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

$$P = N k_\beta T$$

where k_β Boltzmann constan, P represent the pressure and T the absolute temperature

The reactivity of the gas is taken into account in the source term Q_{ij} of the density conservation

$$G_{ij} = \sum_\alpha K_\alpha(T)\left(n_i n_j\right)_\alpha \qquad \text{and} \qquad L_{ij} = \sum_\beta K_\beta(T)\left(n_i n_j\right)_\beta$$

$K_\alpha(T)$ 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:

$$K_\alpha(T) = A \cdot \exp\left(-\theta_\alpha/T\right) \qquad \text{and} \qquad K_\beta(T) = B \cdot \exp\left(-\theta_\beta/T\right)$$

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 .

Results

The system of the chemical kinetics equations can be described by a system of ordinary differential equations (i.e., the algorithm is defined by time integration) of the following form Eichwald et al., 2002.

It should be mentioned here that for the initial condition (i.e., the interelectrode separation, temperature, initial number densities of various species, pressure, potential, Rate Constants, chemical reactions) was obtained by Bouzar et al., 2017 [3].

TABLE 1: The main plasma reactions to générateur the main radical to remove NO_x and their rate constants (in cm^3 molecule $^{-1}$ s^{-1} for bimolecular reactions and cm^6 molecule $^{-2}$ s^{-1} for trimolecular reactions, x[y] denotes x × 10^y)

	Reaction	Rate Constants	References
R_1	$NO + NO_3 \rightarrow NO_2 + NO_2$	$K_1 = 2.00[-11]$	Kossyi et al. (1992)
R_2	$NO + O_3 \rightarrow O_2 + NO_2$	$K_2 = 1.80[-12]$	Kossyi et al. (1992)
R_3	$NO + O_3^- \rightarrow NO_2^- + O_2$	$K_3 = 2.00[-12]$	Kossyi et al. (1992)
R_4	$NO + O_3^- \rightarrow NO_3^- + O$	$K_4 = 1.00[-10]$	Kossyi et al. (1992)
R_5	$NO + O_4^- \rightarrow NO_3^- + O_2$	$K_5 = 2.50[-10]$	Kossyi et al. (1992)
R_6	$NO + HO_2 \rightarrow NO_2 + OH$	$K_6 = 13.5[-11]$	Kossyi et al. (1992)
R_7	$NO_2 + O_2^- \rightarrow NO_2^- + O_2$	$K_7 = 7.00[-10]$	Eichwald et al. (2002)
R_8	$NO_2 + OH \rightarrow HNO_3$	$K_8 = 13.5[-11]$	Eichwald et al. (2002)
R_9	$NO_2 + O_3^- \rightarrow NO_2^- + O_3$	$K_9 = 7.00[-10]$	Eichwald et al. (2002)
R_{10}	$NO_2 + N \rightarrow NO + NO$	$K_{10} = 2.30[-12]$	Eichwald et al. (2002)
R_{11}	$NO_3 + OH \rightarrow HO_2 + NO_2$	$K_{11} = 2.35[-11]$	Eichwald et al. (2002)
R_{12}	$NO_3 + HO_2 \rightarrow HNO_3 + O_2$	$K_{12} = 4.05[-12]$	Eichwald et al. (2002)
R_{13}	$NO_3 + NO_3 \rightarrow NO_2 + NO_2 + O_2$	$K_{13} = 1.20[-15]$	Sieck et al. (2000)
R_{14}	$NO_3 + O \rightarrow NO_2 + O_2$	$K_{14} = 1.70[-11]$	Sieck et al. (2000)
R_{15}	$N + O_2 \rightarrow O + NO$	$K_{15} = 8.90[-17]$	Kossyi et al. (1992)
R_{16}	$N + NO_2 \rightarrow N_2 + O_2$	$K_{16} = 7.00[-13]$	Kossyi et al. (1992)
R_{17}	$N + NO_3^- \rightarrow NO + NO_2 + e^-$	$K_{17} = 5.00[-10]$	Kossyi et al. (1992)
R_{18}	$NO_2 + NO_3 + O_2 \rightarrow N_2O_5 + O_2$	$K_{18} = 3.70[-30]$	Sieck et al. (2000)
R_{19}	$O_3 + H \rightarrow OH + O_2$	$K_{19} = 2.80[-11]$	Mok et al. (1999)
R_{20}	$OH + H_2 \rightarrow H_2O + H$	$K_{20} = 6.70[-15]$	Mok et al. (1999)
R_{21}	$OH + O_3 \rightarrow HO_2 + O_2$	$K_{21} = 6.50[-14]$	Mok et al. (1999)
R_{22}	$OH + HO_2 \rightarrow H_2O + O_2$	$K_{22} = 1.10[-10]$	Mok et al. (1999)
R_{23}	$OH + HNO_3 \rightarrow NO_3 + H_2O$	$K_{23} = 1.30[-13]$	Mok et al. (1999)
R_{24}	$H_2O + e^- \rightarrow OH + H + e^-$	$K_{24} = 2.60[-12]$	Mok et al. (1999)
R_{25}	$CO_2 + e^- \rightarrow CO + O + e^-$	$K_{25} = 8.70[-10]$	Mok et al. (1999)

Figure1 : Time evolution of different species at 50 Td

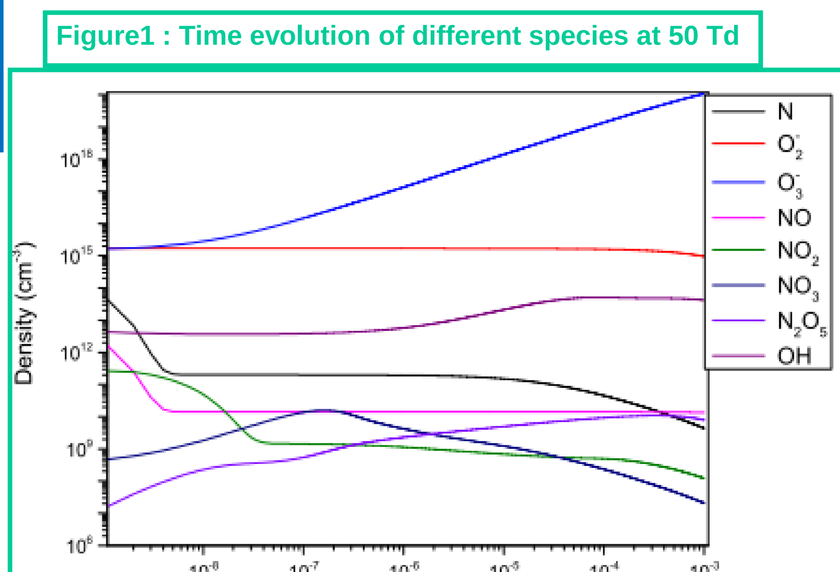


Figure2 : Time evolution of different species at 300 Td

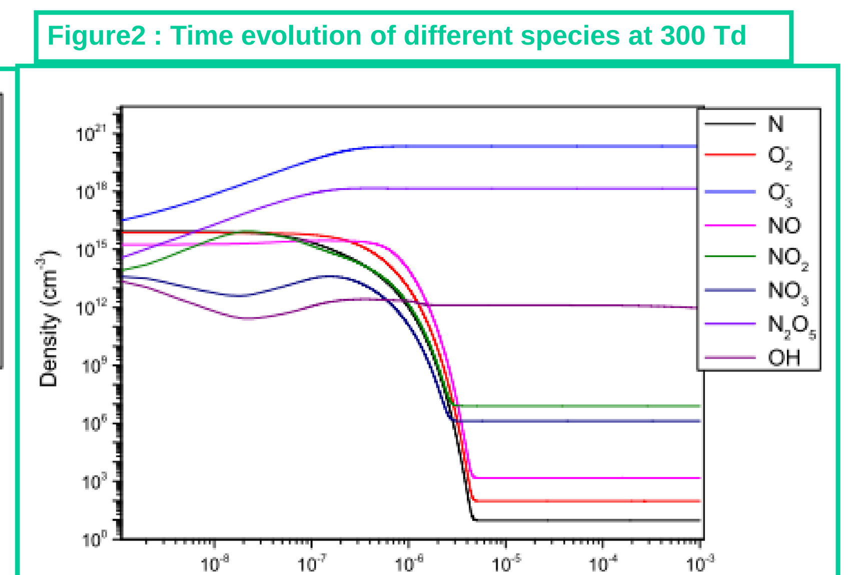


Figure3 : Time evolution of rate depopulation of NO specie for different reduced electric fields [50-300 Td].

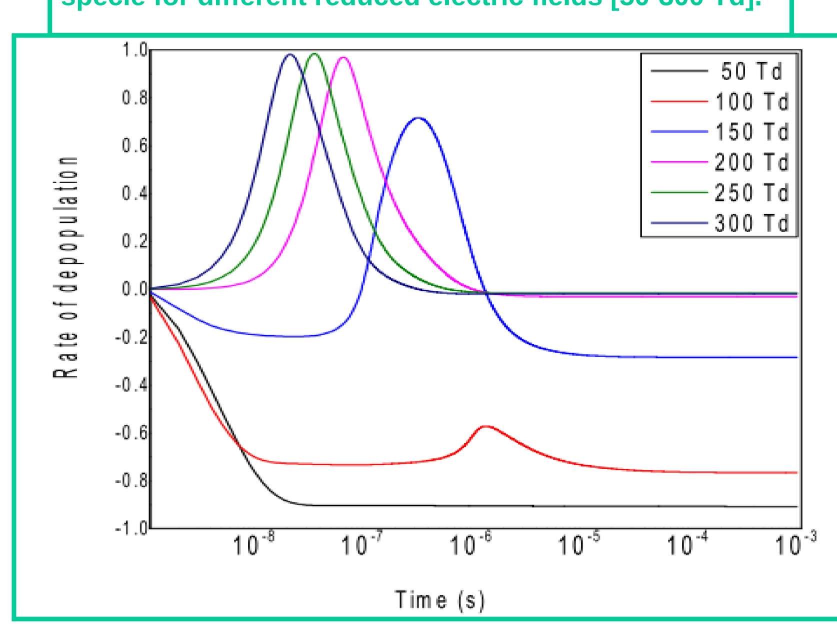
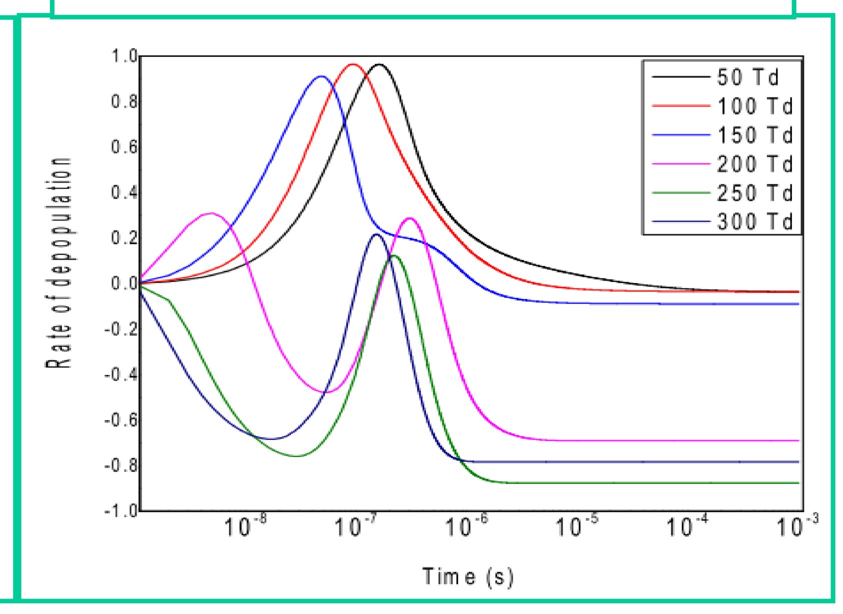


Figure4 : Time evolution of rate depopulation of NO_2 specie for different reduced electric fields [50-300 Td].



Discussion and Conclusions

The problem of removing nitric oxide devoted a lot of work performed for the past 25 years. In this work, we simulate the time behavior of different species and their reaction rates using a zero dimensional model based on chemical kinetic equations These different species react following 100 selected chemical reactions and the analyze investigates the behavior for different values of the reduced electric field. These results permit us to determine the vital role played by the reduced electric field on species evolution, and to higher perceive the various reaction processes affecting the NOx concentration magnitude within the gas mixture. The reduction of oxides of nitrogen is different for all species. In fact, it is observed that the increase and decrease of these species is different and depends strongly on the values of reduced electric fields. Finally, these results permit us to determine the vital role played by the reduced electric field on species evolution, and to more deeply perceive various reaction processes affecting the NOx magnitude within a gas mixture.

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