Chapter

Modeling Study of Impact Effect of Chemical Reactions on Nitrogen Oxide Conversion in N₂/O₂ Mixtures under Various O₂ Concentrations

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Abstract

The main objective of this study is to understand the influence of various chemical reactions that participate on NO creation or reduction in N_2/O_2 mixed gas induced by negative corona discharge under different O_2 concentrations (5%, 10%, 15%, 20% and 25%). The basic chemistry of NO evolution that is presented in this study is based on a comprehensive collection of processes that were gathered into 150 specific chemical reactions involving 25 molecular, excited, atomic, and charged entities. Without the diffusion and convective factors, the density was computed using the continuity equation over a range of electric reduction fields between 50 and 90 Td (1Td = 10^{-21} V.m²), at different points in the ranges 10^{-9} – 10^{-4} s. The outcomes of our numerical simulations demonstrate the impact of various chemical processes on NO production and decrease, including: $N(^2D) + O_2 \rightarrow NO + O$ and: $NO + O + N_2 \rightarrow NO_2 + N_2$ respectively. Our research has shown that at 50 and 70 Td, nitrogen oxide generation is dominated by an O_2 concentration of 5%, whereas at 90 Td, it is dominated by an O_2 concentration of 10%. These outcomes are true for both reactions.

Keywords: plasma chemistry, reaction rate, gaseous mixture, chemical kinetic, gas discharge

1. Introduction

When building and enhancing combustion systems, the emission of nitrogen oxides continues to be one of the main environmental problems [1–5]. There is a lot of research being done on gas discharge plasmas and how they might be used in other fields (physics, chemistry, biology...) [6–10]. They can be used for reforming the poisonous pollutants, such as NO_X , SO_X , CO_X , etc. These studies are based on the numerical equations for the reduction of NO_X gases in reactors. Discharges in N_2/O_2

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mixtures can differ considerably from discharges in pure N_2 or O_2 in a number of characteristics (principally, in chemical and ionic composition). Theoretical modeling of kinetic processes in N_2/O_2 discharges has been developed in several works [11–15].

For a better understanding of the processes taking place in the atmosphere and in a range of modern plasma technologies, the non-equilibrium kinetics of low pressure plasmas in N_2/O_2 mixtures is a crucial area of research. Understanding the operation of plasma reactors used for chemical synthesis and surface treatments of diverse materials, in particular, requires knowledge of the volume and surface kinetics of active species like N, O, $N(^2D)$, or NO [16–21]. On the subject of discharges in oxygen or air, various authors presented theoretical and experimental works [22–25]. Others were interested to study electron swarm parameters in N_2/O_2 mixtures which are of great interest in atmospheric physics, pollution control or for application as electrical insulation media [26–29]. These study at investigating the physical behavior of N_2 and O_2 mixtures in order to predict and optimize their electric strength.

I Stefanović et al. [30], have studied kinetics of ozone and nitric oxides in dielectric barrier discharges in O₂/NO_x and N₂/O₂/NO_x mixtures. They have measured various concentrations of NO, NO₂, NO₃, N₂O₅, and O₃ by classical absorption spectroscopy in dielectric barrier discharges in flowing O₂/NO_x and N₂/O₂/NO_x mixtures. They have reported on a comparison of the measured concentrations with a zerodimensional numerical kinetic model. They have shown that their model accurately describes the kinetics of ozone and the nitric oxides in the DBD in oxygen and dry air with small admixtures of NOx. Xing Fan et al. [31], have been developed a coaxial dielectric barrier discharge (DBD) reactor for plasma and plasma-catalytic conversion of dilute N_2O in N_2 and N_2/O_2 mixtures at both room and high temperature (300°C). They show that N₂O conversion increases with the increase of discharge power and decreases with the increase of O₂ content. They also show that increasing the inlet N₂O concentration from 100 to 400 ppm decreases the conversion of N₂O under an N₂ atmosphere but increases that under an N₂/O₂ atmosphere. They have concluded that concentrating N₂O in the N₂/O₂ mixture could alleviate the negative influence of O₂ by increasing the involvement of plasma reactive species (e.g., $N_2(A^3\Sigma^+)$ and $O(^1D)$) in N_2O conversion. Haefliger et al. [32], have studied experimentally derived rate coefficients for electron ionization, attachment and detachment as well as ion conversion in pure O_2 and N_2/O_2 mixtures. Four ion species and seven rate coefficients make up the model they are utilizing. They compared their findings to a number of sources, and most rate coefficients showed good agreement. They demonstrate that the waveforms' informative content is sufficient to differentiate between the two detaching ions, O and O⁻, and their method may be used to analyze other gases or mixes that undergo electron detachment and ion conversion. For estimating the critical electric field strength of the mixtures, they propose a criterion based on the eigenvalues of the matrix describing the interaction of electrons and ions. Yamamoto et al. [33] developed a method for the breakdown of NOx pollutants that involved a chemical reactor coupled with plasma discharge. Since the plasma nitrogen monoxide was transformed into nitrogen dioxide, the reduction mechanisms' action resulted in the transformation of nitrogen dioxide into nitrogen. They looked at three different plasma reactor models, and they noticed that nearly all of the nitrogen dioxide was breaking down. Mei-Xiang et al. [34] investigated metal catalyst and plasma discharge combination for simultaneous removal of NOx and dust from diesel exhaust. During the plasma creation, the temperature for combustion falls and the efficiency of NOx to NO conversion is reduced. Wang et al. [35] employed the DBD method to reform

carbon dioxide inside the plasma reactor and create nonthermal plasma. Separate studies on the reformation of carbon dioxide by catalytic and nonthermal plasma were conducted. They discovered that employing a DBD reactor significantly reduces CO₂ concentration over time compared to other techniques. Abedi-Varaki et *al.* [36] studied the temporal fluctuations of the number density and reaction rate of the nitrogen monoxide molecules and other generated species inside the DBD plasma reactor using a zero-dimensional model.

In this way, the aim of the present study is to simulate various values of O_2 concentrations (5%, 10%,15%, 20% and 25%), the temporal evolution of 25 chemical species (electrons e, molecules N_2 , O_2 , O_3 , atoms N, O, nitric oxides NO, N_2O , NO_2 , NO_3 , N_2O_5 , positive ions $(O^+, O_2^+, O_4^+, N^+, N_2^+, NO^+)$, negative ions $(O^-, O_2^-, O_3^-, O_4^-, NO_2^-, NO_3^-)$ and metastables species $N(^2D)$, $O(^1D)$. These different species react following 150 selected chemical reactions. The time varied from 10^{-9} to 10^{-4} s. In this numerical simulation we suppose various effects induced by the passage of a corona discharge in a mixed gas. For the sake of simplification, we assume that the gas has no convective movement gradients and the temperature remains constant.

2. Basic formulas

The basic formulas used in the present work 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 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:

$$\frac{dN_i}{dt} = \sum_{i=1}^{j_{max}} S_{ij} \quad \text{where } j = 1, \dots, j_{max}$$
 (1)

where:

$$S_{ij} = \left(G_{ij} - L_{ij}\right) \tag{2}$$

 N_i show the vector of species densities, i=1 up to 25 thought about in the plasma and S_{ij} the source term vector related to the contributions from various processes and dependent on the reaction coefficients. G_{ij} and L_{ij} stand for the gain and loss of species i as a result of chemical reactions from j=1 to $j_{max}=150$, respectively. 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:

$$P = Nk_bT (3)$$

Where P displays the pressure, k_b Boltzmann constant and T the absolute temperature. The source term S_{ij} of the density conservation factored in the gas's reactivity Eq. (1).

$$G_{ij} = \sum_{\mu} \! K_{\mu}(T) \big(n_i n_j \big)_{\mu} \tag{4} \label{eq:4}$$

$$L_{ij} = \sum_{\nu} K_{\nu}(T) (n_i n_j)$$
 (5)

 $K\mu(T)$ and $K\nu$ (T) are the reaction's coefficients μ or ν and (n_in_j) is the product of the species i and j interaction densities with the reaction μ or ν . This Arrhenius formula is satisfied by these coefficients.

$$K_{\mu}(T) = A. \exp\left(-\theta_{\mu}/T\right) \tag{6}$$

$$K_{\nu}(T) = B. \exp\left(-\theta_{\nu/T}\right) \tag{7}$$

Where A and B are the constants factor and $\theta\mu$ and $\theta\nu$ are the reactions activation energy and T is the species absolute temperature.

3. Results and discussion

The chemical kinetics involves 25 different chemical species: electrons (e), molecules N_2 , O_2 , O_3 , atoms N, O, nitric oxides NO, N_2O , NO_2 , NO_3 , N_2O_5 , positive ions $(O^+, O_2^+, O_4^+, N^+, N_2^+, NO^+)$, negative ions $(O^-, O_2^-, O_3^-, O_4^-, NO_2^-, NO_3^-)$, metastable species $N(^2D)$, $O(^1D)$. These different species react following 150 selected chemical reactions, the main ones are given in **Table 1**.

In this section we will analyze the effects of important chemical reactions that participated on creation or reduction of NO specie. In our work, we have found that the following reactions are the most influential on creating NO:

$$N(^{2}D) + O_{2} \rightarrow NO + O \tag{8}$$

$$N + O_2 \rightarrow NO + O \tag{9}$$

$$O_3^- + N \to NO + O_2 + e$$
 (10)

$$O_2^+ + N_2 \to NO + NO^+$$
 (11)

$$O_2^- + NO^+ \to NO + O_2$$
 (12)

and the others following reactions are the most influential on reducing NO:

$$NO + O + N_2 \rightarrow NO_2 + N_2 \tag{13}$$

$$NO + N \rightarrow N_2 + O \tag{14}$$

$$NO + O_3^- \to NO_3^- + O$$
 (15)

$$NO + O(^{1}D) \rightarrow O_{2} + N$$
 (16)

$$NO + O_3 \rightarrow NO_2 + O_2 \tag{17}$$

So, we proposed to represent only the most important reactions namely (R1) and (R10). For that, we analyze for each electric reduced field (50, 70 and 90 Td), the evolution of density and reaction rate between 10^{-9} and 10^{-4} s, under different O_2 concentrations: 5%, 10%,15%, 20% and 25%.

	Chemical reactions	Rate coefficients
R1	$N(^2D) + O_2 \rightarrow NO + O$	$k_1 = 0.97 \times 10^{-11}$
R2	$N + O_2 \rightarrow NO + O$	$k_2 = 0.44 \times 10^{-11}$
R3	$O_3^- + N \rightarrow NO + O_2 + e$	$k_3 = 4.31 \times 10^{-7}$
R4	$O_2^+ + N_2 \rightarrow NO + NO^+$	k_4 = 1.0 \times 10 ⁻¹⁷
R5	O_2^- + NO^+ \rightarrow NO + O_2	$k_5 = 4.0 \times 10^{-7}$
R6	$N_2O_5 + NO_2^- \rightarrow NO + NO_3^- + NO_3$	k_6 = 7.0×10^{-10}
R7	$O(^1D) + NO_2 \rightarrow NO + O_2$	$k_7 = 0.14 \times 10^{-9}$
R8	$N^+ + NO_2 \rightarrow NO + NO^+$	$k_8 = 5.00 \times 10^{-10}$
R9	O_3 + N_2^+ \rightarrow N_2 + O + O_2^+	k_9 = 1.00×10^{-10}
R10	$NO + O + N_2 \rightarrow NO_2 + N_2$	k_{10} = 2.5×10^{-10}
R11	$NO + N \rightarrow N_2 + O$	$k_{11} = 0.32 \times 10^{-10}$
R12	$\mathrm{NO} + \mathrm{O_3^-} \rightarrow \mathrm{NO_3^-} + \mathrm{O}$	k_{12} = 1.0 \times 10 ⁻¹⁰
R13	$NO + O(^1D) \rightarrow O_2 + N$	k_{13} = 1.5 \times 10 ⁻¹⁰
R14	$NO + O_3 \rightarrow NO_2 + O_2$	$k_{14} = 0.18 \times 10^{-11}$
R15	$NO + O \rightarrow N + 2O$	k_{15} = 0.18×10^{-11}
R16	$NO + O_3^- \rightarrow NO_2^- + O_2$	k_{16} = 2.6 \times 10 ⁻¹²
R17	$NO + O_4^- \rightarrow NO_3^- + O_2$	k_{17} = 2.5×10^{-10}
R18	$NO + O_2^+ \rightarrow NO^+ + O_2$	k_{18} = 3.0×10^{-10}
R19	$NO + O^+ \rightarrow NO^+ + O$	k_{19} = 1.0 \times 10 ⁻¹²
R20	$\mathrm{NO} + \mathrm{O}^- ightarrow \mathrm{NO}_2 + \mathrm{e}$	k_{20} = 2.6×10^{-10}
R21	$O_4^+ + O^- \rightarrow O_2 + O_3$	$k_{21} = 4.00 \times 10^{-7}$
R22	$N_2O + O^+ \rightarrow N_2 + O_2^+$	$k_{22} = 2.00 \times 10^{-11}$
R23	$O_4^- + O \rightarrow O_3^- + O_2$	$k_{23} = 4.00 \times 10^{-10}$
R24	O_4^+ + NO \rightarrow NO $^+$ + 2O $_2$	$k_{24} = 1.00 \times 10^{-10}$
R25	$e + O_2 \rightarrow O + O(^1D) + e$	k_{25} = 3.2×10^{-11}
R26	$e + N_2 \rightarrow N + N + e$	k_{26} = 2.0×10^{-11}
-		

Table 1.The primary plasma processes that produce the primary species involved in NO reduction and production, as well as their rate coefficients (rate coefficients are in units of cm^3 -molecule $^{-1}$ ·s $^{-1}$ for two body reactions, and cm^6 . Molecule $^{-1}$ ·s $^{-1}$ for three body reactions). They are taken from the literature [37–40].

Figures 1–3, show the temporal evolution of density of $N(^2D)$ specie which participated on the creation of nitrogen oxide in N_2/O_2 mixture at 50Td under different O_2 concentrations: 5%, 10%,15%, 20% and 25%. As illustrated on these curves, the evolution of NO density depends of O_2 concentrations. However, we notice that when the O_2 concentration increases NO density decreases, except for the value 90Td where we note a decrease in the density at the concentration 5%. Globally, we observe on these three figures, a first step which goes up to 4×10^{-7} s where the density increases, and a second stage which goes up to 10^{-4} s where the density decreases.

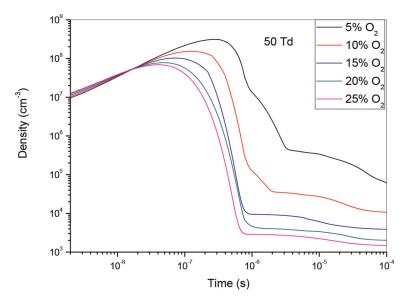


Figure 1. Temporal evolution of N(2D) density that participate in the creation of NO specie in the mixture N_2/O_2 at 50Td under different O_2 percentages: 5%, 10%,15%, 20% and 25%.

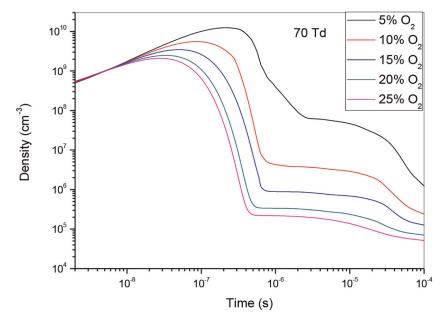


Figure 2. Temporal evolution of $N(^2D)$ density that participate in the creation of NO specie in the mixture N_2/O_2 at 70Td under different O_2 percentages: 5%, 10%,15%, 20% and 25%.

We also notice that the gap between the different curves decreases when the oxygen concentration increases.

So, in **Figures 4–6**, we have represented the temporal evolution of O density of the same O_2 concentrations as before. We note firstly an increase of density until 10^{-6} s,

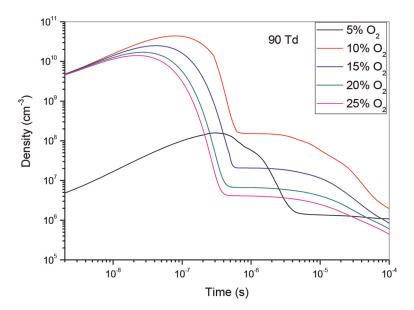


Figure 3. Temporal evolution of $N(^2D)$ density that participate in the creation of NO specie in the mixture N_2/O_2 at 90Td under different O_2 percentages: 5%, 10%,15%, 20% and 25%.

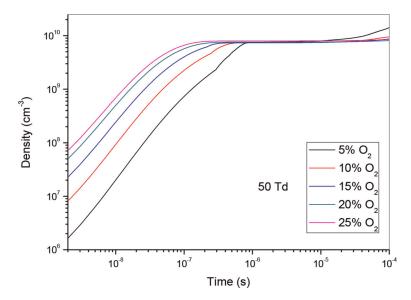


Figure 4. Temporal evolution of O density that participate in the creation of NO specie in the mixture N_2/O_2 at 50Td under different O_2 percentages: 5%, 10%,15%, 20% and 25%.

followed by stabilization. Secondly, we observe that the rise of O_2 concentration induces the increase of atomic oxygen density.

Let us go on to analyze the reaction rate with the same values as before. We have represented in **Figures 7–9**, the temporal evolution of reaction rate of (R1): N (2 D) + O₂ \rightarrow NO + O, that participate in the production of NO specie in N₂/O₂ mixture at 50, 70 and 90 Td, under five various O₂ concentrations: 5%, 10%, 15%, 20% and

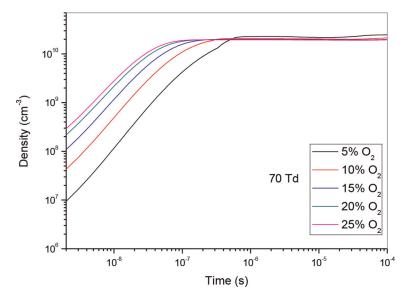


Figure 5. Temporal evolution of O density that participate in the creation of NO specie in the mixture N_2/O_2 at 70Td under different O_2 percentages: 5%, 10%,15%, 20% and 25%.

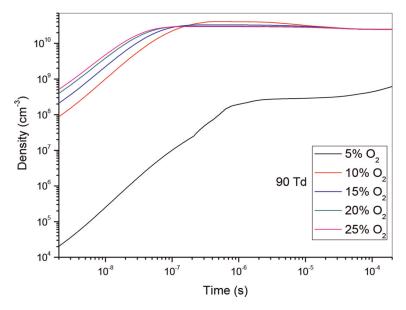


Figure 6. Temporal evolution of O density that participate in the creation of NO specie in the mixture N_2/O_2 at 90Td under different O_2 percentages: 5%, 10%,15%, 20% and 25%.

25%. Let us start with 50 Td. We can say through curves represented in **Figure 7**, that the effect of the reaction passes by three stages:

• Between 10^{-9} and 10^{-7} s, the influence of the reaction increases with the increase of the O_2 concentrations and his domination is obtained for 25%.

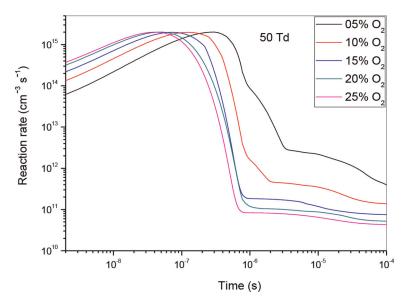


Figure 7.

Temporal evolution of reaction rate of (R_1) : $N(^2D) + O_2 \rightarrow NO + O$, which contributed in the creation of NO specie in N_2/O_2 mixture at 50Td, under various O_2 concentrations: 5%, 10%,15%, 20% and 25%.

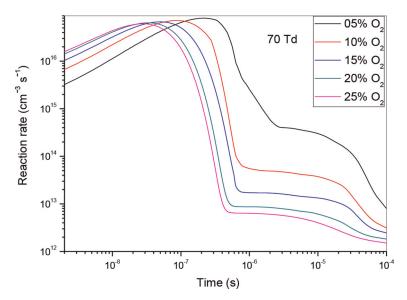


Figure 8. Temporal evolution of reaction rate of (R1): $N(^2D) + O_2 \rightarrow NO + O$, which contributed in the creation of NO specie in N_2/O_2 mixture at 70Td, under various O_2 concentrations: 5%, 10%,15%, 20% and 25%.

- From 10^{-7} to 10^{-6} s, the reaction impact decreases quickly while the O_2 concentrations increases and his domination is obtained for 5%.
- From 10^{-6} to 10^{-4} s, the reaction's impact lessens but only somewhat.

Let us examine what occurs when the electric reduced field is increased to 70 Td. **Figure 8** presents the findings. We see that the curves have the same form as those

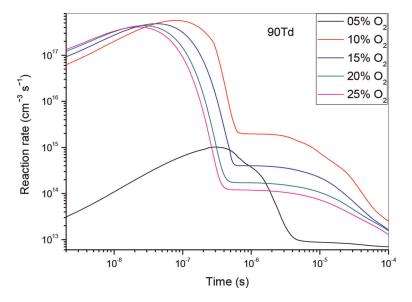


Figure 9. Temporal evolution of reaction rate of (R1): $N(^2D) + O_2 \rightarrow NO + O$, which contributed in the creation of NO specie in N_2/O_2 mixture at 90Td, under various O_2 concentrations: 5%, 10%,15%, 20% and 25%.

previously obtained for 50 Td, but the average reaction time is shorter because of the energy injected into the gas, which is more significant.

To wrap up our research, we have demonstrated in **Figure 9**, the temporal evolution of reaction rate of (R1) which contribute to NO production at 90Td. As before, we observe the same effect for the reaction (R1), excepted the value 5%. Indeed, at this value the reaction rate does not have a great influence on the nitrogen oxide production. So, we can say that at 90 Td it's 10% of O_2 concentration that becomes dominant.

Let us now analyze the influence of reaction (R10) which is the principal reaction in the consumption of nitrogen oxide. For this reason, we have shown in **Figures 10–12** the evolution of the reaction rate for three values of the reduced electric field (50, 70 and 90 Td), and five values of O₂ concentrations (5%, 10%, 15%, 20% and 25%). We notice that NO, can react with the oxidizing radical such as O to form especially NO₂. We note firstly that the effectiveness of these concentrations is higher at the end than at the beginning. Secondly, we observe two stages of evolution:

- At 50 and 70 Td, and between 10^{-9} and 4×10^{-7} s, plus the value of the O_2 concentrations increases more reaction is effective.
- At 50 and 70 Td, and between 4×10^{-7} and 10^{-4} s, the phenomenon reverses and we observe plus the O_2 concentration increases, the effect of the reaction decreases.
- At 90 Td, the phenomena are the same as described before, with the exception of 5%, where the reaction's influence is much weaker than it is at other concentrations. In our opinion, the synthesis of the oxygen atom is insignificant at this energy level and low concentration when compared to other concentrations 10, 15, 20 and 25%.

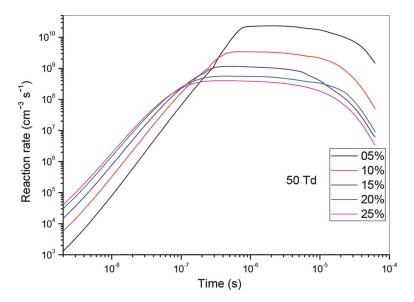


Figure 10. Temporal evolution of reaction rate of (R10): $NO + O + N_2 \rightarrow NO_2 + N_2$, reaction that participate in the reduction of NO specie in N_2/O_2 mixture at 50Td, under various O_2 concentrations: 5%, 10%,15%, 20% and 25%.

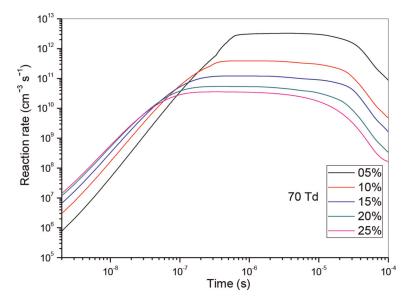


Figure 11. Temporal evolution of reaction rate of (R10): $NO + O + N_2 \rightarrow NO_2 + N_2$, reaction that participate in the reduction of NO specie in N_2/O_2 mixture at 70Td, under various O_2 concentrations: 5%, 10%,15%, 20% and 25%.

To highlight our results, we chose to represent them as a percentage and histogram representations. So, we have represented in the **Figures 13–18** the percentage of the two reactions that participated on the creation and reduction of nitrogen oxide to get an idea about their impact in this conversion (At left: (a) with percentage representation; At right (b) with histogram representation). First of all, let us see **Figure 13(a)**

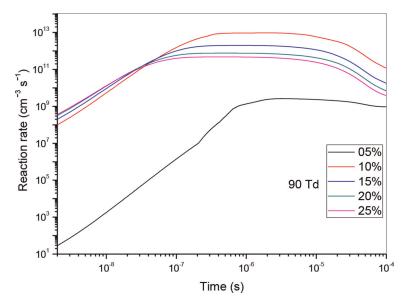


Figure 12. Temporal evolution of reaction rate of (R10): $NO + O + N_2 \rightarrow NO_2 + N_2$, reaction that participate in the reduction of NO specie in N_2/O_2 mixture at 90Td, under various O_2 concentrations: 5%, 10%,15%, 20% and 25%.

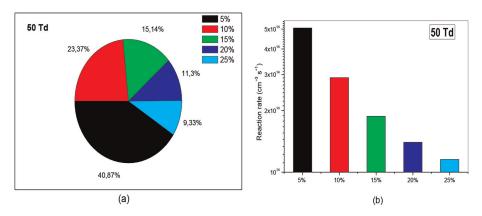


Figure 13. Representation of reaction rate of (R1): $N(^2D) + O_2 \rightarrow NO + O$, that participate in the creation of NO specie in N_2/O_2 mixture at 50Td under various O_2 concentrations (5%, 10%, 15%, 20%, and 25%).

where we have highlighted percentages for each O_2 concentration at 50 Td. We notice that at the concentration 5%, nitrogen oxygen is crated almost four times more than when the concentration is at 25%.

Move us on to the next **Figure 14(a)**, where we have represented the percent influence for 70 Td. We observe also almost the same phenomenon as before. Indeed, we note that the creation of NO specie is still important for the concentration 5%, where we get 48.4%, against 6.96% for the concentration 25%. These results are also verified on the **Figures 13(b)** and **14(b)**, where we can say the phenomenon of NO creation dominates when the O2 concentration equals 5%.

Now let us see what happens when we increase the reduced electric field to 90 Td. The results are given in the **Figure 15(a)** and **(b)**. We clearly observe that when the

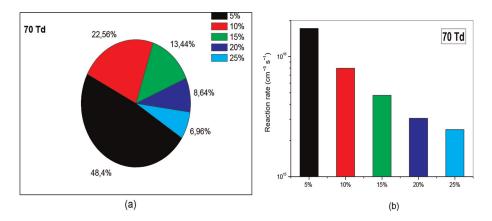


Figure 14. Representation of reaction rate of (R1): $N(^2D) + O_2 \rightarrow NO + O$, that participate in the creation of NO specie in N_2/O_2 mixture at 70Td under various O_2 concentrations (5%, 10%, 15%, 20%, and 25%).

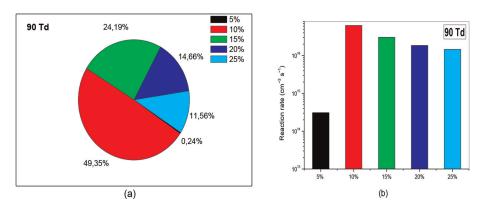


Figure 15. Representation of reaction rate of (R1): $N(^2D) + O_2 \rightarrow NO + O$, that participate in the creation of NO specie in N_2/O_2 mixture at 90Td under various O_2 concentrations (5%, 10%, 15%, 20%, and 25%).

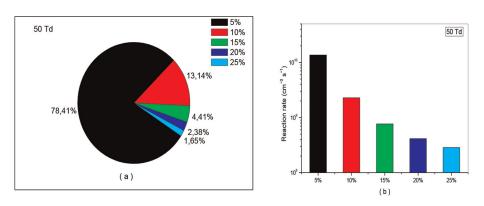
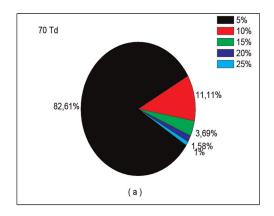


Figure 16. Representation of reaction rate of (R10): NO + O + $N_2 \rightarrow NO_2 + N_2$, that participate in the creation of NO specie in N_2/O_2 mixture at 50Td under various O_2 concentrations (5%, 10%, 15%, 20%, and 25%).



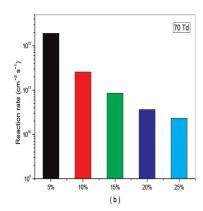
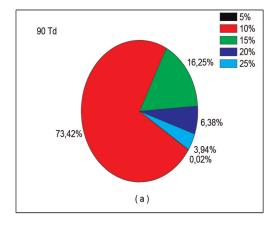


Figure 17. Representation of reaction rate of (R10): NO + O + $N_2 \rightarrow NO_2 + N_2$, that participate in the creation of NO specie in N_2/O_2 mixture at 70Td under various O_2 concentrations (5%, 10%, 15%, 20%, and 25%).



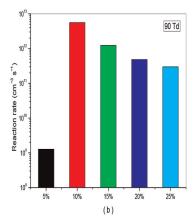


Figure 18. Representation of reaction rate of (R10): NO + O + $N_2 \rightarrow NO_2 + N_2$, that participate in the creation of NO specie in N_2/O_2 mixture at 90Td under various O_2 concentrations (5%, 10%, 15%, 20%, and 25%).

concentration equals 5%, the creation is totally negligible (0.24%) compared to the other concentrations. Now, it's the 10% concentration that takes over and becomes dominant over all other concentrations.

Let us continue our analysis with reaction (R10) which is responsible for consumption of nitrogen oxide. The effects of this reaction have been represented in **Figures 16–18** with percentage (a) and (b) with diagram of different reactions rate. We observe also on these figures the same effect as that observed in the case of creation. The only difference lies in the intensity of the values. For example, at 50 and 70 Td we found in average 80% instead of 44%, and at 90Td we get 73.42% against 49.35%. These results are also verified on **Figures 16(b)**, **17(b)** and **18(b)**.

4. Conclusion

In this study, a zero-dimensional model is considered for numerical studies of NO creation and reduction in N_2/O_2 mixture under various O_2 concentrations

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(5%, 10%,15%, 20% and 25%). In particular, we have analyzed in the ranges 10^{-9} – 10^{-4} s the influence of chemical reactions, which actively participate in the conversion of nitrogen oxide specie at 50, 70 and 90Td. $N(^2D)$ and O are the two species on which we have concentrated.

The obtained data demonstrate that nitrogen oxide conversion varies with oxygen concentration. In fact, it has been found that the rise and fall of various species varies and are highly influenced by the values of O_2 concentrations. These findings enable us to recognize the crucial function that the reaction has in NO conversion, and they may be summed up as follows:

i. N(²D) specie produces most of the NO through the following reaction:

$$N(^{2}D) + O_{2} \rightarrow NO + O.$$

ii. The mechanism of NO reduction is due mainly by O specie through the reaction:

$$NO + O + N_2 \rightarrow NO_2 + (N_2)$$

- iii. We observe that the influence of the reaction (R1) was acquired for the low O_2 concentration of 5% at 50 and 70 Td for creation. In fact, we discovered an average of 44%, compared to 10% at 90 Td, where we got close to 50%.
- iv. In terms of reduction, we also see that at 50 and 70 Td, the reaction's effect (R10) was attained for the low O_2 concentration of 5%, although we had typically attained 80%. The influence of this reaction was discovered for 90 Td at a concentration of 10%, which is equal to 73.42%.

Finally, the acquired data unmistakably demonstrate the significance of chemical processes and oxygen concentrations in the generation or removal of nitrogen oxide.

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