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The kinetics of nitrogen oxides formation in the flame gas

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Abstract: This paper treats about the problem of nitrogen oxides formation in the process of natural gas combustion. The analysis of the influence of selected combustion parameters on the concentration of NO, N_2O and NO_2 in the combustion products was done. From many factors determining NO_x formation two was selected, ie temperature and residence time at the highest temperature zone, considering them to be particularly important. Detailed analysis of the absolute rate of NO_x for various combustion temperatures was done with the use of commercial software CHEMKIN-PRO. Moreover, the paths of formation of above- mentioned compounds were determined.

The main goal of the research is to analyze the impact of selected parameters of combustion process, such as temperature, on formation of thermal nitrogen oxides, with special emphasis on the chemistry of the process. The use of numerical methods to predict the products of combustion process, especially NO_x, is of great importance in terms of ecological and economical aspects

Keywords: combustion, numerical modelling, nitrogen oxides
JEL codes: Q53, Q57

1. Introduction

Nitrogen oxides as one of the most onerous atmosphere pollutants are formed during combustion in energetic boilers, metallurgical and reheating furnaces. Much of them are also emitted from plant of nitrogen industry and installation that produce sulfuric acid by the nitroso method. They are mainly emitted as NO, NO_2 and N_2O. During combustion most of nitrogen oxides arises as nitrogen oxide NO (95-99%) with a minor nitrogen dioxide NO_2 contribution (1-5%). In a combustion technique the concept of NO_x is used as a mixture of NO and NO_2. Devastating effects of nitrogen oxides on the natural environment are commonly known. It is estimated that

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the participation of NO and NO_2 in acid rain formation is about 30%. Nitrogen oxides also cause erosion of the buildings walls and tree damage, as well as accelerate corrosion of metals. Moreover, NO_x is a mainly factor that is responsible for the photochemical smog, that arises in troposphere with the NO_2 participation (Kordylewski, 2000; Weston, 2000; Wilk, 2000; Zajemska and Poskart, 2013).

The kinetics of nitrogen oxides formation in fuel combustion processes is a very complex issue. State of knowledge in this area is constantly enriched with new experience of researchers, not only in term of experimental methods, but also numerical calculations. Breakthrough in the analysis of combustion processes is CHEMKIN program that is a professional product and one of a kind in the world. It was created by American company ‘Reaction Design’. Wide range of applications in many industries, especially in the automotive (Ford Motor Company, General Motors, Honda, l'Institut Français du Pétrole, Mazda, Mitsubishi Motors, Nissan, PSA Peugeot Citroën, Toyota), the world’s scientific and research centers (Uniwersities of Michigan, Tokio, Minnesota, Karlsruhe and Colorado) and also in National Aeronautics and Space Administration (NASA) provides the plenty of possibilities of the CHEMKIN software use (Zajemska *et al.*, 2014).

2. Mechanisms of nitrogen oxides formation in combustion process

In the literature the greatest attention is paid to NO due to the fact that the vast majority of forming nitrogen oxides is in the form of nitrogen oxide. There are three basic mechanisms of nitrogen oxides formation, namely (Bulewicz, 2000; Fenimore, 1971; Gradoń, 2003; Hill and Smoot, 2000; Soete, 1974):

- thermal (Zeldovich’s),
- prompt (flame),
- fuel.

Recently the literature also refers to the mechanism of NO formation by nitrous oxide (N_2O) (Gradoń, 2003). Part of individual ways of NO_x forming depends on the technology and combustion conditions. Fuel nitrogen oxides dominate at 75% or even 95% in typical, conventional energetic boilers equipped with traditional burners, where pulverized coal is burned with high excess of air. Production of thermal NO is less than 15% of the total amount of NO with an excess air ratio $\lambda = 1.2$, while in the stechiometric conditions $\lambda = 1.0$ it is equal 0%.

During combustion of natural gas, what is almost nitrogen- free, the most important factor in the NO_x formation is temperature. Molecular nitrogen comes in this case from air supplied to combustion. Thermal nitrogen oxides are formed from oxygen and atmospheric nitrogen (from an oxidant) at relatively high temperatures ($t > 1350°C$) in the environment of fuels that have low calorific values and their amount strongly depend on temperature (Hill and Smoot, 2000). Thermal NO formation takes place especially for the poor flame ($\lambda > 1$). The value of their concentration is determined by the maximum flame temperature, residence time at the high temperatures zone and local concentration of nitrogen and oxygen molecules. The thermal mechanism base on the following equations (Gradoń, 2003; Hill and Smoot, 2000; Peribáñez *et al.*, 2014; Zajemska *et al.*, 2014):

$$N_2 + O_2 \rightarrow NO + N \tag{1}$$

$$N + O_2 \rightarrow NO + O \tag{2}$$

$$N + OH \rightarrow NO + H \tag{3}$$

The atomic oxygen needed to react with nitrogen in first reaction comes from dissociation of oxygen included in the air, and partly from oxidation of hydrocarbon fuel. Rate of NO formation in thermal mechanism is determined by reaction (1), and increases with the rise of both parameters, temperature and oxygen concentration. The confrontation of NO values, calculated on the base of Zeldovich mechanism, with experimental data, shows much higher NO concentration in flue gas. The reason of such differences is the impact of other mechanisms of NO formation in flames. The last reaction (3) of hydroxyl radical OH with the atomic nitrogen is a supplement of Zeldovich mechanism. It was suggested by Lavoie, Heywood and Keck in 1970, and makes a significant contribution to the formation of thermal NO_x (Gradoń, 2003; Weston, 2000).

Furthermore, during the low-temperature combustion ($t < 1200°C$) of lean mixtures ($\lambda > 1$) of methane or carbon monoxide with air, much higher nitrogen oxides concentration was observed, than as it stems from the Zeldovich's mechanism. The explanation of this process provided Malte and Pratt, who suggested to extend the theory of thermal mechanism. They observed that, the rate of nitric oxide formation through the extended thermal mechanism is much faster than by the Zeldovich thermal mechanism. On the basis of the experiences of Malte and Pratt, Gradoń proposed the mechanism of NO formation by nitrous oxide (N_2O) (Gradoń, 2003):

$$N_2 + O + M \leftrightarrow N_2O + M \tag{4}$$

$$N_2O + O \rightarrow NO + + NO \tag{5}$$

$$N_2O + O \rightarrow N_2 + O_2 \tag{6}$$

The influence of reaction (5) on the rate of nitric oxide formation is high only at temperatures below 1520°C. Above this temperature NO are generated according to Zeldovich mechanism.

In turn, the formation of prompt NO occurs at a low temperature processes, in the first section of flame. A temperature of 1100°C is enough for proceeding the reactions which require less heat or are not influenced by the hearth temperature. Relatively high concentrations of NO occur in the preflame zone with temperatures below 750°C. Prompt nitrogen oxides formation mechanism occurs primarily during the combustion of hydrocarbons rich mixtures with air (Fenimore, 1971; Wilk, 2000). In hydrocarbon flames, both at front and before flame, many hydrocarbon radicals $CH_i\cdot$ exist (such as: CH, CH_2, CH_3, C_2H_4, C_2H_5, C, C_2…) that also have capability to react with N_2, forming transitional product *ie* hydrogen cyanide HCN. This mechanism can be described by reactions, among which the most important are (Hill, 2000; Weston, 2000):

$$CH_2 + N_2 \rightarrow HCN + NH \tag{7}$$

$$CH + N_2 \rightarrow HCN + N \tag{8}$$

$$CH + N_2 \rightarrow HCN + N \tag{9}$$

Forming amino and cyano compounds (HCN, NH, CN) easily oxidize in flame to nitric oxide.

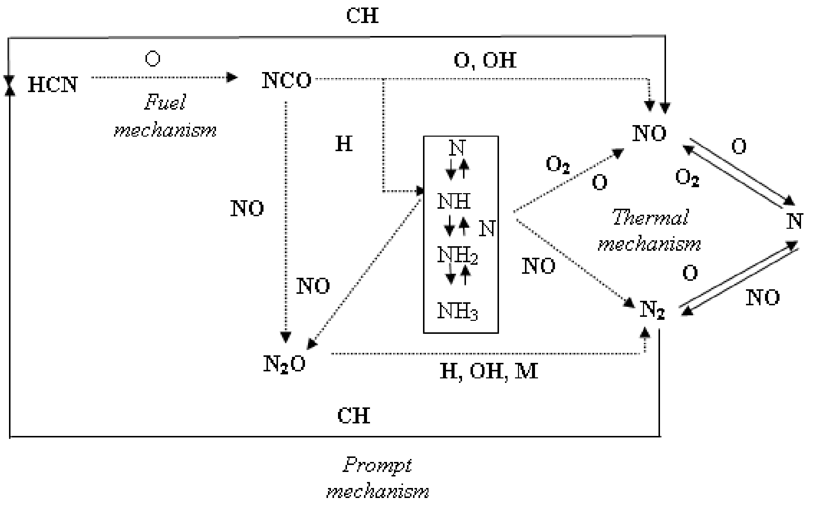
$$CH + N_2 \rightarrow HCN + N \rightarrow \ldots \rightarrow NO \tag{10}$$

Rate of prompt nitrogen oxides formation is equal the rate of combustion. The amount of NO_x depends mostly on molecular nitrogen N_2 concentration and weakly on temperature. The participation of prompt NO_x in total NO emission is quite small and it decreases with temperature rise (Hill, 2000).

Fuel mechanism primarily applies to solid and liquid fuels, that contain nitrogen compounds, called fuel nitrogen. In gaseous fuels chemically bonded nitrogen practically do not exist. Only some of natural gases included admixtures of N_2O and NH_3 (Bulewicz, 2000).

To sum up, processes of formation and decomposition of NO_x in combustion systems are very complex. During combustion, nitrogen from the air or fuel supplied to combustion, is converted to bounded nitrogen in the pollutants, such as: NO, NO_2, N_2O, NH_3 and HCN (Fenimore, 1971) (Fig. 1).

Figure 1. Simplified mechanism of NO_x formation and decomposition



Source: Soete, 1974.

In practice, the combustion process is controlled and operated by several key parameters, such as (Kordylewski, 2000; 2Wilk, 2000; Peribáñez *et al.*, 2014; Zajemska *et al.*, 2014):

- air excess and air staging,
- fuel properties (chemical composition, physical parameters),
- temperature,
- a warm reception,
- the content of oxygen in the oxidizer,
- flow rate and residence time,
- turbulence planes degree,

- the type of flame, etc.

In this article two of these parameters, namely temperature and residence time in the highest temperature zone, have been taken into consideration.

3. The kinetics of the combustion process in terms of numerical methods

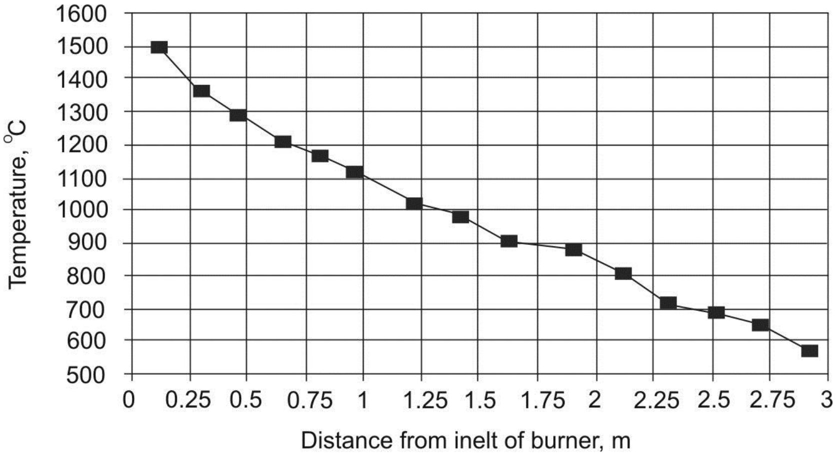
Results of the study (Adamczuk, 2010; 2011; Magdziarz *et al.*, 2011; Rodat *et al.*, 2009; Simmie, 2003; Zajemska and Poskart, 2013) and the current state of knowledge in the kinetics of combustion process shows that problems with the various values of reaction rate constants are a serious impediment to establish the accurate reaction. There is no exist a concept of 'perfect' model, there is also no optimal number of reactions, elements and chemical compounds describing the considered process. Most of researchers in the calculations model applied their own reaction rate constants, designated experimentally. In turn, this leads to create new models. Therefore, during the selection of kinetic data supplied into the model, very important is the choice of one specific mechanism. For the widespread gas fuel, namely methane, the most common reaction scheme of its oxidation is Miller-Bowman mechanism (M-B) (Miller and Bowman, 1989). The other commonly used mechanisms are GRI-Mech (Smith *et al.*), Burcat (Burcat and Gardiner, 2000), Konnov (Konnov, 2000), Curran (Curran *et al*., 2002) and others.

It is known that not all reactions are equally important. Depending on the conditions under which methane oxidation takes place, namely: pressure, temperature, as well as quantity and composition of the oxidant, some reactions are dominant and the others could be neglected because their influence on the process is insignificant. Literary sources available in the range of this issue mention different mechanisms in which the amount of reactions occurs more than 2500 and chemical compounds to more than 500, while the basic model of methane combustion can be described by six components, ie. : CH_4, CO, O_2, H_2O, CO_2 and N_2. The components number required to reduce NO concentration is nine (CH_3, CH_2, CH, H_2, H, OH, O, HCN, HCNO). Depending on the analyzed problem the basic model of methane oxidation can be extended to other compound and reactions based on existing mechanism, in particular the Miller- Bowman. Number of compounds used in the mechanism and reactions affects the computation time. The greater number of compounds applied in the calculation mechanism, the longer computation time.

4. Methodology

Numerical analysis of the natural gas combustion of nitrogen oxides formation was made with the use of the latest version of CHEMKIN-PRO program. Composition of natural gas was as follows: CH_4 = 96.7%, C_2H_6 = 0.7%, N_2 = 2.5%, CO_2 = 0.1%. Boundary conditions were based on preliminary laboratory experiment performed in a quartz chamber with a cylindrical cross section with a diameter of 0.12 and 3.2 m length.

Figure 2. Temperature distribution in the experimental chamber



Source: own elaboration.

The input file was created on the basis of the data determined by the experiment, *ie*: the excess air ratio (λ = 1.05), the supplied media fluxes ($\dot{V}_g$ = 0.00028 m^3/s, $\dot{V}_p$ = 0.0028 m^3/s), temperature profile, which ultimately included the following:

- fuel-air mixture mass flow - 0.003748 kg/s,
- reactant mole fractions determined on the basis of fuel and air composition - CH_4 = 0.08936, C_2H_6 = 0.00065, CO_2 = 0.00009, N_2 = 0.71931, O_2 = 0.19059,
- residence time in the highest temperature zone - 1s,
- temperature profile in the chamber (Fig. 2) ,

- input media temperatures - 1773 K,
- pressure - 1 atm.

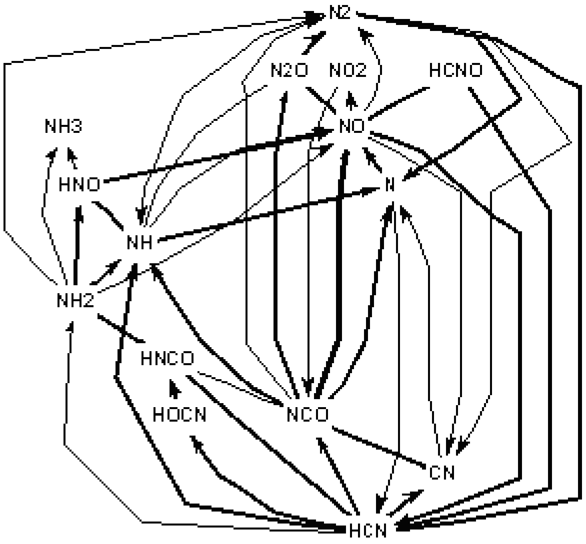
The model determining the combustion process, taking place in the 'Perfectly Stirred Reactor', was adopted in calculations. The basic chemical model was a methane combustion model which includes 132 chemical reactions and 35 elements and compounds, namely: H_2, H, O, O_2, OH, HO_2, H_2O_2, H_2O, N, N_2, NO, NH, NH_2, NH_3, HNO, NO_2, N_2O, CH_4, CO_2, CO, CH_3, CH_2, CH, HCO, C, C_2H_4, C_2H_3, C_2H_5, C_2H_6, CN, HCNO, HCN, HOCN, HNCO, NCO. In this mechanism all the reactions describing the ways of nitrogen oxides formation, *ie* thermal, prompt, fuel and by N_2O, were taken into account.

5. Results and discussion

As a result of numerical calculations were determined:

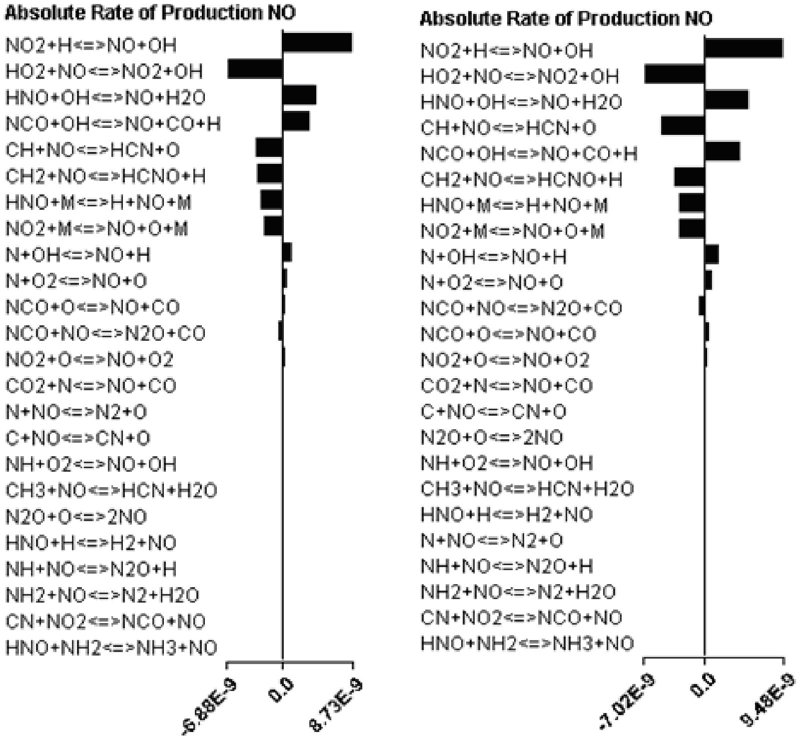
- paths of NO, NO_2 and N_2O formation during natural gas combustion (Fig. 3),
- absolute rate of NO, NO_2 and N_2O formation (Figs. 4-6),
- dependence of NO, NO_2 and N_2O on temperature (Figs. 7-9),
- dependence of NO, NO_2 and N_2O on residence time (Figs. 10-12).

Figure 3. Reaction path analyzer of NO, N_2O and NO_2 formation (1773 K)



Source: own elaboration.

Figure 4. Absolute rate of NO formation at temperatures 1773 and 2100 K



Source: own elaboration.

The figure shows that the temperature has significant influence on the rate of NO formation. At higher temperatures such as 2100 K it can be seen that the rate of NO production is slightly higher than at temperature 1773 K. This impact is in particular evident in reaction (11):

$$CH+NO=HCN+O \tag{11}$$

and in reactions (12)-(18)

$$NO_2+H=NO+OH \tag{12}$$

$$HO_2+NO=NO_2+OH \tag{13}$$

$$HNO+OH=NO+H_2O \tag{14}$$

$$NCO+OH=NO+C+H \tag{15}$$

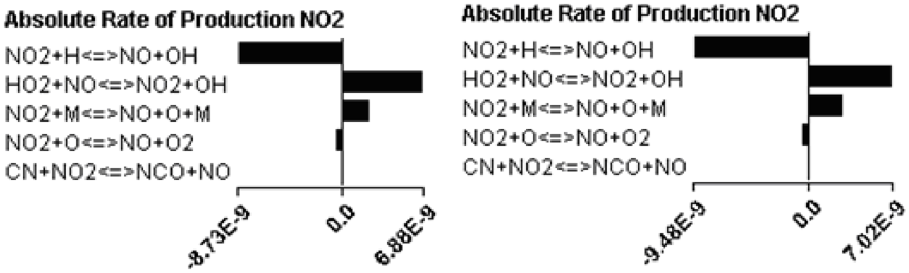
$$CH_2+NO=HCNO+H \tag{16}$$

$$NO_2+M=NO+O+M \quad (17)$$

$$N+OH=NO+H \quad (18)$$

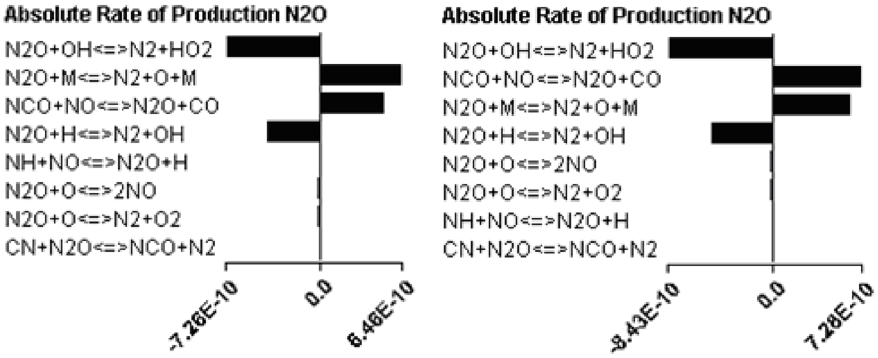
A similar situation occurs in the NO_2 and N_2O formation (Figs. 5 and 6).

Figure 5. Absolute rate of NO_2 formation at temperature 1773 and 2100 K



Source: own elaboration.

Figure 6. Absolute rate of N_2O formation at temperatures 1773 and 2100 K



Source: own elaboration.

Absolute rate of NO_2 formation for reaction:

$$NO_2+H=NO+OH \quad (19)$$

at temperature 1773 K reaches a value –8.73E-9, whereas at temperature 2100 K it is equal –9.48E-9 and for reaction (20):

$$HO_2+NO=NO_2+OH \quad (20)$$

is respectively equal 6.88E-9 and 7.02E-9.

The absolute rate of N_2O formation for reaction (21):

$$N_2O+OH=N_2+HO_2 \quad (21)$$

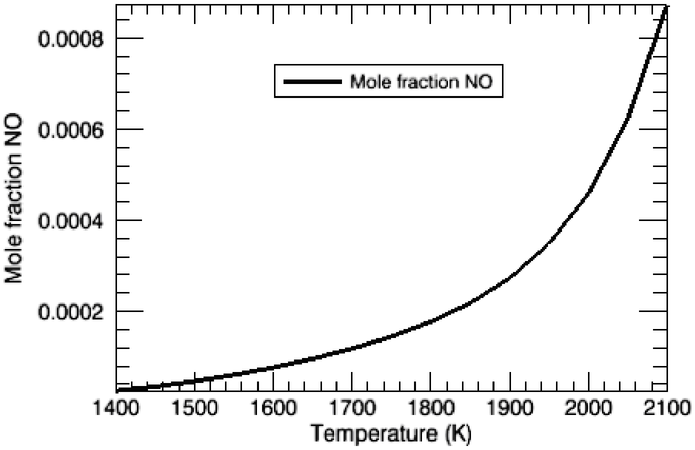
at temperature 1773 K is equal –7.26E-10, whereas at temperature 2100 K it reaches a higher value equals to –8.43E-10. Increase of the absolute rate of N_2O formation in reaction (22):

$$N_2O+M=N_2+O+M \tag{22}$$

is equal 6.48E-10 at temperature 1773 K and 7.28E-10 at temperature 2100 K.

The Figures 7-9 present the impact of combustion temperature on NO, NO_2 and N_2O formation. Calculations were performed for a residence time equals to 1 s.

Figure 7. The influence of temperature on NO formation



Source: own elaboration.

The numerical calculations provide that the mole fraction of NO increases with the rise of temperature. At temperature of 1400 K the concentration of NO in the combustion products is equal 100 ppm and begins to increase slowly, reaching a value of 180 ppm at temperature of 1800 K. At temperatures above 1800 K NO concentration begins to increase more quickly, whereas at temperatures above 1900 K rise more rapidly, reaching a value of 840 ppm at maximum temperature of the analyzed range, *ie* 2100 K. A similar situation is observed for NO_2 (Fig. 8). The only difference is that the concentration of NO_2 in the exhaust gases in the considered temperature range is much smaller than the concentration of NO and it is within the range of 0.01-0.25 ppm.

Figure 8. The influence of temperature on NO_2 formation

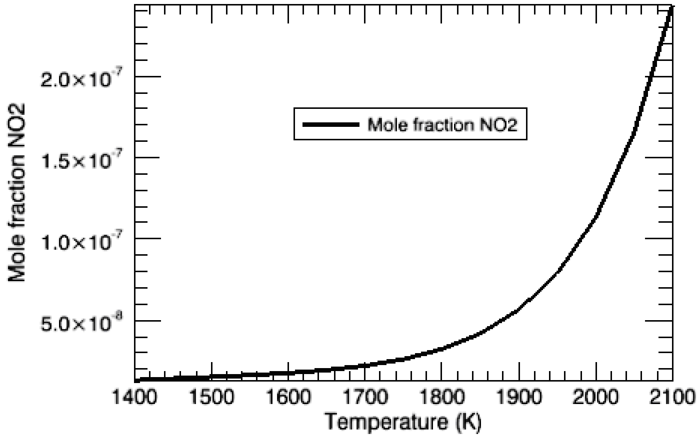


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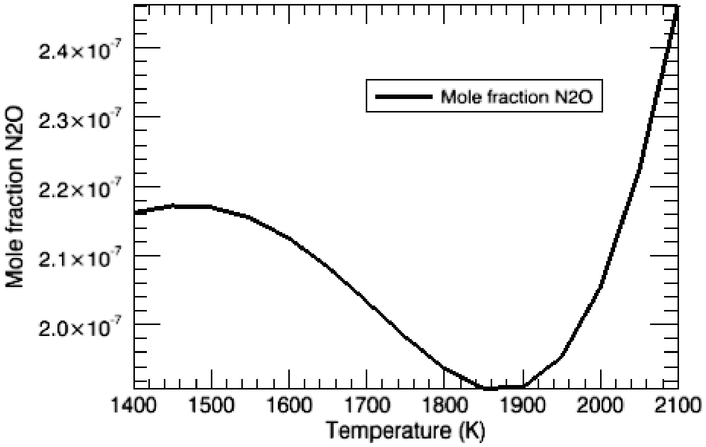
Figure 9. The influence of temperature on N_2O formation



Source: own elaboration.

A different situation occurs in the case of N_2O (Fig. 9). Initially, the concentration of nitrous oxide decreases, reaching a value of 0.19 ppm at temperature of 1850 K. At temperatures above

1850 K a sharp increase in concentration to the value of 0.245 ppm at a temperature of 2100 K is observed. The content of N_2O in the exhaust gases is comparable to the content of NO_2.

Figure 10. The influence of residence time on NO formation

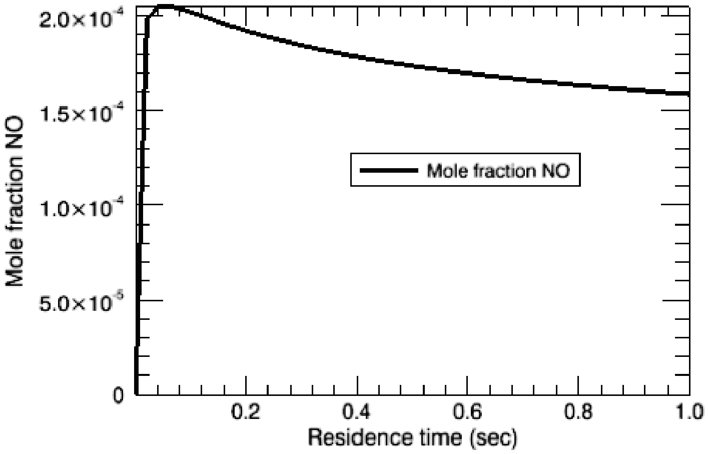


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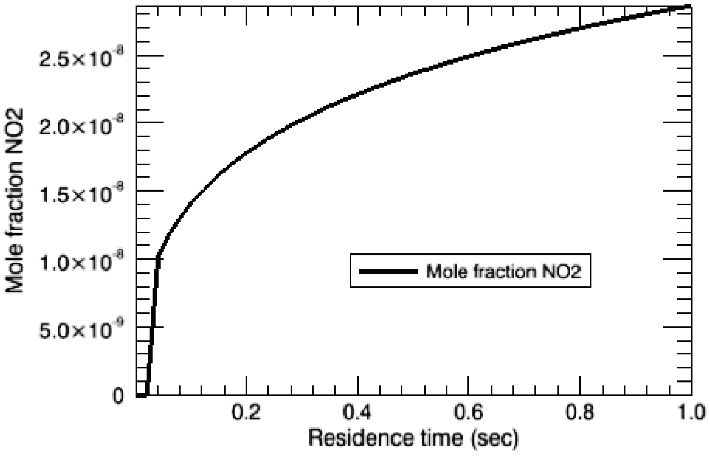
Figure 11. The influence of residence time on NO_2 formation



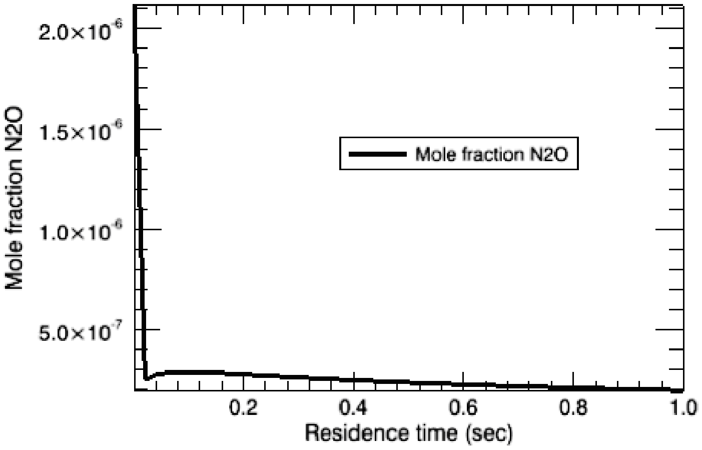
Source: own elaboration.

In the numerical calculations the effect of residence time on the NO, NO_2 and N_2O formation at the highest temperature zone in the temperature equals to 1773 K was also analyzed. The results of these calculations were presented in Figures 10-12.

Figure 10 provides that the residence time has a significant influence on the amount of produced nitrogen oxides. In the case of NO the concentration increases rapidly in a relatively short residence time equals 0.01 second, reaching a value of 200 ppm. With the residence time increase the nitric oxide concentration starts to decrease gradually, reaching a value of 160 ppm at 1 s. Regarding the influence of residence time on the NO_2 formation, it can be seen that this dependence has a slightly different course than for NO. The content of NO_2 in the exhaust gases within the whole range of the considered residence time is increasing and reaches a value of 0.028 ppm at 1 second (Fig. 11).

A different situation is observed for N_2O (Fig. 12). Its content is rapidly decreasing in a residence time shorter than 0.1 s, reaching a value of 0.3 ppm. Further extension of time has little impact on the nitrous oxide contribution in the exhaust gases.

Figure 12. The influence of residence time on N_2O formation



Source: own elaboration.

6. Conclusion

The current state of knowledge and results of our studies show that many parameters have impact on the quantity of formed nitrogen oxides. The most important of them, namely temperature and residence time, were analyzed in this article. The use of professional software CHEMKIN-PRO allows to perform detailed analysis of the nitrogen oxides formation process in terms of their content in the exhaust gases depending on different parameters describing the combustion process. It also allows to determine the absolute rate of NO_x formation and analyze the chemical pathways of their formation. The authors considered that obtained results of numerical simulation of N_2O require a thorough analysis. The results provide several valuable observations in the field of NO_x formation. Calculations show that, the mechanism of NO formation via the N_2O plays an important role, which was noticed in the work of Gradoń (Gradoń, 2003). But unfortunately in simplified numerical calculations it is generally neglected. Furthermore, the analysis, carried out in this article, of the influence of excess air ratio on NO_x content in the exhaust gases at varying values of residence time and temperature will make a significant and valuable contribution in the field of numerical calculations. That issue will be presented in the nearest future in subsequent publications.

The results of numerical calculations may be useful in diagnostics of fuels combustion for different conditions of the process. The application of numerical methods with the use of CHEMKIN-PRO software enables to predict the chemical composition of flue gas in heating devices, including reheating furnaces of complex geometry. Knowledge of pollutant formation mechanisms for specific conditions of the combustion process provides the opportunity to control and minimize the emission in the entire range of operation. Analysis of major pollutants formation paths, such as NO_x, as a function of residence time may be an important element of consideration for the newly designed chambers of heating furnaces. The results of numerical calculations can be the basis of the diagnostics of combustion process in terms of emitted pollutants, as well as may also be useful during efforts to optimize the entire combustion process.

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Kinetyka formowania tlenków azotu w płomieniu gazowym

Streszczenie

W niniejszym artykule poruszono problematykę formowania tlenków azotu w procesie spalania gazu ziemnego. Przeanalizowano wpływ wybranych parametrów spalania na udział NO, N_2O i NO_2 w produktach spalania. Spośród wielu czynników determinujących tworzenie się NO_x wybrano dwa, a mianowicie temperaturę i czas przebywania w strefie najwyższych temperatur, uznając je jako szczególnie istotne. Za pomocą komercyjnego oprogramowania CHEMKIN-PRO

dokonano szczegółowej analizy absolutnej szybkości NO_x dla różnych temperatur spalania. Ponadto, sporządzono ścieżkę formowania ww. związków.
Zasadniczym celem badań jest analiza wpływu wybranych parametrów procesu spalania, takich jak temperatura, na formowanie termicznych tlenków azotu, ze szczególnym uwzględnieniem chemii procesu. Wykorzystanie metod numerycznych do przewidywania produktów spalania, m.in. NO_x, jest niezwykle istotne w aspekcie ekologicznym i ekonomicznym.

Słowa kluczowe: spalanie, numeryczne modelowanie, tlenki azotu