TECHNOLOGY OF GASEOUS FUEL COMBUSTION RESPECT TO NOX FORMATION

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NO_x formation is one of the main ecological problems nowadays as nitrogen oxides is one of main reasons of acid rains. Nitrogen oxides (NOx) are formed as a result of oxidation of nitrogen which occurs in the air and in a fuel.The aim of this work is to research the formation of NOx in combustion of gaseous fuels. The ANSYS model was designed according to the calculation to provide full combustion and good mixing of the fuel and air. In this paper we research influence of combustion air composition by simulation combustion with the different N2/O2 air ratio on NOx formation.The theoretical and experiential knowledge allow understanding and predict the mechanisms of NOx formation.

KEYWORDS

nitrogen oxides, combustion, ANSYS, N2/O2 air ratio

1. INTRODUCTION

The most important problem of modern engineering is environmental contamination by toxic products of combustion of fossil fuels. Already, the pace and extent of human impact exceeds the adaptive capacity of the biosphere and therefore irreversible processes in nature, leading to environmental catastrophes. The major pollutants of the combustion in the atmosphere are carbon monoxide CO, nitrogen oxides NO, NO2, sulphur dioxide SO2 and hydrocarbons [Jandacka 2015]. The most toxic emissions are nitrogen oxides. Continual growth in computing power has been the single greatest factor in a corresponding increase in the size and complexity of combustion models. Growth can be measured in terms of the number of computational grid points in CFD calculations, in the number of chemical species in chemical kinetic models, in the spatial resolution of direct numerical simulations (DNS) of turbulent flows, or in the number of reactive surface sites in a CVD or surface combustion simulation [Westbrook 2005].

2. CHARACTERISTICS OF THE SELECTED COMBUSTION

To understand the mechanism of NOx formation we tried to simulate combustion of the burner with fire-box. The combustion will be calculated in ANSYS 14.0 as turbulent diffusion non-premixed combustion.

In the heterogeneous and homogeneous coupled reactions, the intermediate and final product is simultaneously desorbed from the heterogeneous reactions and then can affect the homogeneous combustion [Qingbo 2016].

The intensity of the diffusion combustion depends on the intensity of mixing. Since the mass transfer in turbulent flow is many times more intense than in laminar, the method of turbulent diffusion of non-premixed combustion gases is more important for industrial purposes [Rimar 2014].

Turbulent diffusion combustion is carried by dual feed gas and air through the burner into the combustion chamber. Air may be supplied through burner or through separate nozzles. In our model burner has big air nozzle around small gas nozzle (Fig. 1).

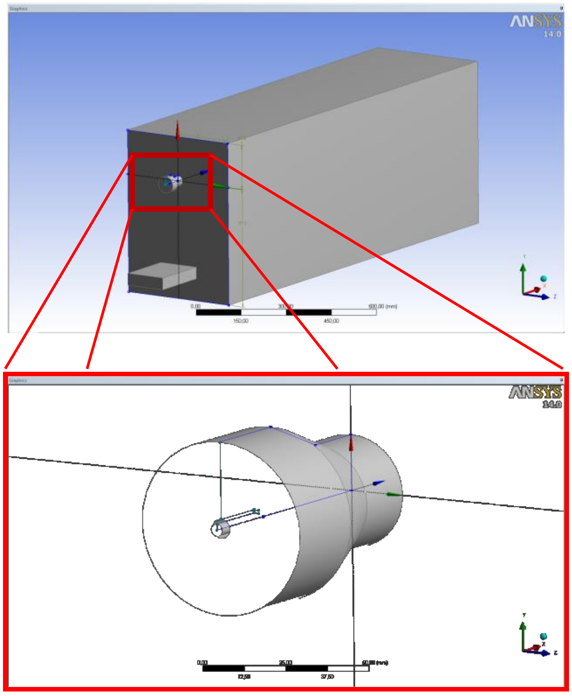


Figure 1. Model of the burner

3. CALCULATION METHOD

To calculate non-premixed combustion of the fuel of next composition

Element	Amount
CH4	0.95%
H2	0.01%
N2	0.04%

Table 1. Composition of the fuel

All necessary air is goes through one nozzle and its quantity is calculated to provide full combustion of the gas with excess air ration m=1.1.

The turbulent was calculated by k-epsilon method, as one of the most suitable [Rajzinger 2015].The turbulent jet has the property of self-similarity, and turbulent diffusion coefficient is proportional to the nozzle diameter and the velocity. The position of the ignition and combustion zone, defined as the locus of points where a mixture of stoichiometric composition at the burner of this size should not depend on the exhaust velocity. Also ignition zone length should not depend on the exhaust velocity. The calculated diameter for a given fuel must be the same for different sized burners. But only the dependence of the relative length of the ignition zone is on the stoichiometric oxygen concentration in the environment [Rimar 2014a].

The length of ignition diffusion zone of the flame depends on the heat of the combustion gas, as for combustion of a mass unit of gas we need to get oxygen. The lower oxygen content in the environment, the longer ignition zone we have. Conversely, by increasing the oxygen concentration in the environment the torch ignition zone length decreases.

These provisions are derived from theoretical studies, confirmed by experiments.

Heat released during chemical reaction by turbulent heat conduction and diffusion of hot combustion products goes to the fuel mixture, providing its ignition and flame spread. Therefore, the position of the combustion zone is determined by the terms of the turbulent diffusion, and burning velocity. An additional condition for stable combustion is the presence of a necessary flame propagation velocity, as otherwise may happen flameout [Rimar 2015].

Ignition of turbulent diffusion torch is similar to the ignition in turbulent combustion of homogeneous gas mixture. A turbulent gas jet carries the hot combustion products during its propagation in the combustion chamber together with the air, also resulting mixture heating and ignition.

The total flame length is longer than the length of the ignition zone by the length of afterburning zone. In this zone occurs afterburning plurality of moles for which the torch is fragmented under the influence of turbulent fluctuations. The mixing process takes place mainly by molecular diffusion, which proceeds slowly. Also, concentration of combustible gas and oxygen is small in the burnout zone. Under these conditions the combustion takes place relatively slowly, causing a considerable length of afterburning zone.

The length of the afterburning zone is equal to the length of travel pass of moles per time of burnout[Rimar 2014b].

The NOx formation will be calculated according to the ANSYS Fluent model and will consider all major mechanisms of NOx formation (Fig. 2).

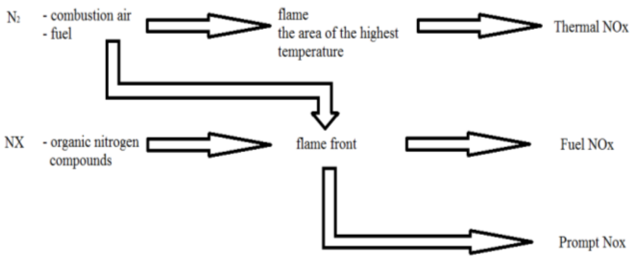


Figure 2. Mechanisms of the NOx formation

Thermal NOx- The concentration of “thermal NOx” is controlled by the nitrogen and oxygen molar concentrations and the temperature of combustion. Combustion at temperatures more than 1,300 C forms significant concentrations of thermal NOx typically in the area of the highest flame temperatures.

Fuel NOx- Fuels that contain nitrogen (e.g., coal) create “fuel NOx” that results from oxidation of the already-ionized nitrogen contained in the fuel.

Prompt NOx - Prompt NOx is formed from molecular nitrogen in the air combining with fuel in fuel-rich conditions which exist, to some extent, in all combustion processes. The nitrogen then oxidizes along with the fuel and becomes NO_x during combustion, simply as fuel NOx. At temperatures more than 1,400 C in areas of high temperatures N_2 starts exothermal reaction with fuel compounds while the products of reaction similar to fuel NX which increase their total NOx pollution[Kizek 2015].

According to the given mechanisms of the nitrogen oxides formation during the fuels combustion, we can compose list of the factors that influence the NOx formation:

- Local gas temperature in the combustion chamber;
- The gas residence time in high temperature zone;
- Levels of oxygen and nitrogen in the combustion zone;
- Air temperature at the combustor inlet.

In this work we will research only the levels of oxygen and nitrogen in the combustion zone and local gas temperature in the combustion chamber. Also we will try to analyse the influences of other factors.

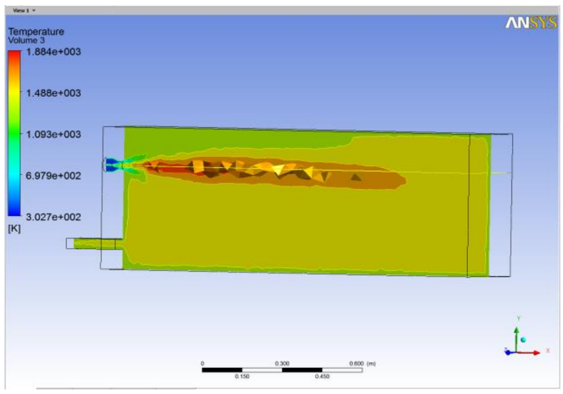
To confirm this and to understand the NOx formation in combustion of fuel with different composition of air Tab.2.

element	Exp. 1	Exp. 2	Exp. 3
N2	0.79%	0.78%	0.77%
O2	0.21%	0.22%	0.23%

Table 2. Composition of the air

4. RESULTS OF THE CALCULATION

We have made a simulation of the non-premixed combustion to confirm calculated characteristics of the burner and the fire-box as well as to determine flame, NO and NO2 fronts. Gas goes through the gas nozzle of d=2.7 mm with the pressure p= 90 kPa. The necessary air comes to diffusor through air the nozzle to provide full combustion of the natural gas with excess air around m=1.1. The gas and air temperatures at the inlet are t_{ng}=30C t_a=60 °C. Temperature of the walls is stable t_w=1000°C. Dimensions of the fire box were calculated to provide necessary space for the flame.
Impact of the oxygen concentration on flame temperature and the character of combustion is on the Fig.3.



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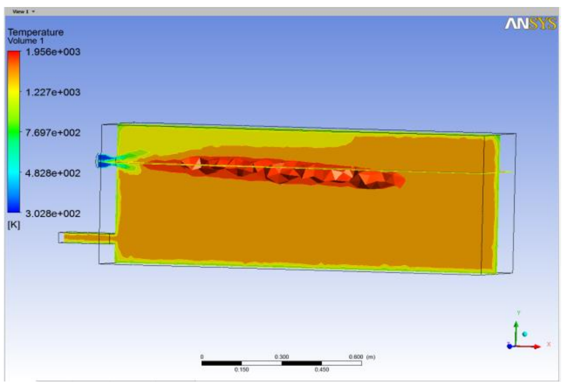

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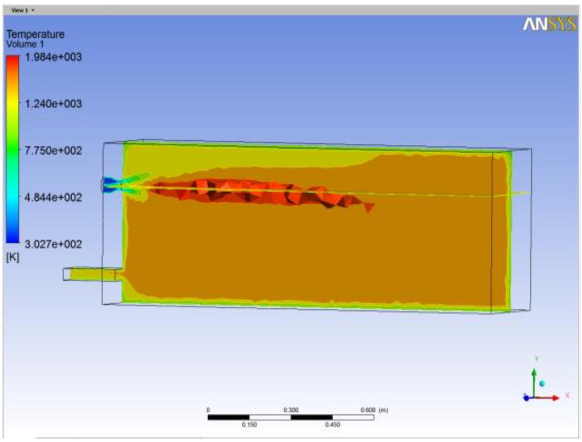

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Figure 3. Temperature front of the burner and fire-box in combustion a – air composition 1, b – 2, c – 3.

As you can see from the Fig.4increasing of O_2 concentration can significantly influence on the combustion temperature and temperature front.

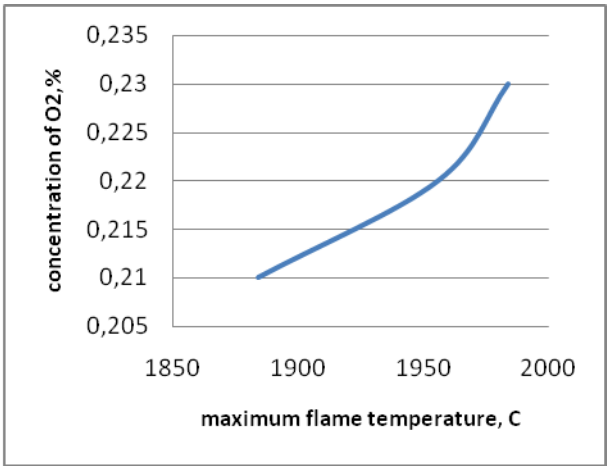
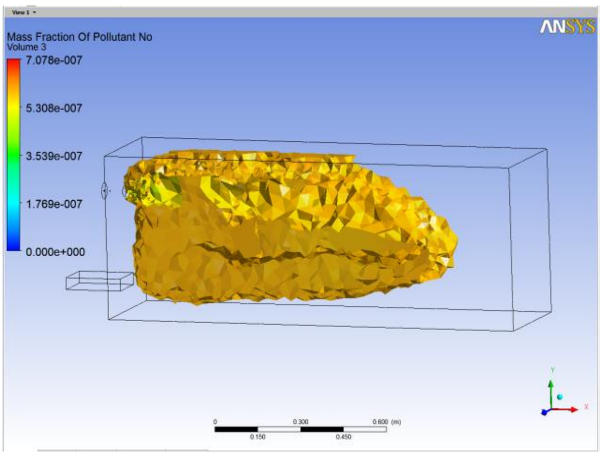


Figure 4. Dependence of O_2 concentration on maximum flame temperature

Increasing of the maximum flame temperature an as a result volumes of higher temperature in fire-box leads to increasing of NO formation what can be seen on the Fig. 5.



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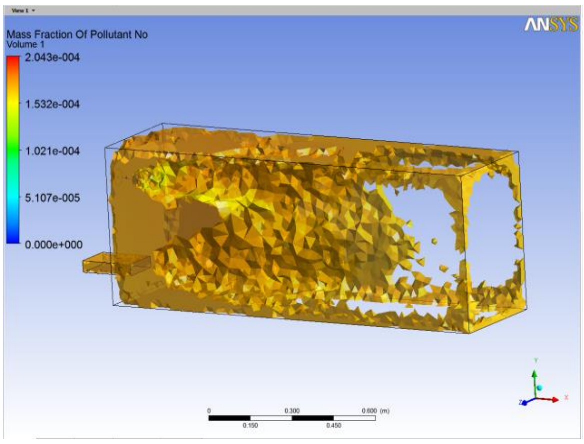

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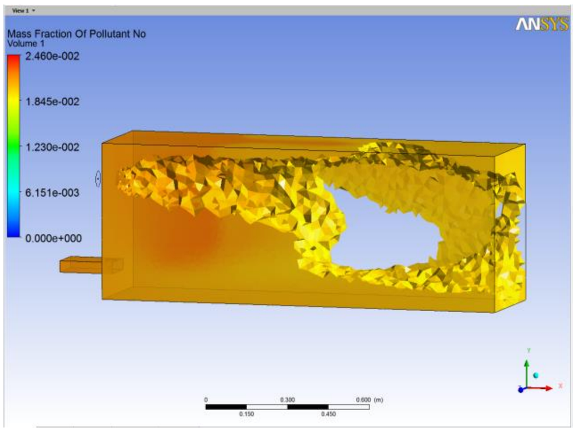

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Figure 5. Areas of NO formation above 3 ppm in a – experiment 1, above 30 ppm in b – 2, above 300 ppm c – 3.

There can be seen increasing of O_2 in combustion air has double influence on combustion process.

On the one hand the amount on N_2 in combustion air decrease, and reduce the total amount on N_2 in combustion area. On the other hand, the bigger amount of O_2 considerably increase flame temperatures what lead to formation of significant part of thermal NO_2.

Thermal oxides of nitrogen are formed by the reaction of oxidation of atmospheric nitrogen and free oxygen in the combustion process. The major amount of thermal nitrogen oxides is formed in a narrow temperature range close to the maximum temperature in the zone of active burning. According to the J. B. Zeldovich mechanism of formation of thermal nitrogen oxides was proposed by and includes the following reactions:

$$O + N_2 = NO + N, \quad (1)$$

$$N + O_2 = NO + O \quad (2)$$

$$OH + N = NO + H \quad (3)$$

NO formation begins at a distance of 1 mm from the visible flame front and reaches a maximum in the flame front. The ratio of NO_2/NO will decrease with increasing of the temperature. NO_2 decomposition occurs during the period = 4*10^-3 with the interval length of 1 mm from the initial boundaries of the visible flame front. NO_2 decomposition in the preflame area in the front of the flame coincides with the formation of a zone of "prompt" NO, in a zone of intensive growth of nitric oxide concentration. NO_2 decomposition in the flame effect starts using to clean gases containing high concentrations of NO2 (flue gases and other chemical industries).The process of final oxidation of NO in NO2 in flames with molecular oxygen has reactions of high activation energy and great response time, so it cannot give significant amounts of NO2. Of the two most probable oxidizing NO to NO2 (atomic oxygen and peroxide radicals - HO2) is practically important only HO2 [De Soete 1975].

The main factors affecting the formation of thermal nitrogen oxides are: temperature in the zone of generation of NOx, concentration of atomic oxygen and residence time in the combustion zone. The concentration of nitrogen oxides increases linearly with increasing concentration of atomic oxygen and exponentially with increasing temperature [Varga 2015].

In the same time reduction of the temperature will lead to decreasing total efficiency of the heat machine, and also will move priority of NOx formation to the prompt and fuel mechanisms.

The gas residence time in high temperature zone and air temperature at the combustor inlet will also have a significant influence on the NOx formation. The good fixing and recirculation of the exhausted gases, as it lead to increasing of the flame temperature, will increase amount NOx in the fire-box. Increasing of the air temperature will have the same results but with other efficiency.

5. CONCLUSIONS

The theoretical and experiential knowledge which you can read above allow understanding and calculating the mechanisms of NOx formation and the main management points of control thermal machines respect to its efficiency and ecological problems.
The good management of thermal processes should consider with next points:
- control areas of maximum temperature,
- control of combustion excess air to provide necessary its volume,
- control time of fuel elements stays in the burning zone,
- control air and fuel temperature before its combustion.

The formation of fuel nitrogen oxides occurs in the initial part the flame, in the area from the prompt NO formation to the areas of thermal NO.
The degree of transition of nitrogen-containing compounds in the fuel NO increases rapidly with an increase in excess air coefficient.
On the length of the flame is strong influence make the burner construction and method of organization of the combustion process in the furnaces for different purposes.
It should be noted that due to the mass transport of fuel, air and combustion products by moving a plurality of individual combustion moles turbulent flame front is a wavy obtained, blurred, torn into pieces and poorly stable. In addition, turbulent diffusion torch, as well as laminar diffusion torch, for the same reasons inherent in the formation of incomplete chemical combustion.

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