Analysis of numerical models for the formation of NO_X for combustion of gases in the strong swirl flow

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Abstract

The present work is a continuation of the work presented previously [1] at a conference ECM2013 which took place in Lund. That work is presented the results of numerical simulations of the combustion process in swirl flow. The swirl flow is generated by specially designed swirler. In present paper will be presented the results of numerical analysis of the combustion process of non normative natural gases with particular emphasis on the production of nitric oxides. This analysis was performed using different models of combustion process and the formation mechanisms of nitric oxides available in ANSYS Fluent.

Introduction

Energy policy of the EU [2] emphasizes the use of renewable energy. Special emphasis is placed on the use of alternative fuels such as biogas, syngas or other gases. These kind of gases can be used for supply the power plants or small energy units based on micro gas turbine or gas engines.

Another type of gases, which can be used as alternative fuel to common fossil fuels are natural gases with non-normative composition such as low calorific natural gases, shale gases or tight gases. These fuel contains a significant amount of nonflammable components like nitrogen or carbon dioxide. The inert gases can be removed using special installation, but these processes are quite expensive due to that energetic use of non-normative natural gases (NNNG) is not profitable. Other possibility of using of NNNG is direct combustion energetic machines like gas turbine.

Non-normative natural gases are very important for Poland, because there is a lot of natural gas fields with NNNG. At this time gas consumption in Poland is about 15,8 mld Nm^3, out of which 20% are natural gases with nonstandard composition. There are a few power plants fired by gas from non-common gas pipe lines mainly located in west part of Poland (power plant in Gorzow Wielkopolski, Zielona Gora).

Combustion processes of such fuels need to know a thermodynamic parameters such as laminar flame speed, adiabatic flame temperature or turbulent flame speed as well as mechanism of formation of toxic compounds especially nitric oxides (NO_x). The numerical value S_L for pure methane is about 42 cm/s (p=1bar, T_{sub}=300) [3] and T_a is about 2230K. For the same conditions of combustion of NNNG1 with chemical composition as given in Table 1 the value of S_L is 38 cm/s and T_a = 2170K. [4]. Different values of the adiabatic temperature and combustion process and laminar flame speed have some effect on flame stability described by such phenomena as flameout or flasback [5] and also on the volume of emissions of toxic compounds into the atmosphere.

The mechanisms of formation of nitric oxides are well known for standard gaseous fuels, and can be calculate by commonly used numeric software. The main available models of formation of nitric oxides are implemented directly in the structure of the calculation code without the use of an additional sources. They are based mainly on well-known model of the formation of NOx - Zeldovich model. For example numerical code Ansys Fluent allows to use for NO_X calculation three kinds of mechanism like: thermal, prompt and/or fuel [6]. There is also possibility to implement an additional NO_X formation mechanism instead of built-in, such as: GRI. 3.0 [7], San Diego Mechanism [8] or like presented in [9]. These mechanisms contains a significant amount of forward and backward chemical reactions of NO_X formation.

In the paper authors have mostly concentrated on the process of calculation of NO_X formation based on built-in codes in post-processing mode. The calculation were made for natural gases with composition presented in table 1. The results of CFD calculation were compared with experimental data.

Nomenclature

c – bulk velocity
c_{syn} – bulk velocity for syngas
S- swirl number
λ – excess of air
ϕ – equivalence ratio
T_{sub} – substrates temperature
T – temperature
r – radius
u- velocity
p – pressure in the combustion chamber
T_a– adiabatic flame temperature
S_L – laminar flame speed [cm/s]
LHV – Low Heating Value

Experimental setup

The experiments were carried out on the test rig shown in Fig. 1. The rig was equipped with a set of measurement openings and quartz windows allowing laser-optics experimental research. The combustion chamber was fitted with a swirl burner shown in Fig.2.

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Swirl flow was produced by a swirler with helical blades with angle of 30° for which swirl number S calculated from the geometry of the swirler was S – 1.26.

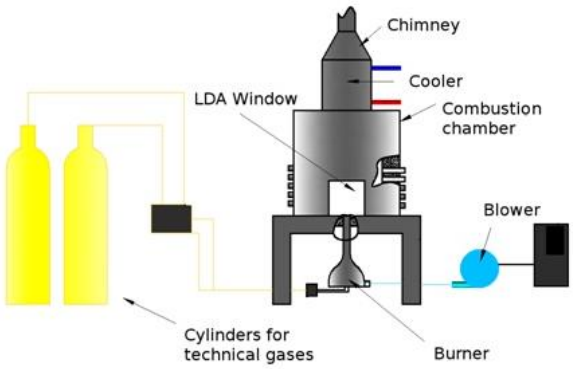

Fig. 1 Experimental test rig

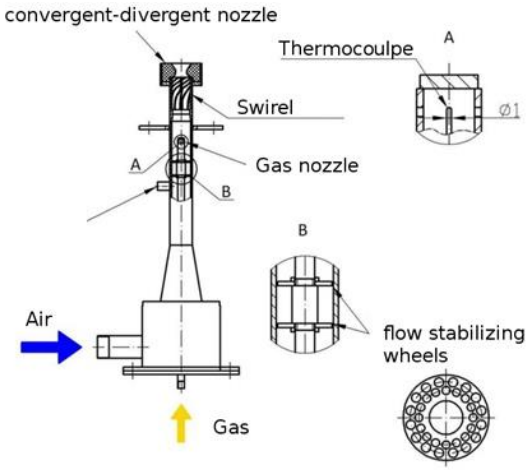

Fig. 2 Scheme of gas burner

Fuel was fed into the burner from a gas mixer about 15 cm before the nozzle exit, where it was mixed with air. The flow of fuel was controlled with mass flow meters. The investigations were done for four different fuels: pure methane, and three non-normative natural gases, with the constant value of equivalence ratio equal ϕ=0.95

Table1 Fuel mixtures

	CH_4 [%]	CO_2 [%]	LHV [MJ/m^3]
Methane	100		36
NNNG 1	90	10	32,4
NNNG 2	75	25	27
NNNG 3	70	30	25,2

All the measurements were done for atmospheric pressure and the temperature of air fed into the burner of 300K.

The flow phenomena in the combustion chamber were investigated with laser-optical method LDA. A two-color laser anemometer with wavelengths of 514.5 and 488 nm made it possible to measure two velocity components u_x and u_y , the third velocity component, radial velocity, was not measured, but from [10] we can assume that its value in relation to components u_x and u_y is very small with no effect on flame stability. Titanium dioxide TiO_2 with nominal diameter of particles from 1 to 5 um was used for seeding.

The exhaust gases extracted from the exhaust duct through the suction pyrometer probe were conducted via a cooling system to a set of gas analyzers manufactured by Emersson for measuring CO, CO_2, NO_X and oxygen.

All measurement data collected in the experiments were being registered on-line and recorded on a computer disc.

Numerical investigations

The numerical computations were made so as to generalize the experimental data and to compare quantitatively the results of numerical simulation with the actual experimental data. To increase the accuracy of calculation was used a full hexahedra mesh. This type of mesh gives more stable results than a tetrahedra mesh. This type of mesh is also characterized by a higher speed of calculation. In order to build a good quality computational mesh, it was necessary to divide the model into smaller components, as shown in Figure 3. This allowed for much greater control of the process of creating the mesh and to control its parameters.

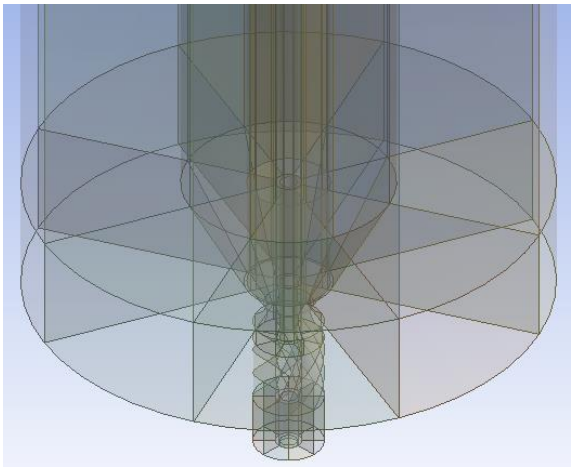

Fig. 3 Geometry of the model

The geometrical model of the combustion chamber created for the numerical calculations underwent some idealization. Additionally, a stable temperature of the walls of the entire model was assumed, which is never the case in experiments (the temperature changes, and there is also some minor heat exchange between the flow and the surroundings). Such assumptions made the comparison of a numerical model and the actual experiment more difficult, but that could not be avoided due to license restrictions on the program used.

Presented below are the settings of the program used in the calculations:

– Mesh settings:

- type of elements: hexahedra
- number of elements: about 320 000
- skewness: less than 0,8
- aspect ratio: maximum 40, in the nozzle maximum 10

– FLUENT settings:
- reference pressure: 1 atm
- turbulence model: k-ε, RSM
- reactions: methane air 2 step, flamelet based on GRI 3.0
- combustion model: Eddy Dissipation, PDF
- combustion mechanism: methane-air 2 step, GRI 3.0
- thermal radiation: Discrete Ordinates
- Inlets: mass flow inlet
- Outlet: pressure outlet
- Walls: adiabatic, emissivity 0,7
- convergence criteria: energy imbalance less than 1% of power in fuel
- excess of air λ=1,05
- substrates temperature Tsub = 300K.

The numerical computations of the flow with combustion were made with the program Ansys FLUENT version 14.5.7. The authors used two different combustion models: Non-Premixed Combustion and Eddy Dissipation model.

In Non-Premixed Combustion model GRI 3.0 mechanism was used to generate a Flamelet database. Then the PDF (Probability Density Function) table was generated, which contains 20 compounds. This table contains the main substrates and products of combustion (O2, N2, CH4, CO, CO2), additional toxic compound (NO) and radicals O, H, OH. It allows to immediately receive the results of emissions of nitric oxides without additional calculations in post-processing. A disadvantage of this model is that one Flamelet database can be used only for one fuel-air mixture composition.

This model required to use of two separate inlets, fuel and air, which was taken into account when creating the geometry and mesh.

The use of this combustion model simultaneously with the turbulence model RSM (Reynolds Stress Model) caused an initiation of the reaction before the swirler and the stabilization of the flame at the outlet of the swirler blades. It can be observed significant increase of the temperature on the edge of mixing the fuel and air (fuel was fed in the middle, air was delivered in the outside). This phenomena is presented in Figure 4.

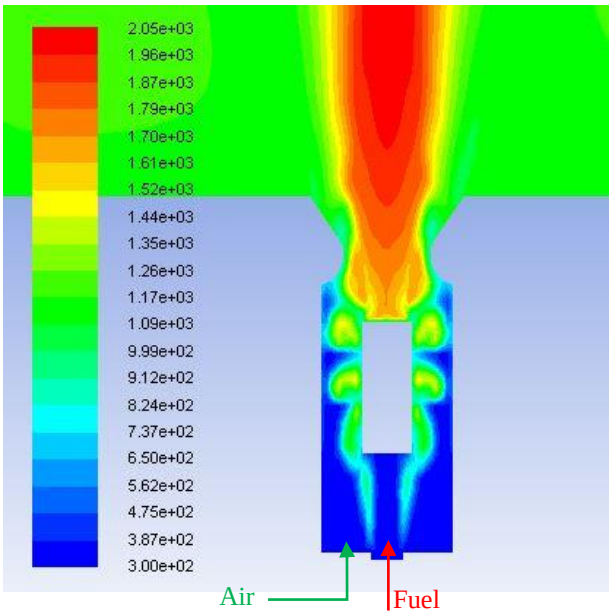

Fig. 4 Distribution of temperature at a cross section for Methane, Non-Premixed model

Such a distribution of the temperature profile has also influence on the velocity distribution in the flame. This resulted in formation of a high velocity stream, which was inhibited before the outlet of the chamber. The character of this stream was shown in Figure 5.

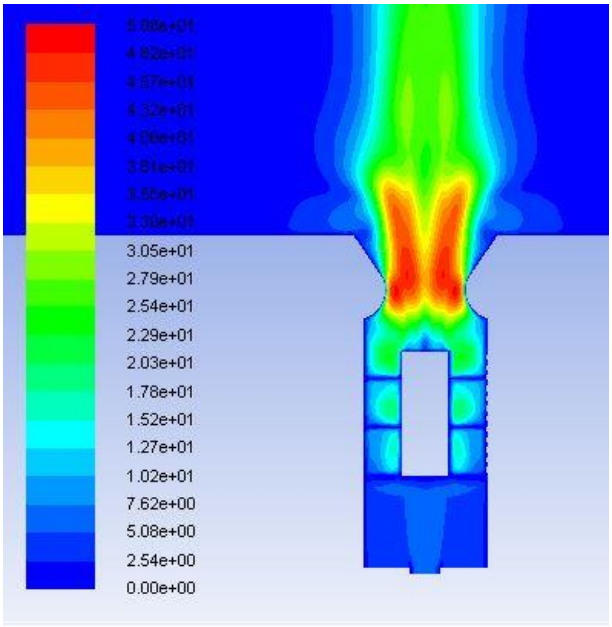

Fig. 5 Velocity distribution at a cross section for Methane, Non-Premixed model

The second combustion model used in the calculation was an Eddy Dissipation (ED) model. Combined with this model was used combustion mechanism Methane-Air 2 Step [6], which is implemented in Ansys FLUENT. Advantage of this mechanism is its simplicity and taking into account the reaction of carbon monoxide as an intermediate product in the combustion of methane.

In this model it was possible to simulate the premix flame.

During the analysis of the results obtained from this model it was also noted that the start of the combustion reaction takes place already in swirler. An increase of temperature is clearly visible on the blades of swirler before convergent-divergent nozzle. This phenomena is shown in Figure 6.

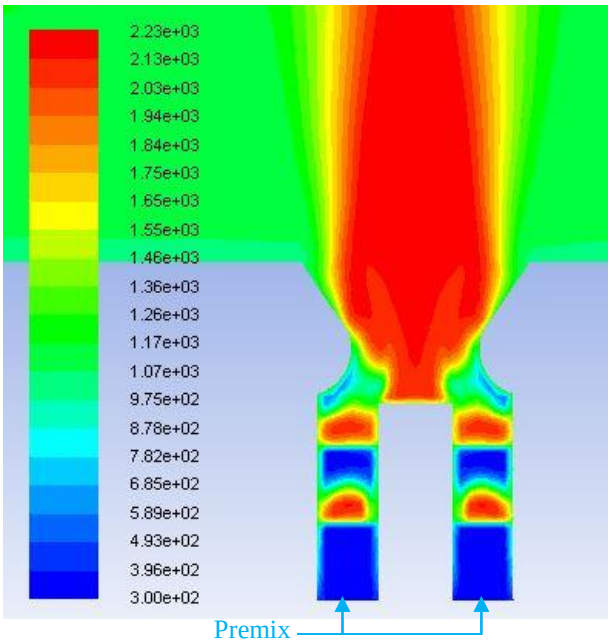

Fig. 6 Velocity distribution at a cross section for Methane, ED model

Also in this case, the flame and flue gases do not create a swirl flame. The internal and external recirculation zone, typical for swirl burner, was not observed. The character of the flow is shown in Figure 7.

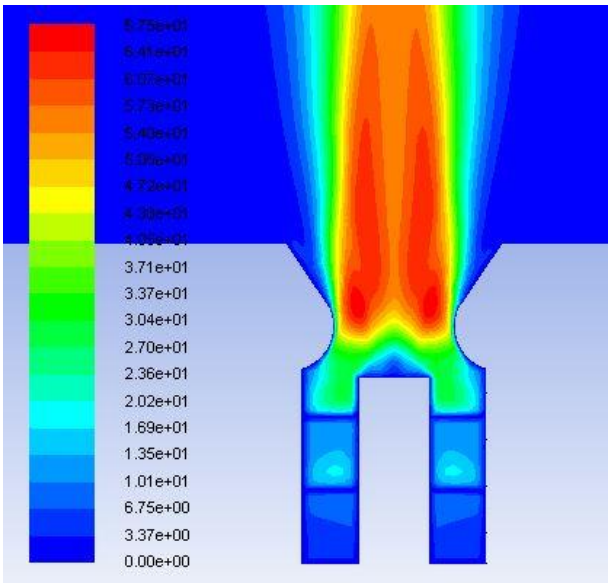

Fig. 7 Velocity distribution at a cross section for Methane, ED model

Similar phenomena were also observed in the cases of the calculations for the other fuel composition listed in Table 1.

For more detailed analysis an additional computational calculation were done. To perform those calculations, Ansys CFX version 13.0 software was used. More detailed data about used combustion models are described in [1]. However, the most significant assumptions used in those calculations is:

– combustion model: Eddy Dissipation
– combustion mechanism: methane air WD1 NO PDF
– mesh type:
  - tetrahedra on swirler and nozzle
  - hexaherda in the main chamber

In figures 8 and 9 are presented the results of Ansys CFX calculation.

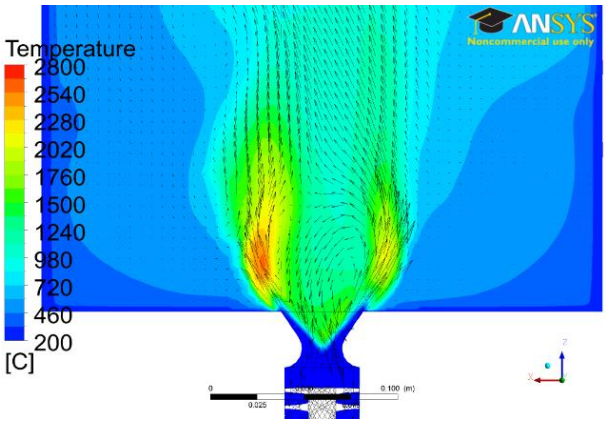

Fig. 8 Temperature distribution for NNNG 1

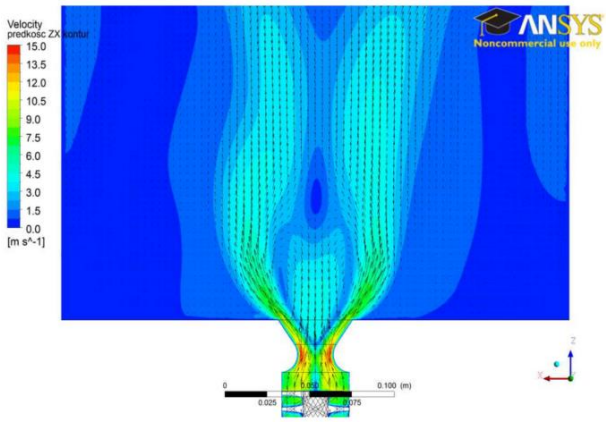

Fig. 9 Velocity distribution for NNNG 1

In these figures, the inner recirculation zone is clearly visible. It should be noted also the asymmetry of the flow, which results from the use of inferior quality mesh. However the nature of the flow is much closer to reality than presented in the figures 4 and 6. An example of velocity measurement in the combustion chamber is presented in Figure 10.

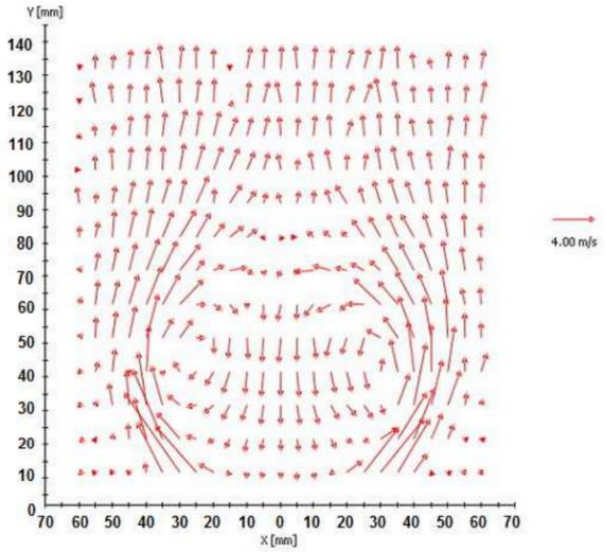

Fig. 10 Velocity distribution in the combustion chamber for NNNG 1

Velocity vectors that have been shown above, were measured using Laser Doppler Anemometer.

Results and Discussion

Despite obtaining such large differences in temperature and velocity profiles inside the combustion chamber, it did not affect the results of toxic compound emission measured in the exhaust duct.

As mentioned earlier, the main aim of this study was to present the results of calculations of emissions of nitric oxides depending on the model and the mechanism of combustion. In the case of PDF model with the GRI 3.0 mechanism it was not necessary to apply additional calculations for nitric oxide emissions. In the second case, where the ED model with Methane-Air 2 Step mechanism was used, it was necessary to use an additional model to calculate the emissions of nitric oxides. For this case the prompt and thermal (with the condition of local T-max factor equal 1.05) mechanisms of creation of nitric oxides was used. These mechanism are built into the FLUENT program. Table 2 summarizes the results of emission in the exhaust channel for the described models comparisons with experimental results, while Figure 11 shows it in graphical form.

Table 2 NO emission

	NO [ppm] measurement	NO [ppm] ED model	NO [ppm] PDF model
Methane	62	31	67
NNNG 1	43	22	57
NNNG 2	28	11	51
NNNG 3	21	9	53

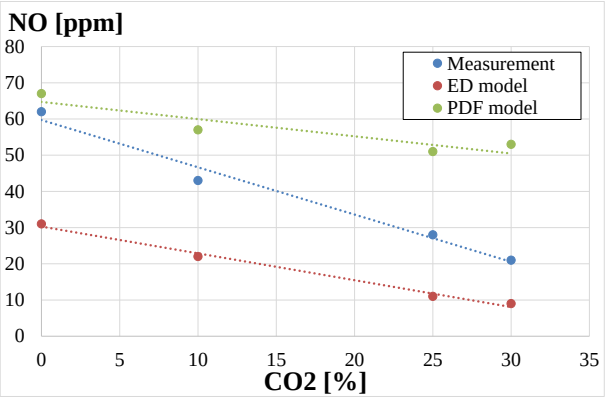

Fig. 11 Emission of NO depend on the amount of CO_2 in fuel

In the picture above it can be seen that the character of changes in emissions of nitric oxides in the exhaust duct is the same for both models and is consistent with results from experimental instigations. The nitric oxides emission decreases with increases of share of carbon dioxide in the fuel.

It should be noted, that the difference in the results of NO_X emission for different NO_X formation mechanism is significant. For the case of calculation using PDF model is almost six times bigger than for ED model. This shows a large discrepancy between the combustion models.

In the above analysis does not take into account the results of emissions of nitric oxides from the calculations performed in the ANSYS CFX 13.0. The emission in these cases exceeds the value of 20.000 ppm, which shows a large error in the calculation for adopted model.

Conclusions

The paper has presented a preliminary analysis of CFD calculations of combustion process of non-normative natural gases (NNNG). The results of investigation presents that used calculations models of combustion process do not coincide with the experimental data.

Carbon dioxide contained in the fuel has influence on the adiabatic temperature of the flame, which was calculated with Cantera [11] and was shown in [12]. The lower temperature in the combustion chamber has influence on the emission of nitric oxide.

On the quality of the numerical simulation results have a very large impact:

- the computing mesh (quantity and quality of the cells),
- used numerical program;
- adopted models and the mechanisms of combustion process.

Future work is aimed at selecting the computational model, which gives the results similar to the experimental data in terms of velocity profiles, temperature profiles and toxic compounds emissions, especially NO_X.

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