Numerical simulation of premixed methane/air and synthesis gas/air flames for turbulence swirling jet

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Abstract. This paper reports on the investigation of combustion features of turbulent swirling methane/air and synthesis gas/air flames via using modern CFD-approaches. For methane/air mixture the equivalence ratio \( \Phi \) was 0.7 which is near to the lean blow off limit. Two regimes with 1:1 and 1:2 ratios of hydrogen and carbon monoxide in the fuel mixture have been considered for synthesis gas combustion. For validation of numerical models, the reliable experimental data has been used. It is found that LES approach demonstrates good agreement with the experimental data. Comparison between methane/air and synthesis gas/air flames demonstrates that in the latter case the size of recirculation zone and the flame temperature are decreasing. But, addition of carbon monoxide in synthesis gas/air mixture leads to flame temperature rise.

1. Introduction

One of the promising technologies to increase efficiency and reduce harmful emissions from the combustion of coal fuel is intra-cycle gasification, production of synthesis gas and its combustion in a gas-turbine plant [1, 2]. The study of the combustion processes of syngas, consisting mainly of carbon monoxide and hydrogen with an admixture of compounds such as methane, CO2, H2O, etc., is of considerable scientific interest. The development of clean and efficient technologies for burning hydrocarbon fuels, based on their conversion to synthesis gas and its further combustion, requires in-depth knowledge of the chemical processes occurring in the process of syngas combustion [3]. Experimental and numerical studies that can provide a deeper understanding of the kinetics of reactions and other fundamental features of the syngas mixtures combustion are important for the development of syngas turbines and future use of systems with integrated coal gasification or biomass.

The aim of this work was numerical simulation of the flow structure and the characteristics of combustion of swirling flames of synthesis gas/air and methane/air at atmospheric pressure using modern mathematical models and verification based on detailed experimental data. Simulation of turbulent combustion is one of the most challenging task for CFD. In order to correctly predict the flow structure in highly swirled turbulent flames, the task is complicated by the need to use resource-consuming nonstationary eddy-resolving turbulent models based on large eddy simulation (LES) method.
2. Methods
The turbulent swirling methane/air and synthesis gas/air flames were investigated by using a numerical simulation (the swirl rate $S = 1.0$). For simulation of turbulent flames, the method of Large Eddy Simulation (LES) with Wall Adapting Local Eddy-viscosity model (WALE) was used. As the main model of turbulent combustion, a partially premixed combustion (progress variable approach) approach with the FGM model (flamelet generated manifold) was used. To simulate the kinetics of gas-phase reactions, various mechanisms were used (GRI-Mech 3.0 for methane/air flame and H2/CO kinetic mechanism that contains detailed mechanism of hydrogen oxidation for synthesis gas/air flame). Radiation heat transfer was performed using the method of discrete ordinates which implemented on non-orthogonal grids and it corresponds to the hydrodynamic grids. The absorption coefficient was calculated using the weighted-sum-of-gray-gases model. Based on steady RANS (Reynolds Averaged Navier-Stokes) simulation, including two-equation k-w SST, the velocity and local variances of turbulent flow in pipe before nozzle were evaluated. The results of RANS simulation were used as boundary conditions at inlet of the nozzle.

![Figure 1. Example of unstructured computational grid in the nozzle region.](image)

The unstructured grid (see Fig. 1) was used. The total number of nodes was approximately 3.5 million. Discretization of the transport equations was performed based on finite volume method. Pressure-velocity coupling for incompressible flow was achieved by the SIMPLEC procedure. For approximation of convective terms the central difference scheme was used. For approximation of convective terms of turbulence properties equations, the second-order upwind scheme was used. The diffusion terms were approximated with a second-order scheme. The implicit second-order scheme for time integration was applied. The time step was $5 \cdot 10^{-3}$ seconds (average CFL < 2). The problem was solved in a three-dimensional formulation. The calculations were performed on a computing cluster consisting of 60 high-performance cores.

3. Verification
For validation of numerical models, the results of three-dimensional simulation of swirling turbulent methane/air flame (swirl rate $S = 1.6$, Reynolds number $Re = 30000$) were compared with reliable experimental data (for more detail about experimental data see Sidney Flame Database, http://sydney.edu.au/engineering/aeromech/thermofluids/swirl.htm). The height and width of computational domain were 350 mm and 130 mm, respectively. For simulation, the unstructured grid with local refining in the regions of the near-nozzle and flame formation was used. The total grid size was approximately 1.1 million nodes. At the testing stage the large number of modern turbulence models were critically evaluated, including popular URANS approach with vortex viscosity (k-ω SST), unsteady Reynolds stresses models RSM LRR (Launder-Reece and Rodi), and LES approach with WALE. Analysis of the results of numerical simulation using various turbulence models showed...
that LES approach demonstrate the best agreement with the experimental data. So, the figure 2
demonstrated quantitative comparison between LES simulation and experimental data. One can
observe good agreement for the flame temperature, carbon dioxide, mean velocity components, and
mean and variances of the fuel concentration.

\[ T[K] \]

\[ f \]

\[ \text{rms}(f) \]

\[ \text{CO}_2 \]

\[ U_{\text{axial}} \]

\[ U_{\text{tangential}} \]

Figure 2. Comparison between experimental data and LES simulation. Profiles of mean temperature,
carbon dioxide, various velocity components, and mean and variances of the fuel concentration. The
data obtained in cross-section at the distance from the nozzle 50 mm.

4. Results and discussions
For LES simulation, the synthesis gas and methane combustion regimes were selected as a result of
simulation using the GRI-Mech 3.0 mechanism. The equivalence ratio $\Phi$ of methane/air mixture was
0.7 which is near to the lean blow off limit. In the case of combustion of synthesis gas ones were
considered two regimes with 1:1 and 1:2 ratios of hydrogen and carbon monoxide in the fuel mixture.
Wherein, the synthesis gas regimes were selected thus to the flame front propagation velocity for all
chosen combustion regimes was approximately 19 cm/s. The specification of the flame regimes
considered is presented in Table 1.

Table 1. Specification of the methane/air and synthesis gas/air flame regimes.

| Case | Air[l/min] | CH4[l/min] | CO[l/min] | H2[l/min] | $\Phi$ |
|------|------------|------------|-----------|-----------|-------|
| 1    | 52.8       | 3.86       | 0         | 0         | 0.7   |
| 2    | 52.8       | 0          | 4.89      | 4.89      | 0.445 |
| 3    | 52.8       | 0          | 7.89      | 3.94      | 0.538 |

[m/s] [K] [Mass fraction]
Spatial distributions of mean velocity, temperature, and OH obtained from LES simulation for various combustion regimes have been presented in figure 3. For quantitative comparison of presented cases, profiles of the above mean distributions at the distance from the nozzle \( y/d = 0.7 \) (corresponds to the maximum width of the recirculation zone) have been demonstrated in figure 4. For all study flame regimes, one can observe inner (around the central recirculation zone) and outer (between the -1.5 -1 -0.5 0 0.5 1 1.5 -1.5 -1 -0.5 0 0.5 1 1.5 -1.5 -1 -0.5 0 0.5 1 1.5

**Figure 3.** Spatial distribution of the mean velocity (red solid line correspond the area with negative axial velocity), temperature and OH for turbulent swirling methane/air and synthesis gas/air flames.

**Figure 4.** Profiles of mean axial velocity, temperature and OH for various turbulent swirling flames for cross-section \( y/d = 0.7 \).
annular jet core and the surrounding air) mixing layers, the expansion of the jet downstream. The flow structure looks very similar for all study combustion regimes. However, in the case of combustion of synthesis gas/air mixture (cases 2 and 3) the size of recirculation zone is less than for methane/air flame. For combustion of synthesis gas/air mixture with 1:1 ratio of hydrogen and carbon monoxide the flame temperature is approximately at 25% less than for methane/air flame. However, addition of carbon monoxide in synthesis gas mixture leads to significant increasing of flame temperature and it is comparable with the temperature of methane flame. The spatial distribution of OH shows that the hot combustion products are generally located in the inner mixing layer. Hence, for all study cases, the flame front is located only in the inner mixing layer. For combustion of synthesis gas/air mixture, the decrease of OH concentration is observed as compared with methane/air flame. As expected, the addition of carbon monoxide leads to increasing of OH concentration.

Conclusions
Combustion features of turbulent swirling methane/air and synthesis gas/air flames have been studied numerically using modern CFD-approaches. For synthesis gas, two cases have been considered with 1:1 and 1:2 ratios of hydrogen and carbon monoxide in the fuel mixture. Based on reliable experimental data (Sidney Flame Database) validation of several numerical models has been performed. LES approach with WAVE model demonstrates good agreement with the experimental data. Based on LES-simulation results, distinctions of the recirculation zones shape between methane/air and synthesis gas/air flames have been obtained. In the case of the synthesis gas combustion, both the size of recirculation zone and the flame temperature are decreasing. In the other hand, addition of carbon monoxide in synthesis gas/air mixture leads to significant increasing of flame temperature. In the latter case, the temperature of the synthesis gas/air flame is comparable with the temperature of methane/air flame.

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References
[1] Ryzhkov A F, Gordeev S I and Bogatova T F 2015 *J. Therm. Eng.* **62** 796–801
[2] Chacartegui R, Sánchez D, Muñoz de Escalona J M, Jiménez-Espadafor F, Muñoz A and Sánchez T 2012 *J. Fuel Process. Technol.* **103** 34–45
[3] Whitty K J, Zhang H R and Eddings E G 2088 *Comb. Sci. Tech.* **180** 1117–36