Numerical simulation of unsteady combustion at elevated pressure and initial temperature of the mixture for the model combustion chamber

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Abstract. The paper presents the results of investigation of combustion features of a fuel-lean methane-air swirling flame in a model combustion chamber using numerical simulation at an elevated pressure and initial temperature of the mixture. The equivalence ratio is 0.7, the initial temperatures of the mixture are 300 and 500 K, and the overpressure corresponds to 2 and 4 bars. Setting the increased pressure as the output boundary conditions in the numerical simulation of combustion in a model combustion chamber is shown to be efficient. It is found that a change in the initial temperature of the mixture from 300 to 500 K (at a fixed Reynolds number equal to 30000) leads to a significant change in the combustion regime. So, in the case of the initial temperature of the mixture equal to 300 K, the recirculation zone is formed only near the walls of the combustion chamber, and the flame has a compact shape, and is stabilized inside the premixer. With elevated initial temperatures of the mixture, a stagnation region is formed on the jet axis, and the flame displacement downstream relative to the premixer exists.

1. Introduction

Stringent environmental regulations for harmful emissions of modern gas turbines and high cost of the fuel promote the development of promising technologies that serve to achieve efficient GT-burners with low-emission. In particular, lean premixed combustion (LPC) is an effective strategy to reduce NOx emissions. [1,2]. However, the LPC has serious disadvantages, since such flames are more susceptible to thermoacoustic instabilities, which can lead to resonance effects in combustion chambers [3]. For flame stabilization the flow swirl is often used. Nevertheless, the swirling flow is characterized by the presence of centrifugal instability of the flow which occurs in cases when the intensely swirling flow enters the combustion chamber through the region of sudden expansion. With a sufficiently high swirling of the flow, a breakdown of the vortex core occurs. The vortex breakdown is related to the formation of a recirculation zone and often leads to an instability and dramatically intensifies local mixing [4]. Nevertheless, the role of the precessing vortex core in the flame stabilization during the combustion of a swirling flow still remains insufficiently studied [5]. Numerical simulation of a turbulent flow using vortex-resolving methods with detailed chemical kinetics contributes to a better understanding of the effect of the inhomogeneity of velocity, temperature and concentration fields on flame stability and on the formation of harmful emissions. In particular, the Large-eddy simulation (LES) method is currently most often used for numerical simulation of flame stabilization in a swirling flow [6-9]. The aim of this work is to investigate the combustion of a turbulent swirling flame of a
premixed fuel-lean mixture at an elevated pressure and initial temperatures of the mixture using numerical simulation.

2. Methods
In this work, the combustion of a swirling turbulent methane-air mixture realized in a model combustion chamber is numerically simulated. Figure 1a shows the 3D geometry of the GT-burner. The model gas turbine combustor includes an annular preliminary chamber, premixer mounted in the plenum chamber (similar to that in [10]), a combustion chamber with a cooled confuser and an outlet nozzle. Air is supplied directly into the premixer and fuel is supplied through a central channel with a diameter of 5.8 mm. The mixing of fuel and air is performed directly in the combustion chamber. The equivalence ratio is 0.7. The swirler outlet diameter is 37 mm and the combustion chamber width is 180 mm. Figure 1b shows a photograph of a swirling flame during the combustion of a fuel-lean mixture in a combustion chamber of similar geometry designed and put into operation at the IT SB RAS.

Figure 1. 3D geometry of the combustion chamber (a), photograph of the flame (b), example of the computational domain (c).

Figure 2. The difference in the computational grid aimed at reaching the elevated pressure in the combustion chamber. Implementing the effect of the critical flow (a) and setting the elevated pressure as the boundary condition at the outlet (b).
Figure 1c shows the 3D geometry of the computational domain. The height of the computational domain is 400 mm, the width is 320 mm. The computations are carried out using unstructured grids. The total number of nodes in the computational grid is about 12 million. Two different approaches are used to reach elevated pressure in the model combustion chamber. In the first case, the outlet nozzle of the combustion chamber has a diameter of 8 mm, and as a result of the implementation of the effect of the critical flow in the combustion chamber, elevated pressure is provided. In the second case, the outlet diameter is 32.5 mm, but the elevated pressure is set as the boundary condition at the outlet from the combustion chamber. An example of computational grids for the first and second cases in a central cross-section of the combustion chamber is shown in Figure 2.

For simulation of turbulent flames, the large eddy simulation (LES) approach with Wall Adapting Local Eddy-viscosity model (WALE) is used. A progress variable approach with the FGM model (flamelet generated manifold) and GRI-Mech 3.0 mechanism is used as a model of turbulent combustion and to simulate the kinetics of gas-phase reactions. The simulation of radiation heat transfer is carried out using a discrete ordinate model, and the absorption coefficient is calculated using the weighted-sum-of-gray-gases model. The convective terms of the transport equations are approximated by a second-order upwind scheme. As a scheme for approximating convective terms of the Navier–Stokes equations in the LES method, a central difference scheme is used. Nonstationary derivatives are approximated by an implicit second-order scheme. The time step satisfies the condition keeping the premixer exit average CFL < 2 (Courant–Friedrichs–Lewy condition). The mass flow rate of air and fuel is set according to Table 1. The Reynolds number was fixed at a value of 30 000.

Table 1. Experimental parameters for combustion regimes. \( Q_{\text{air}} \) and \( Q_{\text{fuel}} \) denote the flow rate of air and fuel, respectively. \( T \) denotes the initial temperatures of the mixture.

| \( Q_{\text{air}} \) [g/s] | \( Q_{\text{fuel}} \) [g/s] | \( T \) [K] | \( \text{Re}_{\text{air}} \) |
|-------------------|-------------------|---------|-------------------|
| 16.1209           | 0.654674          | 300     | 30000             |
| 23.640371         | 0.960041          | 500     | 30000             |

3. Results and discussion

Using non-stationary numerical simulation, the features of combustion of fuel-lean premixed flame at an elevated pressure and initial temperatures of the mixture in a model combustion chamber are investigated.

Figure 3. Spatial distribution of the average radial (a) and axial (b) velocity components and temperature (c) in the case of implementation of the effect of the critical flow in a model combustion chamber for the combustion of a fuel-lean methane-air flame.
In the case when the elevated pressure in the combustion chamber is due to the implementation of the critical flow effect (the diameter of the outlet nozzle of 8 mm), it can be observed that the air flow corresponds to a swirling annular jet released from the premixer and mixed with the fuel supplied from the central channel. It is also possible to observe the recirculation zone at the jet axis and near the walls of the combustion chamber (see Figures 3a and 3b). The distribution of the temperature field visually corresponds to the lifted flame, stabilized at some distance downstream from the swirler (see Figure 3c). However, the flame photograph in Figure 1b shows that it has a more compact shape and is stabilized inside the premixer. Probably, the numerical simulation error is caused by a large difference in velocity in the area near the premixer exit and in the outlet nozzle. For both the radial and axial components, the difference is approximately 50 times. In this regard, in the area of the outlet nozzle, the CFL magnitude is 65, which leads to incorrect results of numerical simulation. Reducing the time step between iterations or the size of the computational grid cell in the area of the outlet nozzle assumes to be irrational due to a significant increase in the time necessary for numerical simulation.

Figure 4. Spatial distribution of the average radial (a) and axial (b) velocity components and temperature (c) in a model combustion chamber for the combustion of a fuel-lean methane-air flame. The initial temperature of the mixture is 300 K and the overpressure is 2 bars.

Figure 5. Spatial distribution of the average radial (a) and axial (b) velocity components and temperature (c) in a model combustion chamber for the combustion of a fuel-lean methane-air flame. The initial temperature of the mixture is 500 K and the overpressure is 2 bars.
In the case of setting an overpressure of 2 bars as the boundary condition at the outlet from the combustion chamber and increasing the diameter of the outlet nozzle, changes are observed both in the flow pattern and in the distribution of the temperature field (see Figure 4). Thus, in the presented fields of average velocity, one can observe a decrease in the absolute magnitude of the velocity and the jet opening angle. Moreover, the recirculation flow is observed only near the walls of the combustion chamber. The temperature field becomes more compact and one can see that the flame is stabilized inside the premixer, which is in good agreement with the photograph of the flame shown in Figure 1b.

To investigate the effect of the elevated initial temperatures of the mixture on combustion processes, the temperature of the mixture is increased by 200 degrees. At the same time, to keep the magnitude of the Reynolds number, the mass flow rates of air and fuel are changed. The results of numerical simulation of combustion with the elevated initial temperatures of the mixture and a fixed overpressure at the exit from the combustion chamber equal to 2 bars are shown in Figure 5. One can observe a significant change in the flow pattern, the occurrence of a stagnation zone on the jet axis, an increase in the combustion zone, and a displacement of the flame downstream relative to the premixer exit. At the same time, the magnitude of the velocity at the exit from the combustion chamber remain within reasonable limits in comparison with the velocity of the fuel jet near the central channel. However, an increase in the mass flow rate of air and fuel in real conditions with a permanent diameter of the outlet must necessarily lead to an increase in pressure in the combustion chamber. Figure 6 shows the numerical simulation results at the elevated initial temperatures of the mixture of 500 K and with a fixed overpressure at the exit from the combustion chamber equal to 4 bars. At the same time, significant changes in the flow pattern and the temperature field distribution are not observed. The absolute magnitude of velocity decreases, the flame becomes more compact and displacement nearer to the exit at the premixer.

Figure 6. Spatial distribution of the average radial (a) and axial (b) velocity components and temperature (c) in a model combustion chamber for the combustion of a fuel-lean methane-air flame. The initial temperatures of the mixtures is 500 K and the overpressure is 4 bar.

Conclusions
In this work, the combustion of a turbulent swirling flame of a premixed fuel-lean mixture at an elevated pressure and initial temperatures of the mixture has been investigated by using the modern methods of numerical simulation. The combustion chamber has been designed for the elevated pressure to be realized through the implementation of the effect of the critical flow. It is found that the numerical simulation of combustion processes in the combustion chamber in this formulation is incorrect or ineffective, due to the significant difference in the local velocity magnitude in the area near the swirler and at the exit from the combustion chamber. Good results are shown by the approach in which the
diameter of the combustion chamber outlet is significantly increased, while the elevated pressure is set as the boundary conditions at the outlet from the combustion chamber. As a result, during the combustion of a fuel-lean methane-air flame without the elevated initial temperatures of the mixture and with fixed overpressure of 2 bars, a quite compact flame is realized, and the recirculation zone is present only near the walls of the combustion chamber. It is found that elevated initial temperatures of the mixture (at a fixed value of the Reynolds number) lead to a significant change in the flame shape and flow structure. One can observe a significant change in the flow pattern, the occurrence of a stagnation zone on the jet axis, an increase in the combustion zone, and a shift of the flame downstream relative to the premixer. A stagnation region is formed on the jet axis and the flame is displaced downstream. An increase in the pressure at the outlet of the combustion chamber to 4 bar does significantly change the combustion regime.

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