Large-eddy simulation of flow structure after a bluff-body flameholder with different chemical kinetics mechanisms

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Abstract. The majority of modern power generating systems operates on a principle of fuel combustion in turbulent flow. A design and a final adjustment of that kind of products often involve use of methods of computational fluid dynamics. In the last decades, large eddy simulation (LES) proved its efficiency in a solution of turbulent flows' simulation problems. That method is more versatile in comparison with RANS and requires less computing resources and time than direct numerical simulation method. The process of combustion, in a case of an implementation of methods of computational fluid dynamics, can be described using global oxidation reactions of fuel, as well as with a use of detailed kinetic mechanisms. In the presented study, results of calculations of flow after flameholder in a case of an implementation of LESmethod with kinetic mechanisms of chemical reactions of varied number of reactions are presented and analyzed. At the first stage, a calculation of flow without combustion was conducted, a sub-grid viscosity model is selected, which most accurately describes flow characteristics, such as axial velocity and gas flow through a recirculation zone. Further, combustion of pre-prepared mixture of a stoichiometric composition was simulated, using a one-, two- and multiple-step kinetic mechanisms of chemical reactions. Results showed that in a case of an implementation of one- and two-step mechanisms flame flashback is appearing, which was not registered during experimental studies. At the final stage a capability to predict lean blow-out of flame was studied. It is shown, that one and two step reaction mechanisms predict lean blow-out of flame in a case of an equivalent ratio leaner, then it was obtained during the experiment. The value of an equivalent ratio of lean blow-out of flame in a case of multi-step mechanism use proved to be much closer to the experimental value.
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Introduction

Combustion process in gas flow in a real conditions occurs through thousands of different chemical reactions with hundreds of chemical components involved . At the same time, in a case of industrial products, a situation is complicated by a presence of turbulence. One of the most realistic approaches for a combustion simulation in turbulent flow is a direct numerical simulation (DNS). Direct numerical simulation is carried out in order to understand fundamental aspects of combustion processes (e.g. autoignition, flame stabilization mechanisms, diffusion in a case of combustion) and depending on a task, which was set, it is using kinetic mechanisms for varying number of reactions [1]: from single-step [2] to detailed [3-6].

Direct numerical simulation of combustion in turbulent flow is very difficult even with an application of modern supercomputing technology and, generally, is carried out for low Reynolds numbers and simple fuels. Thus, for example, in the studies [7, 8] combustion of hydrogen with detailed kinetic mechanisms was simulated. Although a number of reactions in them doesn't exceed 21 and a number of components is 9 [9], when Reynolds number is not more than 10000, total calculation time was about 29 million processor hours [7].

Another approach to a simulation of turbulent flows is method of large eddy simulation (LES). In terms of universality and requirements to computational and time resources, that approach lies between direct numerical simulation (DNS), in which all spatio-temporal scales of turbulence are solved, and a solution of Reynolds-averaged Navier–Stokes equations (RANS). LES is based on a mathematical separation of flow on large-eddy and small-eddy motion using a filtering procedure. An influence of small-eddy motion is described by an approximate, so-called sub-grid, models. A local size of grid element, generally, serves as a filter. Advantages of LES are a possibility to obtain parameters of average flow, as well as spectral characteristics, spatial and time scales of turbulence. At the same time, it is necessary to ensure that filter size and the time step will allow to solve largest eddy structures, which are outside of inertial interval of turbulence kinetic energy spectrum [10]. For a developed turbulent flow of a cross-section, that area is described by Kolmogorov-Obuhov law (law of “5/3”) [11]:

$$E(k) = C_k \varepsilon^{2/3} k^{-5/3},$$

where E – energy spectrum, C_k =1.5 – Kolmogorov constant, k – turbulence kinetic energy, ε – dissipation velocity of turbulence kinetic energy.

Poinsot and Veynante [12] underlined superiority of LES for combustion processes simulation in industrial application, in comparison with RANS (universality and accuracy) and DNS (requirements for computing resources) approaches.

In a case of direct numerical simulation of combustion processes chemical kinetics, generally, is calculated using Arrhenius equations. In a case of LES, tabulated chemistry is often used [13-16]. However, that approach has some limitations: for example, the use of tabulated chemistry is impossible, if it is necessary to simulate combustion of several different fuels or oxidants [17]. Modeling of combustion in terms of LES is carried out using special sub-grid models, because combustion process itself usually occurs at scales smaller than a grid size.

The purpose of the presented paper is to study a possibility of LES application for a calculation of combustion processes of pre-prepared mixtures without an implementation of sub-grid combustion models. In order to do that, a comparison of combustion's calculation results in LES statement using kinetic mechanisms varying number of reactions was conducted.

Materials and methods

As a subject of the study a bluff-body was selected, with a shape of regular triangular prism and base length h = 25 mm, which was set in a channel of square cross-section 50×50 mm. Velocity of incident flow was 10 m/s, velocity profile is uniform. Turbulence intensity at an inlet – 2 %.The scheme of the experimental area is presented in figure 1. The source data and the results of the experimental measurements are taken from the paper [18]. In the calculation length of channel before stabilizer is equal 4h and down the stream from stabilizer –10h.

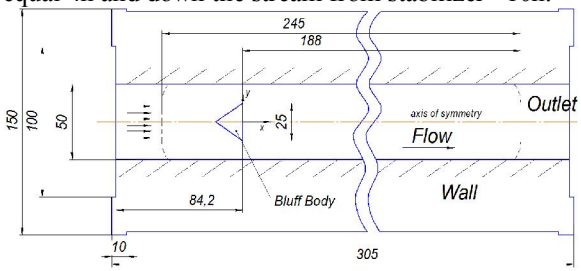


Fig. 1. Scheme of the experimental area

The calculation was carried out in three-dimensional nonstationary statement in ANSYS Fluent 14.5 software package [19]. In order to create a block-structured finite-element grid geometric model of the calculated area was divided into 7 blocks (fig. 2).

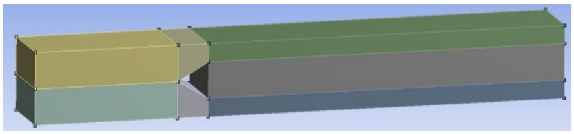


Fig. 2. Geometric model of the calculated area

The calculation in LES statement was conducted on a grid of 3.69 million. With time step 0.1 ms.

In the beginning, the calculation without combustion was conducted in order to analyze quality of a grid and select sub-grid viscosity model.

At the next stage, a study of a combustion of pre-prepared propane-air mixture with equivalent ratio φ=1 was conducted. The calculation of gaseous fuel combustion process was described using a model of finite rate of chemical reactions, which presumes using Arrhenius equation without taking into account sub-grid transfer. In the presented study, three kinetic mechanism of chemical reactions were used: two of them are realized in ANSYS Fluent 14.5 (global reaction and two-step mechanism) and reduced kinetic mechanism, proposed in the paper [20], which contains 17 components and 28 reactions.

For the single-step global reaction of propane oxidation was used:

$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O \qquad \text{(R1)}$$

For two-step mechanism following reactions were used:

$$2C_3H_8 + 7O_2 \rightarrow 6CO + 8H_2O, \qquad \text{(R2)}$$

$$2CO + O_2 \rightarrow 2CO_2, \qquad \text{(R3)}$$

$$2CO_2 \rightarrow 2CO + O_2. \qquad \text{(R4)}$$

Velocity of conversion component i in reaction $\hat{R}_{i,r}$was described by the equation:

$$\hat{R}_{i,r} = \Gamma(\nu''_{i,r} - \nu'_{i,r})(k_{f,r}\prod_{j=1}^{N}[C_{j,r}]^{(\eta'_{j,r}+\eta''_{j,r})}),$$

where $\nu'_{i,r}$, $\nu''_{i,r}$ – stoichiometric coefficients for reagents and products of reaction r, respectively;

$k_{f,r}$ – constant for a forward reaction, described by Arrhenius equation;

N – number of chemical components in the current element;

$C_{j,r}$ – molar concentration of a component j in a reaction r;

$\eta'_{j,r}$ – factor of exponent (degree) for an ingredient j in a reaction r;

$\eta''_{j,r}$ – factor of exponent (degree) for a product j in a reaction r.

Constant of forward reaction $k_{f,r}$ is defined as: $k_{f,r} = AT^{\beta}e^{-\frac{E}{RT}}$

where A, β – parameters of preexponential multiplier;

T – temperature;
E – activation energy;
R – universal gas constant.

Parameters of reactions are presented in table 1.

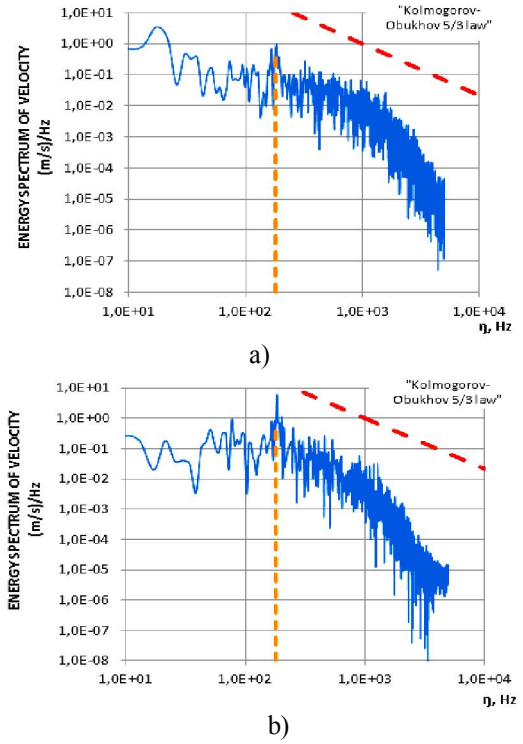
Table 1. Parameters of reactions

Reaction	$\eta'_{1,r}$	$\eta'_{2,r}$	$\eta''_{1,r}$	$\eta''_{2,r}$	A $(kmol/m^3)^{1-n}s^{-1}$	E (j/kgmol)	β
(R1)	0.1	1.65	0	0	4.836e+09	1.256e+08	0
(R2)	0.1	1.65	0	0	5.62e+09	1.256e+08	0
(R3)	1	0.25	0	–	2.239e+12	1.7e+08	0
(R4)	1	–	0	0	5e+08	1.7e+08	0

A calculation was conducted using cluster "Sergey Korolev" [21] with an implementation of 512 computaional processors.

Results and discussion

Figure 3 shows results of Fourier transformation for magnitude flow velocity, which was obtained as a result of a calculation of nonreacting flow using dynamic sub-grid model of Smagorinsky-Lilly [22]. A change in velocity with time was registered from two points with following coordinates: #1 x_1=1h, y_1=0.5h; #2 x_2=3h, y_2=0.5h. The graph shows that, for both points there is an area, which corresponds to the law "5/3" of Kolmogorov-Obuhov. Also, a marked peak was discovered at a frequency around 170-190 Hz, which corresponds to experimental data [18].



a)

b)

Fig. 3. The results of fast Fourier transformation for velocity in two points a) point #1, b) point #2

For a selection of sub-grid viscosity model, calculations using the following models were carried out: dynamical model of Smagorinsky-Lilly (SL) [22], Wall-Adapted-Local-Eddy (WALE) [23] и Wall-Modeled (WM) [24]. In figure 4 graphs for changes of axial velocity V_x along central line of the model (x-axis) and air flow rate in the recirculation zone along its length, where G_{RZ} – flow rate through a zone of inverse flows (RZ), G_{air} – air flow rate at an entry in an estimated area, L_{RZ} – length of RZ.

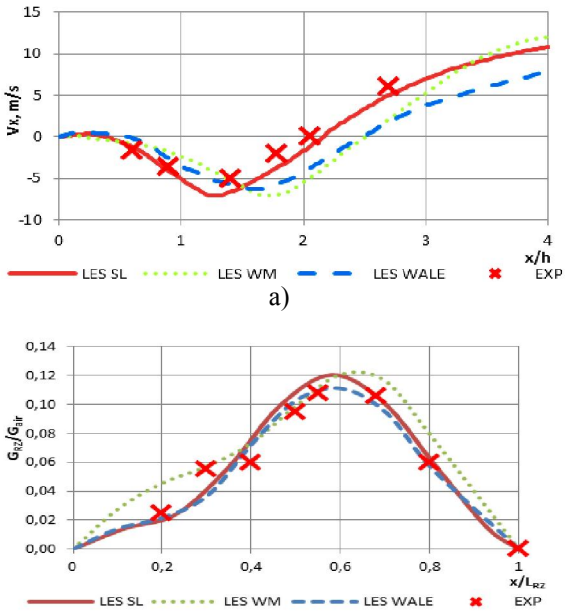


Fig. 4. Axial flow rate along a central line (a) and air flow rate in the recirculation zone (b)

The presented data shows, that all used models give similar results and adequately reflect averaged in time flow characteristics. However, results, that are the closest to the experimental data, were showed by dynamic model of Smagorinsky-Lilly, which was selected for further calculations.

For a calculation of combustion processes the following algorithm was used. In the beginning, a calculation of flow of pre-prepared mixture without fuel combustion with an equivalent ratio φ=1 was conducted. Then, after flame stabilizer, flow temperature locally increased above the values necessary for ignition (1500 K). Then, a calculation was conducted over time period, which is equal to $3t_{ВП}$, where $t_{ВП}$ – characteristic time. According to recommendations [25] the characteristic time is defined as:

$$t_{ВП} = \frac{V}{Q},$$

where V – volume of calculated area, Q – volume flow rate at an inlet.

In figure 5 fields of instant temperature and velocity of heat generation (which are characterizing a position of flame) in a case of an implementation of various kinetic mechanisms in calculations are presented.

In a case of the one-step mechanism use, a flame flashback along the solid walls of the model is occurring. At the same time, flame front extends from walls to flow's axis. After the stabilizer flame front is virtually non-existent. In a case of the two-step mechanism a flame flashback also takes place along boundary layer, however, flame doesn't spread to a channel's axis. And finally, in a case of the multi-step mechanism use a flame flashback is not observed, the entire process of combustion occurs after flame stabilizer. Front flame is deformed by large eddy structures. At that, it is more stretched, in it a smooth increase of temperature is observed , and, then, temperature is increasing sharply. There are also local breaks in flame front. Structure of temperature field in a case of a calculation using the two-step and multistep mechanisms are similar, especially in a near wake after a stabilizer (zone of inverse currents).

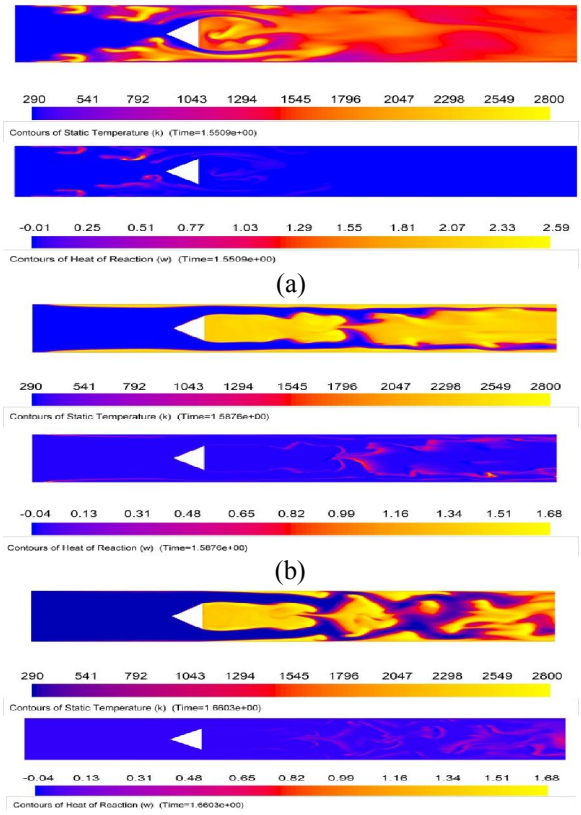


Fig. 5. Instant temperature of flow and velocity of heat generation in a case of an implementation of 1 step mechanism (a), 2 step mechanism (b) and multistep mechanism (c)

In order to determine boundaries of lean blow-out of flame the following algorithm was used. After a calculation of combustion processes with φ=1 at an entry in a calculated area, equivalent ratio decreases incrementally. For a determination of lean blow-out of flame, on each time step average mass temperature of flow in cross-section at a distance of x=2h was registered.

A change in temperature over time in a cross-section x=2h during a calculation using global reaction is presented in figure 6a. From the graph it is clear that lean blow-out of flame occurs when φ=0.38-0.4; the experimental value is φ=0.52 [18]. The results of a calculation of lean blow-out of flame in a case of two-step mechanism implementation showed similar results (fig. 6b).

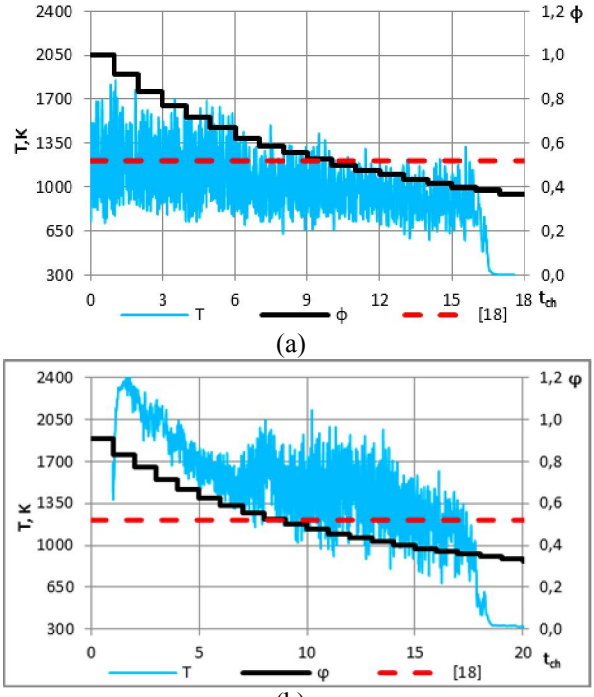


Fig. 6. Temperature of the cross-section x=2h in a case of calculation using 1 step mechanism (a) and 2 step mechanism (b)

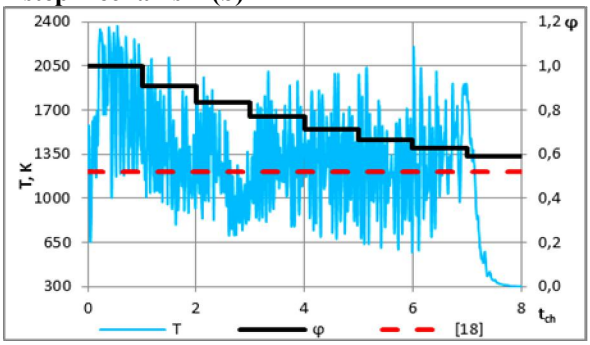


Fig. 7. A change in temperature during a calculation using a reduced kinetic scheme [18]

A change in temperature over time in the cross-section x=2h during a calculation using kinetic mechanism, proposed in the paper [20] is presented in figure 7. In that case, flame extinction in the cross-section x=2h occurs with φ=0.61. However, that value is higher than the experimental one. Perhaps, this is related with an insufficient mesh resolution, then, as a result front surface of laminar flame appeared to be less than in reality, as a consequence, turbulent velocity of flame's spreading is underestimated. The solution of that problem might lie in an implementation of models of thicken flame front [26], for which in a calculation of thickness of flame front and velocity of its spreading, grid resolution or a use of special procedures for sub-grid simulation is taken into consideration [12].

Generally, since in a case of implementation of the one- and two-step mechanisms, lean blow-out of flame occurs with a leaner φ and with the multi-stage mechanism with a richer φ, then was obtained during the experiment, it can be stated that chemical kinetic mechanism makes a decisive contribution in a simulation of lean blow-out of flame, even without use of sub-grid combustion models.

CONCLUSION

The presented study indicates that the combustion model, based on global reaction, overstates reactivity during combustion. During a simulation of a combustion of pre-prepared mixtures that can lead to a flame flashback, which is not observed during full-scale experiments. For an adequate simulation of combustion processes it is necessary to use multistep mechanisms of chemical reactions that are configured for a description of main features of the combustion process (delay time of ignition, normal velocity of flame spreading, equilibrium temperature of combustion products) under the specific conditions.

LES showed good agreement with experimental data on a distribution of velocity along the central line and air flow rate through recirculation zone. Also, a possibility in principle for a study of lean blow-out of flame phenomenon with a specified law of φ change as a function of time.

Also, it is established that in near blow-out regime, flame stabilization is determined by a behavior of large-scale vortical structures: their time of existence in a near wake after a stabilizer, a frequency of a decent from edges and an interaction between them.

Further development of the presented study may lie in an investigation of combustion processes with defined properties of a reaction mechanism (ignition delay time, normal velocity of flame spreading, equilibrium temperature of combustion products), as well as an influence of various models of sub-grid combustion. Additionally it is necessary to consider a problem of an influence of grid resolution on results of a calculation.

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