Numerical simulation of hemispherical hydrogen–air flame propagation with heat losses

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Abstract. The article presents numerical simulation of the propagation of hydrogen–air flame in adiabatic conditions and with the heat absorption on the wall. The results of experiments in a cylindrical shell of 4.5 m\textsuperscript{3} are compared with the results of numerical simulation. The quantitative agreement between the experimental and numerical results is achieved. It is shown that the numerical model of the combustion with the heat losses under the conditions of the experiment may account the heat losses as an integral effect of the heat absorption.

1. Introduction

The problem of propagation and acceleration of flames in gas mixtures is interesting both for fundamental science in connection with the complex nature of the interaction of chemistry, thermodynamics and hydrodynamics of the process, and for applied science in the field of energy burning and safety. Creation of internal combustion engines and pulsating detonation devices is associated with the problem of initiation and development of combustion [1,2]. In pulsating detonation devices, it is required to accelerate the flame and form a detonation wave in a short section; in internal combustion engines, it is necessary to ensure the combustion speed within certain limits. Exceeding this speed leads to excessive loads and destruction of the engine. Low combustion rate reduces fuel combustion efficiency and efficiency. In tasks related to the safety of [3], the maximum reduction in the flame speed is required to reduce pressure loads and complete the operation of fire extinguishing systems.

The smooth flame front in gas mixtures is unstable. The acceleration of the gas flame front at the initial stage after initiation is caused by the curvature of its front [4] and the hydrodynamic stretching of the flame [5]. The flame front curvature is caused by its thermodiffusion [6] and hydrodynamic [7,8] instability. The increase in the density of the flame surface [9] is a necessary condition for the acceleration of the front. Hydrodynamic stretching is caused by the presence of walls that change the direction of the gas flow. When approaching the flame front to the wall of a volume having a gas flow parallel to the flame front. These flows increase the surface of the flame and the flow rate of the combustible mixture along the walls.
The increase in the density of the flame front surface and the hydrodynamic stretching of the flame increase with the degree of expansion of the gas during combustion [10]. The degree of expansion is calculated as the ratio of the density of the fuel mixture to the density of the combustion products and depends solely on the thermodynamic characteristics of the combustion process. The second important characteristic of the flame front, which determines its instability and the speed of the combustible mixture in front of it, is the normal speed of the flame. It is determined by the chemical kinetics of the combustion process and the removal of heat from the volume of combustion products affects it slightly. Thus, it can be assumed that the heat loss on the walls of the volume in which combustion occurs, have an impact on the flame propagation through the thermodynamics of the process.

A number of codes and models are being developed to describe the different combustion modes and the corresponding level of explosive loads. The situation with turbulent deflagration [11] is more complicated. Our current level of understanding and computer capabilities do not allow us to model turbulent combustion from the first principles. Simplified models are used to describe both turbulence and chemistry. These models typically include several empirical constants that should be adjusted when compared with experimental results. Current computer codes are able to reproduce some details of experiments on turbulent deflagration, however, the accuracy of these calculations is still a matter of doubt. In addition, calculations with existing models of turbulent combustion are resource-intensive. The computer code CREBCOM (CRiteria and Experimentally Based COMbustion) was developed to describe flame propagation and explosive loads. There are several codes and models, which include modeling of heat loss, but most of them are designed and adapted for the simulation of internal combustion engine [12, 13]. The modified CREBCOM code was the first code to use a heat loss model to model combustion in large volumes.

The influence of heat loss in the walls of [2] and non-diffusion heat transfer in the volume of reagents [14] has already been discussed in the literature. This work is devoted to the study of the flame acceleration in the hydrogen–air mixture with intense heat absorption of one of the walls of the volume. In addition to the fundamental importance of the task is the application in the field of fire and explosion safety of petrochemical facilities, nuclear industry and nuclear power.

In this paper, a modified computer code CREBCOM is used to simulate experiments with high heat loss in a layer of steel wool.

2. CREBCOM code description

2.1. Description of the calculation algorithm

The computer code CREBCOM (criteria and experimentally based combustion) uses a semi-empirical approach, based on determining the characteristic modes of combustion according to their degree of danger, and applying criteria to determine the most dangerous possible modes of combustion for specific initial conditions and geometry. Next, in the code, the corresponding three-dimensional combustion model is chosen, describing the flame propagation and pressure load for the selected combustion mode: slow flames, fast flames, detonation. This approach combines a system of criteria and models of combustion in a single computer environment that allows a conservative estimate of the loads that occur during the combustion of an air–fuel mixture. In this case, the term “conservatism of calculations” assumes that the pressure value calculated in the code will be no less than that obtained in a real experiment or emergency situation. The CREBCOM code system was verified in detail to calculate all possible combustion regimes in the hydrogen–air mixtures [15].

The code B0B [15], used in the calculations of experiments with steel wool, is part of the CREBCOM code system and is used to simulate slow and fast burning processes. The burning model used in the code is quite simple: it assumes that the burning rate depends only on the
properties of the mixture and does not take into account all aspects of the complex interaction between hydrodynamics and the rate of energy release in the combustion process.

Figure 1. Experimental $R$–$t$-diagrams.

The numerical scheme of the B0B code uses a three-dimensional explicit first-order scheme with differences in flux. Verification of the hydrodynamic part of the code on analytical problems and experimental data showed its high accuracy and efficiency. At the same time, large numerical diffusion, a well-known deficiency of first-order schemes, does not play a special role due to the combustion model used in the code.

The code uses a simplified thermodynamic model in which the equation of state of an ideal gas is applied to gas mixtures with constant heat capacities. For thermodynamic calculations, the CHEMKIN-II [16] package is used.

The combustion model used in the B0B code assumes that the burning rate in each cell is constant and ignition occurs in the next cell when the reagent gas in the neighboring cell burned to a certain value $e$, which is indicated explicitly. Other words, $e$ is the ratio of burned gas in a cell to total amount of gas in a cell. The burning rate is defined as $\partial C/\partial t = K_0/x$, where $C$ is the mass fraction of reactants, and $K_0$ is the burning rate constant and $x$ to be the cell size.

2.2. Heat loss model

The code uses a burning model with a constant speed, which depends on the composition of the mixture, but does not change during the combustion process. Using the effective burning rate constant for a given composition of the mixture and the initial conditions, but independent of local conditions of flow, can be considered as a zero approximation of the real energy release and absorption function. The constant burning rate, together with the use of equations that ignore heat loss, leads to an overestimation of the rate of heat release and the total energy of the system. Without the heat loss model, the pressure values $p(x, y, z, t)$ are also overestimated in the calculations with the code B0B. Therefore, accounting for heat losses becomes extremely important if we want to improve the accuracy of the description of the combustion process and reduce the conservatism of calculations.
3. Experimental data

The experimental part of the study was carried out on an installation consisting of a cylindrical shell with a diameter of 1.5 m and a height of 2.4 m, made of high density polyethylene (HDPE) with a thickness of 0.1 mm bounded by a metal frame. The lower part of the structure was covered with a solid aluminum plate. For experiments with steel wool, it was covered with a layer of steel wool 50 mm thick. The installation was located inside the VBC-2 explosive pressure chamber, which is part of the Moscow Regional Explosive Collective Use Center at the Russian Academy of Sciences. The shell was filled with a hydrogen–air mixture with a hydrogen content of 15 vol% at normal atmospheric pressure at a temperature $T \approx 293$ K. The mixture was ignited by the explosion of thin nichrome wire. The energy released on the wire was 5 J. In all experiments, the distance from the ignition point to the surface was 100 mm and remained constant. A detailed description of the experimental procedure, the experimental results and analytical interpretations are reported in [17]. Experimental dependences of the flame front position versus time in cases of flame propagation along a flat aluminum wall and a layer of steel wool are shown in figure 1.
Figure 3. The position of the flame front in the horizontal and vertical directions as a function of time: the results of calculations and experiments. Red symbols are the results of calculations with high heat losses.

4. Numerical results
The calculations were performed on a grid of $100 \times 100 \times 250$ cells with cubic cells. The linear cell size was 10 mm and did not change during the counting process. The total number of cells in the calculations was 2 500 000.

Results of the numerical simulation of the experiment are shown in figures 2 and 3. Figure 2 shows the temperature and flow velocity fields at the time instant of 101.5 ms above the layer of steel wool. One can see the characteristic elongated shape of the flame, named in the papers [5,10] “finger flame”. A similar flow pattern is observed in the experiment. The $R-t$-diagram shown in figure 3 shows the position of the flame as a function of time from the moment of ignition in two directions. In the case of flame propagation with heat losses, the numerical results coincide with the experimental ones. Thus the numerical model of the combustion with the heat losses under the conditions of the experiment may account the heat losses as an integral effect of the heat absorption.

Heat loss in hot products is an integral part of the combustion process. Experimental data show that for detonation, the rate of heat loss is negligible from the rate of heat release, otherwise the detonation decays. Therefore, for most cases where detonation takes place, heat losses can be neglected. On the other hand, the problem of estimating thermal loads and pressure loads is not limited to the short period of the detonation wave. Therefore, the heat loss model can also be important for the detonation code.

Experimental data on the values of heat losses in combustion processes are almost completely absent. In experiments on combustion in pipes, the pressure measured by a manometer is always noticeably lower than the theoretical value of the pressure of complete combustion $P_{aicc}$ and quickly continues to fall. This shows that the rate of heat loss is significant, but no quantitative estimates can be made from these data. Theoretical estimates also do not provide reliable quantitative values of losses. The numerical model of heat losses should include the thermal
conductivity of the walls and, possibly, the convection and radiation term. This problem can be solved with the availability of detailed and reliable experimental data suitable for verification of the model.

The dependence of the amount of heat absorbed by a layer of steel wool on time was calculated in a two-dimensional formulation based on the experimentally obtained dependence of the flame front radius on time and the calculated thermal conductivity of steel wool. More details about the method for the calculating heat absorption are presented in [18].

5. Conclusions

Numerical simulation using the CREBCOM code shows that the calculations are consistent with experimental results.

The numerical model of the combustion with the heat losses under the conditions of the experiment may account the heat losses as an integral effect of the heat absorption.

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