Flame acceleration and transition to detonation in acetylene-based mixtures

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1 Introduction

Despite the general trend towards decarbonization and tightening of requirements for the emissions from the energy and propulsion systems, hydrocarbon fuels remain the main source of energy for a wide range of industries. At the same time, more efficient combustion of hydrocarbons, environmental friendliness and safety can be achieved by developing new combined fuels and organizing combustion modes that provide high combustion efficiency, intensive energy release and low emission of carbon oxides. Among the variety of hydrocarbon compounds, acetylene deserves special attention. It finds applications in many areas from gas welding and metal cutting to fuelling of rocket engines. An important feature of this hydrocarbon is the ability to maintain the combustion process in a wide range of mixture compositions and thermodynamic conditions of the system. The addition of acetylene to the fuel-air mixture improves the combustion stability [1], which is a key step towards the organization of efficient combustion modes for gaseous fuels and the reduction of associated harmful emissions. Also, acetylene can act as an alternative to traditional fuels in internal combustion engines [2]. At the same time, its use is associated with high risks of developing abnormal combustion modes, including detonation, which can damage the chemical reactor and create a threat of emergency situations accompanied by large-scale destruction and causalities [3–5]. This motivates further research in the field of non-stationary combustion of gas mixtures based on acetylene, including flame acceleration, and the transition from deflagration to detonation. An efficient approach to the study of such high-intensity processes is a combination of natural experiment and computational analysis.

To date, a fairly representative experimental base has been accumulated on the problem of the transition from deflagration to detonation in gas mixtures based on acetylene [6–8], while the bulk of the computational and theoretical work on this issue was carried out using simplified models of a single-step [9] or reduced [10] chemical kinetics. Numerical calculations of unsteady combustion processes, including flame acceleration and transition to detonation [11], require a careful choice of a computational approach and chemical kinetic model describing the transformation of the fresh mixture into combustion products. In particular, it is known that the use of single-step mechanisms of chemical kinetics

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can lead to controversial results on the flame acceleration modes and the mechanisms of transition to detonation in gas mixtures [12, 13]. The choice of computational approach is no less important. In [14] several contemporary and traditional numerical schemes were tested on the specially developed benchmark problems to assess the capabilities of numerical schemes to be applied for transient combustion analysis. Among others the non-dissipative CABARET numerical algorithm [15] was evaluated and it was shown that it can be successfully used for the detailed simulation of non-stationary combustion processes. Present paper is devoted to the numerical analysis of the flame acceleration process in channels filled with acetylene-based mixtures with the use of CABARET numerical scheme and reduced chemical kinetic scheme proposed in [16].

2 Problem setup

Problem setup for the numerical analysis is schematically presented in Figure 1. Here semi-opened channel of 2 cm width and 100 cm length is filled with stoichiometric acetylene-oxygen mixture diluted with 25% nitrogen. Channel walls are non-slip and isothermal with wall temperature $T_{wall} = 300$ K. Mixture is ignited near the middle of the closed end of the channel in the circular area of 1 mm radius initially heated up to 1500 K. Fresh mixture is initially under pressure of 20 kPa and temperature 300 K. After the ignition flame propagates from the closed end of the channel towards the opened end of the channel.

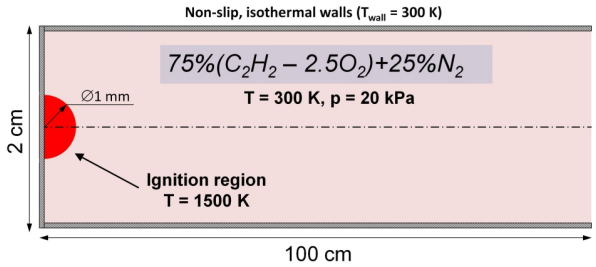

Figure 1: Schematic of the problem setup for the numerical analysis

Numerical simulation was performed via solving full system of Navier-Stokes equations with an account of compressibility, viscosity, multicomponent diffusion, thermal conductivity and chemical transformations in two-dimensional setup. Contemporary non-dissipative algorithm CABARET was employed for solving governing equations system [15]. Reduced chemical kinetics scheme consisting of 25 elementary reactions among 17 active components [16] was used to model acetylene oxidation.

Experimental facility and details of the experimental routine can be found in recent papers [8, 17]. In the experiments round tube with diameter 6 cm was used, the mixture and initial conditions were the same as in numerical setup presented above.

3 Results

Let us analyze flame acceleration process in the considered problem setup. Comparison between experimental and numerically obtained flame dynamics is presented in Figure 2a. In Figure 2b characteristic flame structures on various stages of the acceleration process are given. Flame acceleration process in acetylene-based mixtures proceeds via four characteristic stages [17, 18]. After the ignition flame expands isotropically until it reaches the side walls of the channel. Reaching the side walls, flame begins to propagate towards the opened end of the channel and one can observe exponential manner of the

flame acceleration establishes at this initial acceleration stage. Here elongated flame structure or the so-called "finger flame" is developing due to the flame interaction with the flow in the fresh mixture ahead of the flame front (see "1" in Figure 2b), which is decelerated near the side walls due to the viscosity effects [11]. After the flame moves away from the closed end of the channel the transition from the elongated flame to the "tulip flame" structure proceeds. The beginning of this transformation is accompanied by the acute reduction in flame acceleration rate, which is highlighted by the mark "1" in Figure 2a. During the transition from "finger" to "tulip" flame structure, it achieves almost planar form ("2" in Figure 2b). The deceleration of the flame in the bulk of the flow is determined by the formation of the rarefaction wave inside the combustion products area and the non-uniform flow structure due the flow viscous deceleration near the side walls of the channel. After the tulip structure is formed ("3" in Figure 2b) the secondary flame acceleration stage begins. At this stage flame elongates near the side walls of the channel due the flame-boundary layer interaction ("4" in Figure 2b) until the conditions sufficient for the detonation formation are established. From the Figure 3 one can see that flame dynamics is reproduced qualitatively with numerical simulation. Quantitative disagreement can be related to the two-dimensional setup, lower acceleration rates are obtained [11], and by the difference in channel width (2 cm height in calculations vs 6 cm diameter in experiment).

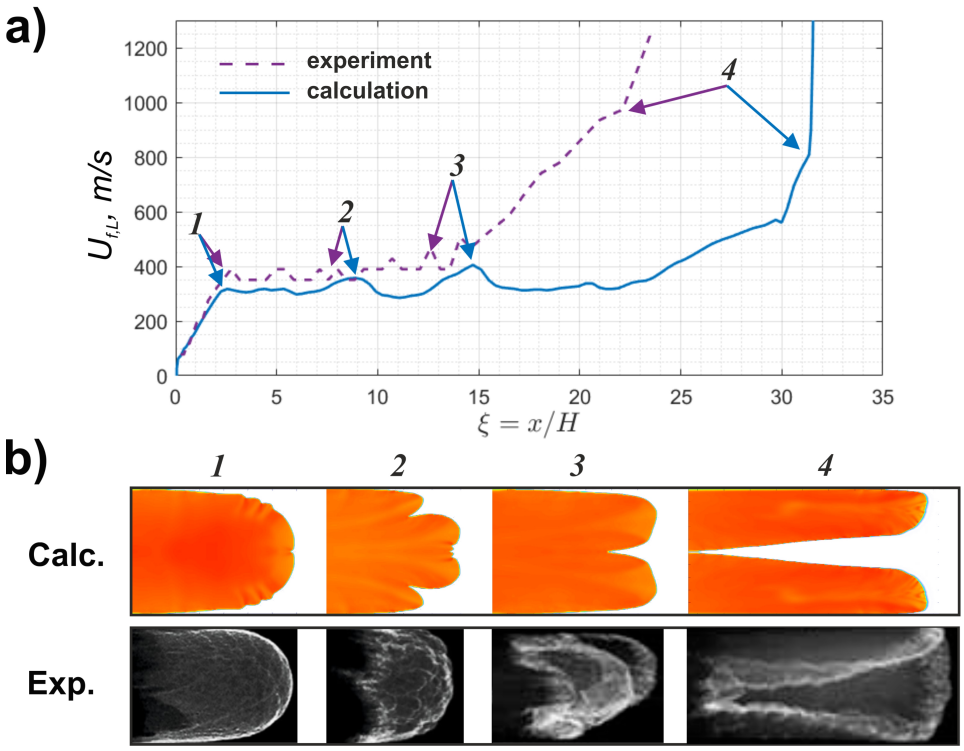

Figure 2: a) Flame front leading point velocity $U_{f,L}$ dependence on the leading point coordinate x divided by the channel height (for calculations) or radius (for experiment) H. b) Characteristic flame front structures on different stages of the flame acceleration process.

In numerical analysis deflagration to detonation transition process in the considered conditions proceeds via the mechanism of the flame choking and local compression on the scales of the reaction zone, described in detail in [19]. According to this mechanism, after the flame achieves sonic speed in combustion products, compression waves emitted by the accelerating flame become localized inside the reaction zone. That causes local compression of the gaseous mixture, which in turn can result in rise of the burning rate. This positive feedback leads to the formation of pressure peak immediately inside the reaction zone (see Figure 3a). After the pressure achieves sufficiently high values, the shock wave

is formed with the intensity high enough to initiate detonation propagation process. In Figure 3b temperature and pressure profiles across the leading point of the flame are presented. It can be noted that the pressure peak is formed and localized at the flame front and the transition-to-detonation proceeds in the vicinity of the leading point of the flame. Such a detonation formation mechanism in the considered mixture and conditions was also observed experimentally (see Figure 4).

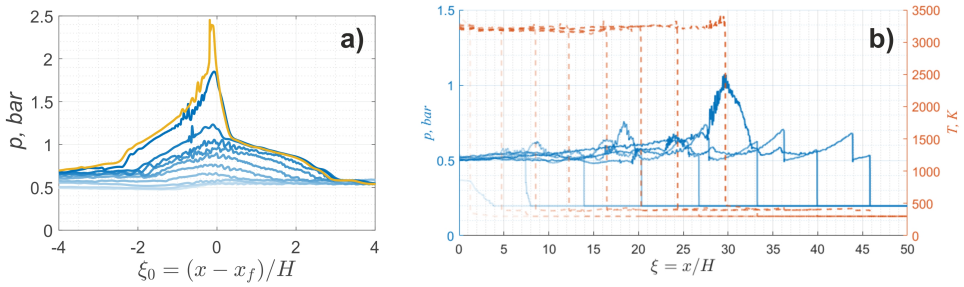

Figure 3: a) Pressure distribution near the leading point of the flame in the coordinate system associated with the leading point location x_f. b) Temperature (orange) and pressure (blue) profiles across the leading point for different time instances ($\Delta t = 200$ us).

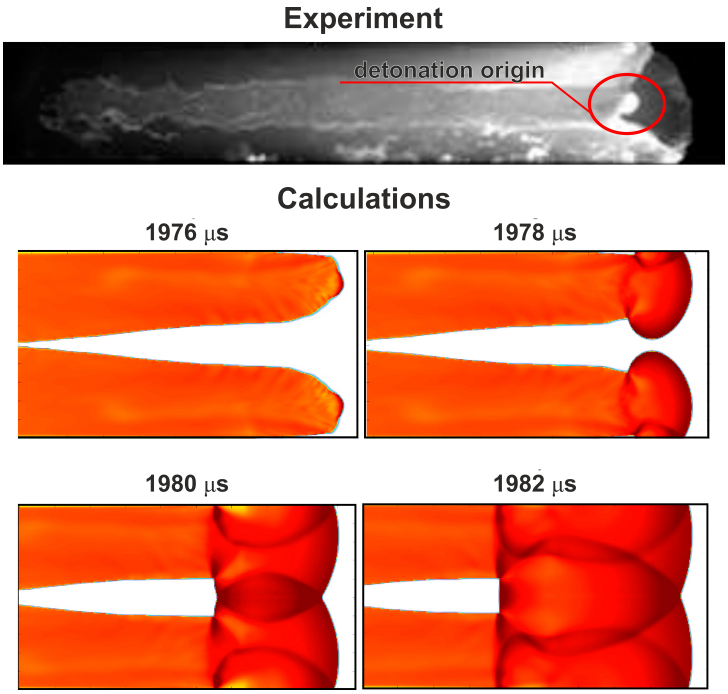

Figure 4: Transition to detonation origin and dynamics. Experiment (top) and calculations (bottom).

4 Conclusions

Flame acceleration and deflagration-to-detonation transition processes are investigated via joint numerical and experimental analysis. Novel non-dissipative computational approach CABARET and reduced chemical kinetic scheme [16] were employed to perform numerical analysis. The results of mathematical modeling agree qualitatively well with the experimental ones. Different stages of the flame acceleration are analyzed experimentally and numerically. At the first stage flame elongates in the bulk flow and the "finger flame" structure is formed with exponential manner of acceleration. After the flame

propagates away from the closed end of the channel the acceleration rate suddenly drops and the flame structure transforms into the "tulip flame". Secondary flame acceleration of the "tulip flame" structure leads to the establishment of conditions for the transition to detonation in the vicinity of the flame front via the mechanism of the flame chocking and local pressure rise.

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