On the Gasdynamic Mechanisms of Reaction Wave Development in Shock Tube

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1 Introduction

The reactor based on the shock tube represents one of the most widely utilized techniques for studying chemical kinetics of reactive systems. According to the ideal shock tube theory reacting gas is compressed inside the shock front that leads to its ignition with a certain delay time corresponding to the thermodynamic state behind the shock. However, the process in the real experiment is usually much more complex compared with the ideal theory and ignition arises in significantly non-ideal conditions. Especially this issue is relevant to the case of relatively long ignition delays when the flow instabilities have time to develop on the background of slow chemical kinetics. In such conditions, the so-called mild ignition proceeds via local ignition events in the regions of higher temperature [1]. Herewith, the exothermal reaction locally starts earlier than estimated for average thermodynamic state behind the shock wave. As a result flame front appears earlier than the entire mixture compressed behind the shock wave begins to react volumetrically [2]. Finally, the measured ignition delay occurs to be shorter than calculated value [3].

In case of fast enough exothermal reaction with short ignition delay temperature, gasdynamical non-idealities lead to the spatial perturbations in the reaction zone that in particular define wave structures on the detonation front (detonation cells) [4].

In view of issues discussed above it is of fundamental interest to get clear understanding of the gasdynamical mechanisms responsible for non-idealities of the flow behind the shock wave propagating through the reactive mixture. To obtain clear view on the physical processes of interest the specific experimental diagnostics is needed. Additional information can be also obtained with the use of precise numerical analysis which became available over the last decades. Thus, in recent papers [5,6] two-dimensional calculations allowed vizualization of vortical structures arising due to the shock-boundary layer interaction and determining the non-uniformity of temperature field behind the reflected shock. Recently in [7,8] the detailed numerical analysis of the boundary layer development both behind the incident shock and behind the reflected shock was carried out. It was shown that the gasdynamic instability of boundary layer develops via the same scenario as in incompressible case and that one of the

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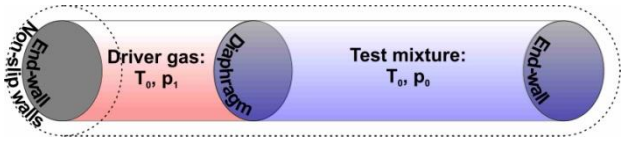
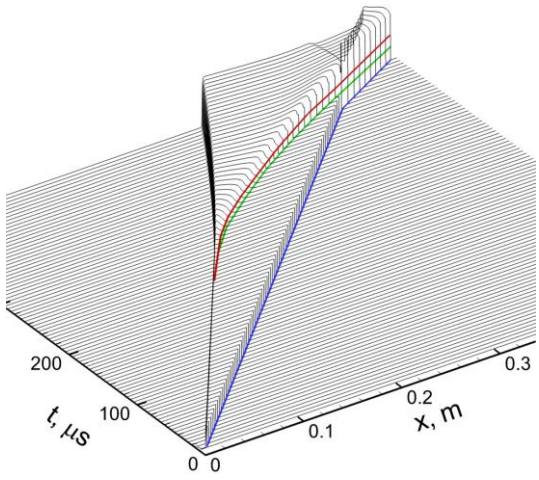
leading roles in hot kernels formation belongs to the roller vortices developing on the scales of boundary layer. This paper is devoted to the issue of detonation onset in the shock-compressed mixture where the reaction starts in the form of ignition kernels. Despite such scenarios were widely studied experimentally in natural conditions [9-11] and in the special problem setups with externally induced ignition [12] there is still lack of understanding of the process.

2 Problem setup

Let us consider the problem of the detonation formation behind the incident shock wave in the shock tube filled with a premixed gaseous mixture. The problem setup is presented in figure 1a while figure 1b shows the overall process on the x-t diagram. The process starts with the driver gas expansion from the high pressure chamber. Driver gas pushes the test mixture causing the formation of the shock wave. Chemical reactions start in the test gas compressed by the shock wave. Herewith, firstly endothermic reactions proceed giving birth to active radicals. After induction delay is passed the exothermal reaction starts that result in the mixture ignition. The longer is the period during which the test mixture is compressed the higher is the reaction progress value. Therefore, in ideal case the ignition most probably to arise directly ahead of the contact surface. Further ignition propagates non-stationary behind the shock wave leading to the detonation onset.



(a)



(b)

Figure 1. Left (a): Schematic problem setup, Right (b): x-t diagram of the general pattern of the process. Black lines – temperature profiles obtained from 1D calculations. Blue line – path of the leading shock wave, red – reaction front, green – compression wave generated ahead of the non-steady reaction wave.

In the framework of current study, the process of detonation generation by the incident shock wave in the tube is considered for different test mixtures which compositions correspond to different levels of reactivity. In particular, stoichiometric hydrogen-oxygen mixtures diluted with argon and nitrogen are considered. Helium is used as a driver gas. The main attention of the study is focused on the near-limit ignition regimes under almost atmospheric pressure and temperature of about 1000-1050 K.

Numerical analysis presented below is performed in two-dimensional problem setup with the use of the conventional mathematical model for reactive compressible viscous flow and contemporary low-dissipative numerical technique [8].

3 Results and discussion

Let us first consider the process in one-dimensional approximation. As it was already mentioned above, a certain non-uniform field of reaction progress value establishes behind the shock wave. The reaction progress is maximal exactly ahead of the contact surface while the non-uniformity is defined by the finite speed of shock wave relative the compressed mixture. In such conditions the ignition develops in the form of non-steady thermal explosion on the background of spatially non-uniform distribution of induction delay [13]. Herewith, the initial speed of reaction wave can be determined as:

$$U_{sp} = \left(grad(\tau_{ind})\right)^{-1} = D - u_p \quad (1)$$

where U_{sp} is the speed of spontaneous combustion wave determined according to [13], τ_{ind} – induction time, D – shock speed, u_p – flow velocity behind the shock front. Value $\left(D - u_p\right)$ determines the delay between time instants at which two neighboring lagrangian particles pass through the shock front. And exactly this value defines the difference in ignition delay times for these two lagrangian particles.

In general case the spontaneous combustion wave can propagate with almost any speed. With that in mind, in [13] Zel'dovich classified all the possible regimes of combustion resultant from the thermal explosion in the region with spatial non-uniformity of induction delay time. If $U_{sp} < U_f$, where U_f is normal burning velocity, then a classic deflagration wave is forming. If $U_f < U_{sp} < a$, where a is a sonic speed, then a deflagration wave behind a compression wave is forming. At higher U_{sp} a detonation can be formed as soon as U_{sp} becomes greater than sonic speed in the combustion products a_b [14]. At $U_{sp} > D_{CJ}$ a so-called weak detonation forms and finally at $U_{sp} \to \infty$ a volumetric thermal explosion takes place. Here it is important to note that the regime of deflagration wave behind the compression wave as well as the regime of weak detonation in reality is unstable. In the first case, depending on the kinetic parameters of the test mixture the deflagration wave can either accelerate or decelerate in the flow behind the compression wave. As a result, slow deflagration establishes or transition to detonation takes place. In the case of weak detonation, the reaction wave tends to transit into the detonation [15].

In the considered case of reaction initiation by incident shock wave, the speed of spontaneous combustion wave is $U_{sp} = D - u_p < a$, so as soon as ignition takes place the deflagration wave behind the outrunning compression wave is forming in the compressed test mixture (see e.g. Fig. 1b where one can observe both reaction wave and compression wave formed ahead of it). Such a pattern represents one of the possible scenarios of detonation onset behind the incident shock and can be used, for example, to interpret the results of [11] where synchronized pressure and OH* emission records show the same sequence of events in stoichiometric hydrogen-air mixture. According to the data obtained in [11] there are: (1) certain pressure increase behind the leading shock that is related to the flow acceleration ahead of the non-steady reaction front; (2) flame front propagating at some distance behind the leading shock at the background of compression (1); (3) detonation wave formed as a result of reaction wave acceleration. On the other hand, there are scenarios in which the dynamics of the process is much more complex and cannot be reproduced in one-dimensional approximation. Thus, in [10] it is obtained for nitrogen-diluted acetylene-oxygen mixture that the detonation onset is realized as a sequence of series of ignition events arising at ~5-8 mm distance from each other with delay of ~25 μs. According to the data obtained for specific case considered in [10] the detonation is forming only after third ignition event.

Now, consider the peculiarities of the process in multidimensional case. The analysis of the flow structure behind the incident shock shows that the flow is subjected to the development of vortical structures related to the gasdynamic instability of the boundary layer [7,8]. Together with the heat losses through the wall this leads to the temperature redistribution firstly in the boundary region and secondly in the bulk flow as

well. Figure 2a represents the characteristic temperature field in argon-diluted hydrogen-oxygen mixture that reflects the influence of both vortices and "cold" wall. It this particular case the temperature rise on the upper margin of the boundary layer achieves values of $\delta T \sim 40K$. Herewith, it should be noted that the considered temperature range corresponds to the chemical margin (so-called "crossover") where such temperature rise δT can cause a decrease in ignition delay of several orders of magnitude. So in this particular case, the most probable position of ignition kernel is around the intersection of the contact surface and the upper margin of boundary layer. Subsequently the process evolves in a manner close to that discussed above for one-dimensional case. Figure 2b illustrates the non-uniform field of OH radical concentration in the developing ignition kernel. One can observe that the reaction is much more intensive in the boundary region. Moreover, the reaction front propagates there much faster. In considered case of mixture highly diluted with argon the boundary layer is quite thin, and one can observe an accelerating reaction front propagation in a relatively narrow layer along the side wall of the shock tube. The structure of the accelerating reaction zone together with the compression wave on the transient phase is shown in Fig. 2c while Fig. 2d shows the structure of detonation wave formed as a result of transient process.

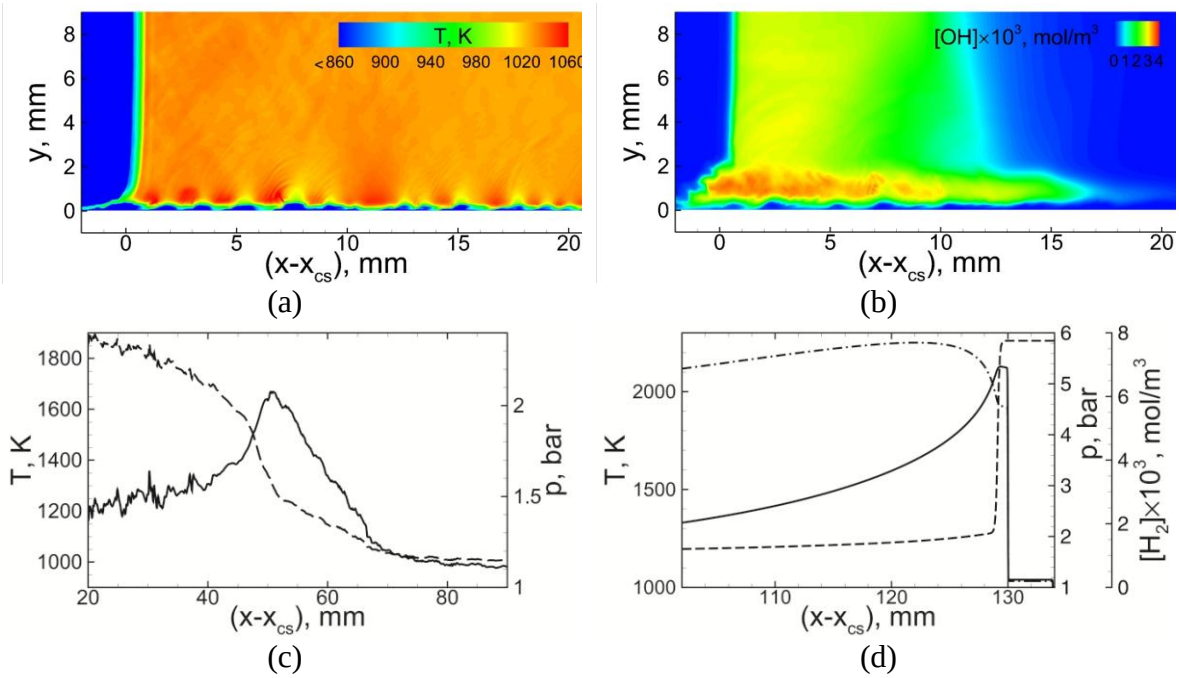


Figure 2. (a): Characteristic temperature field in the vicinity of contact surface. Helium-driven shock wave in 10%($2H_2$+O_2)+Ar mixture, temperature behind the shock front is ~1020K. Time instant: t=200μs; (b): Non-uniform [OH] field after ignition start. Time instant: t=280μs; (c) Flow structure in the complex of reaction wave and compression wave. Dashed line – temperature, solid line – pressure. Time instant: t=350μs; (d) Structure of the detonation wave propagating through the compressed mixture. Dash-dotted line – temperature, solid line – pressure, dashed line – H_2 concentration. Time instant: t=420μs.

Different regime takes place in case of nitrogen dilution. First of all, in 10%($2H_2$+O_2)+N_2 mixture the boundary layer grows faster that results in larger scales of vortices on the developed stage. In addition such a mixture occurs to be less reactive than one considered above that leads to longer ignition delay at the same temperature. Due to the thicker boundary layer a series of larger roller vortices is formed on the developed stage. Characteristic wavelength correspondent to the distance between vortices (or their diameter) can be estimated as 10 mm (in case of 10%($2H_2$+O_2)+Ar mixture the same scale can be estimated as 1 mm, see Fig. 2a). Thereby, the ignition kernels associated with these roller vortices occur to

be separated in space that in particular leads to the spatial separation of ignition events. As a result, here the spontaneous ignition, which seemed to be almost permanent in the previous case, proceeds in a discrete manner. Herewith, the time delay between subsequent ignition events can be estimated as 40–60 μs. The evolution of the process in this regime is presented in figure 3. It is very likely that the same scenario took place in the case considered in [10].

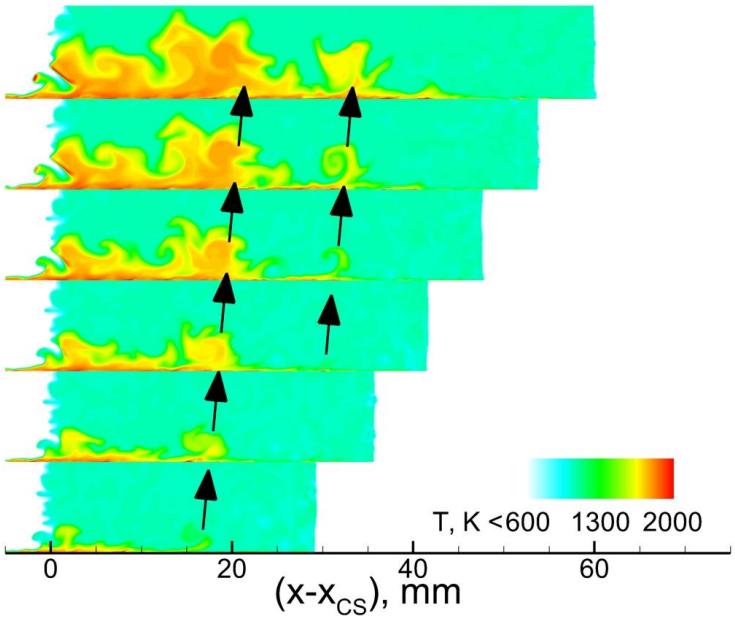


Figure 3. Sequence of temperature fields illustrating the dynamics of 10%($2H_2$+O_2)+N_2 ignition behind the incident shock wave. Time delay between the frames is 20 μs. Arrows show locus of two neighboring ignition kernels.

4 Conclusions

According to the obtained results and their analysis the following conclusions can be drawn.

- The origins of ignition events behind the shock waves in channels and tubes are related to the gasdynamical behavior of the compressed test mixture. In particular, an important role belongs to the roller vortices formed already on the linear stage of boundary layer development.
- The most probable position of first ignition kernel is the intersection of contact surface and boundary layer where locally higher values of temperature and reaction progress are achieved.
- The ignition develops in the form of spontaneous combustion wave with maximal initial speed equal to the shock wave speed relative the moving compressed gas. Since this value is subsonic the spontaneous wave forms the unstable complex consisting of combustion wave behind the outrunning compression wave. In such conditions the combustion wave accelerates finally forming the detonation.
- In case of mixtures diluted with monomolecular gas the boundary layer on the developed stage occurs to be rather thin that determines almost continuous process of detonation formation.
- In case of gas consisting of larger amount of molecules the boundary layer is thicker that determines discrete manner of spontaneous wave propagation in the form of spatially separated kernels.

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