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Hydrogen–oxygen flame acceleration and deflagration-to-detonation transition in three-dimensional rectangular channels with no-slip walls

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ABSTRACT

Hydrogen–oxygen flame acceleration and the transition from deflagration to detonation (DDT) in channels with no-slip walls are studied using high resolution simulations of 3D reactive Navier–Stokes equations, including the effects of viscosity, thermal conduction, molecular diffusion, real equation of state and detailed (reduced) chemical reaction mechanism. The acceleration of the flame propagating from the closed end of a channel, which is a key factor for understanding of the mechanism of DDT, is thoroughly studied. The three dimensional modeling of the flame acceleration and DDT in a semi-closed rectangular channel with cross section 10×10 mm and length 250 mm confirms validity of the mechanism of deflagration-to-detonation transition, which was proposed earlier theoretically and verified using 2D simulations. We show that 3D model contrary to 2D models allows to understand clearly the meaning of schlieren photos obtained in experimental studies. The "numerical schlieren" and "numerical shadowgraph" obtained using 3D calculations clarify the meaning of the experimental schlieren and shadow photos and some earlier misinterpretations of experimental data.

1. Introduction

Since the discovery of detonation more than 150 years ago, a huge number of experimental, theoretical and numerical studies had been taken in attempt to understand nature of the detonation formation. These studies are inspired by their importance for industrial safety [1,2] including nuclear power plants safety [3–7] and their potential application for micro-scale propulsion and power devices [8,9]. Yet many questions still remain unresolved or poorly understood. There was a general dissatisfaction about the reasons which caused one of the worst in the history of mankind accident of Fukushima Daiichi Nuclear Power Plant on March 11, 2011, following after an earthquake and tsunami at the Honshu island. As the fuel rods were overheated the water–Zirconium reaction started liberating hydrogen into the atmosphere under confinement. The hydrogen is one of the most explosive gases and deflagration or even detonation can be easily

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triggered when it is mixed with air at a high pressure. The explosion, which occurred in unit 3 of the Fukushima Daiichi Plant, was much more violent [10] than in unit 1. Presumably it was caused by detonation formation according to the DDT scenario or by non-stationary accelerating deflagration with continuously generated compression and shock waves.

Understanding the nature and the physical mechanisms responsible for initiation of detonation is of paramount importance. Recently the different scenarios of how a detonation can be initiated were studied in details [11]. It was shown that sufficiently fast and large energy addition can facilitate direct initiation of detonation. It can be initiated by initial shallow gradient of reactivity, formed e.g. behind a shock wave in a shock-tube, or it can appear as a result of the deflagration-to-detonation transition. Especially, one of the most difficult and poorly understood problems seems to be the flame acceleration in ducts and subsequent deflagration-to-detonation transition (DDT), which have been intensively studied over the past decades.

The hazardous potential of hydrogen–air and hydrogen–oxygen (H_2–O_2) mixtures has been extensively studied assuming a perfect mixture of fuel and oxidant. Since pioneering studies by Shchelkin, Zeldovich, Oppenheim and their co-authors [12–16] there has been a continuous effort aiming to elucidate the nature of DDT and to reveal a reliable physical mechanism explaining DDT. From the beginning researchers thought that the crucial aspect for the DDT occurring is a high intensity of turbulence in the flow ahead of the flame. A common belief was that a fast flame acceleration and transition to detonation can occur only for strongly turbulent flames. The first explanation of the flame acceleration in tubes with no-slip walls before the DDT occurred goes back to Shchelkin [12]. He argued that due to thermal expansion of the burning matter the flow ahead of the propagating flame becomes turbulent, so that turbulence is the main reason of the flame acceleration. How DDT occurs may vary depending on particular experimental conditions. The rough walls and the presence of obstacles along the channel walls enhance the flame acceleration rate and shorten drastically the run-up distance. The experiments demonstrate much higher acceleration rate for the flames passing through an array of turbulence-generating baffles. Therefore, channels with rough walls or obstacles are often used to study the flame acceleration and DDT since in this case the run-up distance can be better controlled [12–22]. This presumably was the reason why for a long time the attempts to explain DDT were associated with turbulent flames and were based on assumption that DDT might occur only in the case of turbulent flames. All the same DDT occurs in channels with smooth walls [23,24] and in thin capillary tubes [25] where flow remains laminar till the transition to detonation.

In 1947 Zeldovich [26] in his detailed analysis of the Shchelkin's experiments has pointed that turbulence is not a primary factor responsible for flame acceleration in a smooth-walled channel and sequential detonation formation. Explaining the nature of the flame acceleration in the DDT events Zeldovich [26] emphasized the fruitfulness of the Shchelkin idea about the role of a flame interaction with the upstream flow, and questioned the Shchelkin's idea about turbulence as the main reason of the flame acceleration. In his analysis of the flame acceleration in a tube with no-slip walls Zeldovich has shown that stretching of the flame front due to the interaction with a nonuniform velocity field of the upstream flow is the main cause of the flame acceleration, while turbulence plays only a supplementary role if any depending on the current experimental conditions.

Over the past years significant efforts have been devoted to understand the nature of the flame acceleration and the mechanism of transition from deflagration to detonation. Since the early 80's when more or less detailed computations of gasdynamics became available, researchers have made great efforts trying to understand mechanism of DDT by performing 2D simulations. A simple one-step reaction model described by the first order Arrhenius kinetics was widely used for the simulations of DDT. A general conclusion was (see e.g. review [27]) that turbulent flame creates ignition centers ("hot spots") in nearby unreacted material ahead the flame front that lead to detonation formation through the Zeldovich gradient mechanism [28] involving gradients of reactivity. Therefore it was claimed that detonation occurs due to the reaction wave spontaneously initiated in the region between the precursor shock and the flame front and that the transition to detonation occurs via is essentially the Zeldovich gradient mechanism. Similar explanation of DDT [29], which is known as SWACER (the shock wave amplification by coherent energy release), also involves the Zeldovich gradient mechanism and assumes that a proper temperature gradient can be formed between the flame front and the precursor shock wave. However the analysis of experiments [23–25] and high resolution 2D simulations using detailed chemical reaction models [30–32] have shown that temperature ahead the flame front (in "hot spots") is too low to ignite exothermic reaction on the time scales of the whole process. Therefore the earlier studies based on the calculations, which used a simplified one-step chemical kinetics, can be treated as an artificial as such models allow ignition at any low temperatures. Contrary, for detailed kinetics models it was shown [33,34] that the spatial scales of the temperature nonuniformity capable to ignite detonation via the Zeldovich gradient mechanism should be much greater (temperature gradient should be much gently sloping) than those formed either in hot spots or between the precursor shock and the flame front observed in numerical simulations with a one-step chemical reaction model. Even for highly reactive mixtures such as stoichiometric H_2–O_2 the minimum scale of the temperature gradient (inverse gradient steepness $L = (T^* - T_0)/\nabla T$, where T^* and T_0 are maximum and minimum temperatures along the temperature gradient) required for successful detonation initiation is about 10 cm at pressure $P_0 = 1$ atm and it is more than 1 m for H_2–air mixture or at lower pressure, which is by orders of magnitude exceeds size of the hot spots.

From the very beginning of DDT studies the very fact of the flame acceleration in tubes with no-slip walls has been considered as an important factor that influences the DDT process. The flame acceleration and the transition to detonation have been studied using the one-dimensional and multi-dimensional analyses taking into account that the acceleration rate can be enhanced by external turbulence or intrinsic flame instabilities (such as Darrieus–Landau instabilities) [12–22,35–37]. Probably the first quantitative description of the flame acceleration has been obtained by