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 $10 \times 10$ 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.

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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 microscale 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 (H₂–O₂) 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 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 non-uniformity 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 H₂–O₂ 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 H₂–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
Clanet and Searby [38] who have shown that the increase in the flame surface during development of a finger flame from the initial hemispherical shape in a cylindrical tube leads to the exponential increase of the flame tip velocity.

It was shown [30–32] that an exponential increase of the flame speed is intrinsic for the flames accelerating in channels with no-slip walls due to the flame front stretching along the boundary layer in the flow formed ahead the flame front, so that the flame velocity in laboratory system increases as \( U_{f_L} \propto \exp(\alpha U_{f_0} W/D) \), where \( U_{f_0} \) is the normal flame velocity and \( \alpha = \rho_p/\rho_0 \) is the expansion coefficient, \( \alpha \) is a numerical factor of the order of unity. Note, that this solution for the exponential increase of the flame speed is an exact solution with accuracy \( \delta/D \ll 1 \), where \( \delta \) and \( D \) are the width of the boundary layer and the channel width, correspondingly.

The classical formulation of the problem in question for theoretical analysis and an experimental set-up is an initially laminar flame, which is ignited near the closed end of the tube and then propagates towards the open end. The flame accelerates, produces compression and weak shock waves modifying the flow ahead the flame front. Eventually DDT occurs, which appears as a sudden explosion in the vicinity of the flame front.

Recently the quantitative theory of the flame acceleration in a tube with smooth no-slip walls has been developed and validated by comprehensive 2D numerical simulations with detailed chemical kinetics [30–32]. It was shown that the principal feature of the flame acceleration in tubes with no-slip walls, which determines the mechanism of DDT, is the specific evolution of the flame acceleration, which results in the formation of a shock wave in the closed vicinity of the flame front [30–32]. If in the beginning the flame was initiated as a planar one, then the first stage of the initially planar flame evolution is the exponential acceleration due to the stretching of the flame front edges along the thin boundary layer. During this stage the accelerating flame acting as a piston produces compression waves which steepen into the shocks far ahead in the upstream flow. Such stretching of the flame front in the flow generated ahead of its front is restricted by the small width of the boundary layer and later it is replaced by the next stage [30–32], when the flame speed increases according to the power law \( U_{f_L} \propto 1 + \beta t^n \) with \( 0 < n < 1 \). During this stage the compression waves produced by the accelerating flame steepen into the shock waves in the close vicinity of the flame front. When shocks are formed directly ahead the flame surface, the flame starts to consume more compressed and heated fresh fuel formed behind the shock running away from the reaction zone, which results in a larger increase in the burning rate. The increased amount of fresh fuel entering the flame results in the formation of the pressure pulse in the reaction zone. This pressure pulse grows exponentially due to the positive feedback between the strength of the shock and the reaction rate. Consequently, there are two feedback mechanisms leading to the flame acceleration up to supersonic speed. One is driven by the increased temperature, and hence reactivity, of the mixture due to the shock, and the other by the increased density of the mixture entering the reaction zone. The increase of the flame speed advances the gas velocity ahead the flame front. After the flame accelerates up to the local sound speed the generated pressure pulse occurs to be locked in the reaction zone and violently increases due to the positive feedback until it steepens into the shock strong enough to initiate a detonation. This mechanism of DDT is determined only by the intrinsic features of the flame accelerating in the channel with non-slip walls and is considerably different from those proposed earlier based on the gradient mechanism and spontaneous ignition in the hot spots.

A large diversity of the experimental details usually clouds the actual sequence of events and the basic processes leading to the transition from deflagration to detonation. In view of great importance of the problem in question the objective of the present work is to examine in details the features of the flow evolution, their influence on flame dynamics and mechanism of detonation formation within rectangular duct using 3D computations with a detailed chemical reaction mechanism. The precise ways in which transitions to detonation can occur are complex in the extreme, and the important details can be revealed by high resolution three-dimensional numerical simulations.

The paper is organized as follows. Section 2 is the formulation of the problem and numerical method. In Section 3 we perform 3D direct numerical simulations of the initially planar hydrogen–oxygen flame propagating through the channel and the transition to detonation and compare the results of 3D modeling with those obtained from 2D computations. Section 4 presents analysis of the pressure pulse formation and the mechanism of DDT for the three-dimensional flame. In Section 5 we use the results of 3D modeling to reproduce the schlieren images corresponding to those obtained in experimental studies. We discuss interpretation of the experimental schlieren images and compare them with the real three-dimensional flow pattern. We conclude in the last Section.

### 2. Formulation of the problem and numerical method

To reproduce the phenomena of flame acceleration in stoichiometric hydrogen–oxygen mixture and sequential deflagration-to-detonation transition in three-dimensional rectangular channel we have kept the problem setup similar to that used in Refs. [30–32]. The computational domain is taken as a rectangular channel with cross section \( 10 \times 10 \) mm and length 250 mm with closed left end and open right end. The grid system is built out from 50 million up to 400 million points. The flame is ignited by a thin heated layer near the closed-end wall and propagates in the direction \( x \) to the opened end through the channel with non-slip side walls. We used a condition of adiabatic walls to exclude any additional influence of the thermal boundary layer and to extract the features of flame acceleration related to the flame gasdynamics. Such a problem setup allows to obtain solution for initially planar flame evolving within the channel excluding secondary factors. The flow in the channel emerges only due to the expansion of the burned products and already on the very first stage is represented by an approximately uniform velocity profile with a thin boundary layer near the side walls.

The computations solve the multidimensional, time-dependent, reactive Navier–Stokes equations including the...
effects of compressible gas convection, molecular diffusion, thermal conduction, viscosity and detailed chemical kinetics for the reactive species $H_2$, $O_2$, $H$, $O$, $OH$, $H_2O$, $H_2O_2$ and $HO_2$ with subsequent chain branching, production of radicals and energy release in the form

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_x)}{\partial x} + \frac{\partial (\rho u_y)}{\partial y} + \frac{\partial (\rho u_z)}{\partial z} = 0, \quad (1)$$

$$\frac{\partial Y_i}{\partial t} + u_x \frac{\partial Y_i}{\partial x} + u_y \frac{\partial Y_i}{\partial y} + u_z \frac{\partial Y_i}{\partial z} = \frac{1}{\rho} \left( \frac{\partial (\rho D_{ij} \frac{\partial Y_j}{\partial x})}{\partial x} + \frac{\partial (\rho D_{ij} \frac{\partial Y_j}{\partial y})}{\partial y} + \frac{\partial (\rho D_{ij} \frac{\partial Y_j}{\partial z})}{\partial z} \right), \quad (2)$$

$$\rho \left( \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x} + u_j \frac{\partial u_i}{\partial y} + u_j \frac{\partial u_i}{\partial z} \right) = - \frac{\partial \rho}{\partial x} \frac{\partial \rho u_i}{\partial x} - \frac{\partial \rho}{\partial y} \frac{\partial \rho u_i}{\partial y} - \frac{\partial \rho}{\partial z} \frac{\partial \rho u_i}{\partial z} - \frac{\partial p}{\partial x} - \frac{1}{ho} \frac{\partial \rho}{\partial x} \frac{\partial \rho u_i}{\partial x} - \frac{1}{ho} \frac{\partial \rho}{\partial y} \frac{\partial \rho u_i}{\partial y} - \frac{1}{ho} \frac{\partial \rho}{\partial z} \frac{\partial \rho u_i}{\partial z} \quad (3)$$

$$\rho \left( \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x} + u_j \frac{\partial u_i}{\partial y} + u_j \frac{\partial u_i}{\partial z} \right) = - \frac{\partial \rho}{\partial x} \frac{\partial \rho u_i}{\partial x} - \frac{\partial \rho}{\partial y} \frac{\partial \rho u_i}{\partial y} - \frac{\partial \rho}{\partial z} \frac{\partial \rho u_i}{\partial z} - \frac{\partial p}{\partial x} - \frac{1}{ho} \frac{\partial \rho}{\partial x} \frac{\partial \rho u_i}{\partial x} - \frac{1}{ho} \frac{\partial \rho}{\partial y} \frac{\partial \rho u_i}{\partial y} - \frac{1}{ho} \frac{\partial \rho}{\partial z} \frac{\partial \rho u_i}{\partial z} \quad (4)$$

$$\rho \left( \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x} + u_j \frac{\partial u_i}{\partial y} + u_j \frac{\partial u_i}{\partial z} \right) = - \frac{\partial \rho}{\partial x} \frac{\partial \rho u_i}{\partial x} - \frac{\partial \rho}{\partial y} \frac{\partial \rho u_i}{\partial y} - \frac{\partial \rho}{\partial z} \frac{\partial \rho u_i}{\partial z} - \frac{\partial p}{\partial x} - \frac{1}{ho} \frac{\partial \rho}{\partial x} \frac{\partial \rho u_i}{\partial x} - \frac{1}{ho} \frac{\partial \rho}{\partial y} \frac{\partial \rho u_i}{\partial y} - \frac{1}{ho} \frac{\partial \rho}{\partial z} \frac{\partial \rho u_i}{\partial z} \quad (5)$$

$$\rho \left( \frac{\partial E}{\partial t} + \frac{\partial (\rho u_x)}{\partial x} + \frac{\partial (\rho u_y)}{\partial y} + \frac{\partial (\rho u_z)}{\partial z} \right) = - \frac{\partial (\rho u_x)}{\partial x} \frac{\partial \rho u_i}{\partial x} + \frac{\partial (\rho u_y)}{\partial y} \frac{\partial \rho u_i}{\partial y} + \frac{\partial (\rho u_z)}{\partial z} \frac{\partial \rho u_i}{\partial z} + \frac{\partial \rho}{\partial x} \left( \sigma_{xx} u_i + \sigma_{xy} u_j + \sigma_{xz} u_z \right) + \frac{\partial \rho}{\partial y} \left( \sigma_{yx} u_i + \sigma_{yy} u_j + \sigma_{yz} u_z \right) + \frac{\partial \rho}{\partial z} \left( \sigma_{zx} u_i + \sigma_{zy} u_j + \sigma_{zz} u_z \right) \left( \frac{\partial \rho}{\partial x} \right) \left( \frac{\partial \rho u_i}{\partial x} \right) \quad (6)$$

Here $P$, $\rho$, $u_x$, $u_y$, $u_z$ are pressure, density, mass, and flow components of the velocity, $Y_i = \rho_i / \rho$ is the mass fraction of the species, $E = \varepsilon + (u^2)/2$ is the total energy density, $\varepsilon$ is the inner energy density, $R_0$ is the universal gas constant, $m_i$ is the molar mass of $i$-species, $R_i = R_0 m_i n$ is the molar constant, $\sigma_{ij}$ is the viscous stress tensor, $c_{ii} = \sum c_{ii} Y_i$ is the constant volume specific heat, $c_{ii}$ is the constant volume specific heat of $i$-species, $h$ is the enthalpy of formation of $i$-species, $\kappa(T)$ and $\mu(T)$ are the coefficients of thermal conductivity and viscosity, $D_i(T)$ is the diffusion coefficient of $i$-species, $(\partial Y_i / \partial t)_{ch}$ is the variation of $i$-species concentration (mass fraction) in chemical reactions.

The equations of state for the fresh mixture and combustion products were taken with the temperature dependence of the specific heats, heat capacities and enthalpies of each species borrowed from the JANAF tables and interpolated by the fifth-order polynomials [39,40]. The transport coefficients were calculated from the first principles using the gas kinetic theory [40,41]. The viscosity coefficients for the gaseous mixture are

$$\mu = \frac{1}{2} \left( \sum a_i \mu_i \right) \left( \frac{1}{\sum a_i} \right)^{-1} \quad (13)$$

where $a_i = n_i / n$ is the molar fraction, $\mu_i = 5/16(\sqrt{m_i kT_i / \pi \Sigma^2 (\hat{q}^{(2)})})$ is the viscosity of $i$-species, $\hat{q}^{(2)}$ is the collision integral which is calculated using the Lennard-Jones potential [41], $\hat{m}_i$ is the molecular mass of the $i$-th species of the mixture, $\Sigma_i$ is the effective molecule size. The thermal conductivity coefficient of the mixture is

$$\kappa = \frac{1}{2} \left( \sum a_i \kappa_i \right) \left( \frac{1}{\sum a_i} \right)^{-1} \quad (14)$$

Coefficient of the heat conduction of the mixture $\kappa$ can be expressed via viscosity $\mu$ and the Prandtl number, which for two- and three-atomic gases can be taken in a range $Pr = 0.71 \pm 0.75$.

The binary coefficients of diffusion are

$$D_{ij} = \frac{3}{8} \frac{2\pi k T_i m_j \hat{m}_j / (\hat{m}_i + \hat{m}_j)}{\pi \rho_i \Sigma_i \hat{q}^{(1+1)} \left( T_i / T_j \right)}$$

where $\Sigma_i = 0.5(\Sigma_i + \Sigma_j)$, $T_j = kT_i / \gamma_j$, $\gamma_j = \sqrt{\epsilon_j} ; \epsilon$ are the constants in the expression of the Lennard-Jones potential, and $\hat{q}^{(1+1)}$ is the collision integral similar to $\hat{q}^{(2)}$ [40,41].

The diffusion coefficient of $i$-th species is

$$D_i = (1 - Y_i) / \left( \sum_{i \neq j} a_i / D_j \right) \quad (16)$$

Concentrations of the mixture components $Y_i$ are defined by the solution of system of chemical kinetics

$$\frac{dY_i}{dt} = F_i(Y_1, Y_2, \ldots Y_N, T), \quad i = 1, 2, \ldots N. \quad (17)$$

The right hand parts of Eq. (17) contain the rates of chemical reactions, which depend on temperature according to the Arrhenius law in a standard form [40].
The elementary reactions of the Arrhenius type together with pre-exponential constants and activation energies used in the simulations were presented in Table 1 of Ref. [32]. Sensitivity analysis [32] has shown reliability of this reaction scheme for a stoichiometric H₂–O₂ mixture and that it is adequate to complete chemical kinetic scheme. The computed [32] thermodynamic, chemical, and material parameters using this chemical scheme are in a good agreement with the hydrogen–oxygen flame and detonation wave characteristics measured experimentally [42].

Numerical method used in the simulations is based on splitting of the Eulerian and Lagrangian stages, known as coarse particle method (CPM) [43]. This scheme appears to be robust when used to model various complex hydrodynamic flows. The analysis of this method applied to a large variety of problems, including problems of hydrodynamic instability, shows that it possesses a high numerical stability, which enables to carry out calculations of shock wave without the aid of artificial viscosity. High stability of the method is achieved by dividing one time-step calculation into three stages. On the first stage, the change of hydrodynamic characteristics on the fixed Eulerian space grid is calculated using the explicit scheme without regard of mass, momentum and energy transfer. The hydrodynamic variables transfer through the cell boundaries on the second stage using the values of hydrodynamic characteristics from the first stage. The third stage consists of final calculation of the values of all parameters for every cell and for the whole system. It was shown [44] that a high numerical stability of the method is achieved if the hydrodynamic variables are transferred across the grid boundary with the velocity, which is an average value of the velocities in neighboring grids. However, in this case the second stage and, as the result, the whole algorithm is of the first order accuracy in space variables. The second order method of the Lagrangian stage makes the scheme unstable in some cases. In contrast to Ref. [43], we used another method to increase accuracy of the second stage. We assume that the velocity between centers of neighboring grids changes linearly and take the mass transfer velocity between the grids equal to the velocity in the point where the mass reaches the boundary between the grids during the time step of the calculation [44,45]. The modified coarse particle method and optimal approximation scheme were thoroughly tested by modeling different combustion problems and engine combustion. The modified CPM and optimal approximation scheme were thoroughly tested and successfully used for simulation engine combustion knock occurrence in SI engine [44,45]. The computational method, its validation, the resolution and convergence tests and comparison with other numerical codes are outlined in Ref. [32]. The resolution tests have shown that 6–8 grid points over the flame width are sufficient for good resolution of the inner flame structure. The convergence of 3D solutions should be kept to reproduce 3D flow structure. In our previous papers [11,32–34] the convergence for the flame front resolution was studied in 2D cases. Here we carried out 3D calculations in the vicinity of the convergence limit obtained there and observed the convergence of the 3D flame surface structure below this limit for the cell size several times smaller than that obtained in [32,33], increasing the number of grid points up to 400 millions points over the computational domain and 24 points per flame front. Thus we chose the required resolution for 3D calculations. The violent pressure buildup on the flame front was verified in [34] where we observed such a scenario of detonation formation in case of flame acceleration ahead the shock wave in the 1D setup for ignition problem. The convergence of solution in the present studies at higher pressures, during the pressure buildup, was tested using more than 50 grid points per flame front reaction zone.

Stiff system of the differential equations of chemical kinetics was solved using the Gear method [46]. The developed algorithm was implemented using the FORTRAN-90, and the simulations were performed using high-performance parallel computers.

3. Flame acceleration and DDT in three-dimensional rectangular channel

Simulations of the flame propagating in channels with no-slip smooth walls filled with the stoichiometric hydrogen–oxygen mixture at initial temperature T₀ = 298 K and initial pressure P₀ = 1.0 bar were performed for the channel of square cross-section (10 × 10) mm and length 250 mm with the minimum computational cell size Δ = 0.025 mm (which resolves flame front using 12 computational cells). A planar laminar flame was initiated near the left closed end of the three-dimensional channel and propagated to the right open end.

The shape of the flame propagating in the channel depends on the small perturbations imposed in the beginning. To analyze the influence of flame surface topology the additional small perturbations were imposed in the beginning of the flame propagation. While in 2D case the main direction of the flame propagation is associated with the side walls, and initially planar flame evolves into the tulip-shaped or single-mode flame which leading tips are moving along the walls (see, e.g. Figure 1 in Ref. [32]), in 3D case the edges between the channel walls are a preferential orientation for the flame propagation. To reduce cost of computations, the shape of the propagating flame depending on the imposed initial small perturbations was analyzed for the case of the channel of square cross-section 5 × 5 mm. Typical flame front structures during the initial stage of the flame propagation are shown in Fig. 1 for: a) initially unperturbed planar flame; b) initial regular perturbation; c) initial random (chaotic) perturbation. In Fig. 1 the type of the perturbations is shown at the rear end wall of the channel. Contrary to 2D case in 3D case the unperturbed planar flame aims to move along the edges between the channel walls and only in case of non-regular initial perturbation it evolves into the non-symmetrical shape with tips moving in the bulk far from the walls. For typical flame shapes one can see that initial perturbations tend to destroy the symmetrical shapes specified by the channel geometry (see Fig. 1). In case of the initially unperturbed planar flame (Fig. 1a) the stretching inside the boundary layers, preferentially at the edges between the channel walls causes formation of the tulip-shaped flame. The initial regular small perturbations (Fig. 1b) result in a single-mode flame shape and stochastic perturbations (Fig. 1c) cause formation of so-called flame brush – strongly corrugated flame surface with several
Fig. 1 – (a–c) Structure of the flame front depending on the initial small perturbations (shown at rear surface of the channel) at $t = 400 \, \mu s$: a) initially unperturbed planar flame, b) initial regular perturbation, c) initial random (chaotic) perturbation.
leading bulged tips. At the same time the overall dynamics of the flame acceleration remains almost the same independently on initial perturbations. Moreover the dynamics is similar to that obtained for 2D case except the higher acceleration rate associated with additional degree of freedom. This is clearly seen from Fig. 3 (below) which shows the flame velocities (solid lines) computed for 3D and 2D channels of the same width $D = 10$ mm.

Fig. 2 – Images at the left show the flame structure and compression (shock) waves (green surfaces) at sequential times 100, 200, 487 and 495 μs in square-cross channel of $D = 10$ mm. Boundary layer is seen as a white strip at the bottom and side walls. The corresponding 2D cross sections of 3D images in the plane $(x, y, z = 5$ mm) are shown at the right part. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
emphasized that the images representing by the cross sections in the plane (x, y) do not correspond to experimental schlieren photographs, but rather similar to the 2D simulation of the process. We will discuss it in details in Sec. 5. The frames of 2D cross sections in Fig. 2 also show the streamlines (arrowed lines) and the velocity profiles in the upstream flow. The boundary layer of width about 0.5 mm in the flow ahead of the flame is slightly thickened towards the flame. It should be noticed that the flow remains laminar everywhere in the channel ahead of the flame all the time till the transition to detonation. Also the upstream flow remains almost uniform in the bulk of the channel with the longitudinal flow velocity which drops to zero within a thin boundary layer. The time required for establishing the Poiseuille flow velocity profile is much longer than the duration of the whole process of DDT. The parabolic velocity profile establishes during the time $t_p = D^2/ν$, where $ν$ is kinematic viscosity [31,32]. For the channel of width $D = 10$ mm, $t_p = 2.5$ s which by many orders of magnitude exceeds duration of the whole process. This also means that till the transition to detonation there is too little time for the flow turbulization.

The transition from deflagration to detonation depends on a variety of circumstances and may develop in a number of physical scenarios. Though in the rectangular cross section channel the preferential location of the leading flame tip propagation and correspondingly the primary origin of detonation occurs near the edge between the channel walls, but it does not mean that the boundary layer itself or shock wave – boundary layer interaction play specific role if any for the mechanism of DDT as it is sometimes claimed (see e.g. Ref. [47]). The precise ways in which transitions to detonation can occur are complex in the extreme, including important details revealed by the frames shown in Fig. 2.

Fig. 3a shows the evolution of the flame speed and the pressure peak at the leading flame tip throughout the process of the flame acceleration and DDT computed for 3D channel. For comparison, Fig. 3b shows the flame speed and the pressure peak evolution computed for 2D channel of the same width $D = 10$ mm [32]. It is seen that the overall dynamics in 2D and 3D cases is similar. For both cases the velocity–time dependence plots demonstrate the same feature of several distinctive stages of the flame acceleration: (0) initial stage of flame expansion out from the ignition zone; (1) the stage of exponential increase of the flame velocity; (2) the stage when the rate of the flame acceleration decreases compared with the previous nearly linear stage; (3) the sharp increase of the flame velocity and actual transition to detonation. The time of transition to detonation in 3D case appears to be about three times shorter mainly because of the shorter stage (1) and as a result more violent conditions at the beginning of the stage (2) which determines the DDT mechanism involving the rise of a pressure pulse in the reaction zone [30–32].

**4. Formation of the pressure pulse and mechanism of DDT**

A propagating flame initiated near the closed end of the channel controls the flow forming ahead of it, which results in
the flame acceleration compatible with the physical boundary conditions. When the flame is initiated near the closed end, the expansion of the high temperature burned gas induces an outward flow of the unburned mixture with the velocity \( u = (\theta - 1)U_{0} \) ahead of the flame front while the flame propagates with the velocity \( U_{c} = \theta U_{0} \) in the laboratory reference of frame [48], where \( U_{0} \) is the normal velocity of laminar flame at the ambient conditions and \( \theta = \rho_{b}/\rho_{u} \) is the density ratio of the unburned \( \rho_{u} \) and burned \( \rho_{b} \) gases, respectively. The velocity in the upstream flow is approximately constant in the bulk and vanishes within a thin boundary layer at the channel walls because of the friction of the no-slip walls. Every part of the flame front moves with respect to the unreacted mixture in the upstream flow with normal velocity \( U_{0} \) and simultaneously it is entrained by the flow ahead of the flame with its local velocity. Thus, the flame shape is defined by the relative motion of different parts of the flame front. As the flame front advances into a non-uniform velocity field, the flame surface stretches repeating to some extent the shape of the velocity profile in the upstream flow. The surface of stretched flame increases and it consumes fresh fuel over a larger surface area which results in an increase in the rate of heat release per unit projected flame area. The increase in the rate of heat release due to the flame stretching gives rise to a higher volumetric burning rate, and a higher effective burning velocity based on the average heat release rate per frontal area of the stretched flame sheet. A higher burning velocity results in an enhancement of the flow velocity ahead of the flame, which in turn gives rise to a larger velocity gradient field and enhances the flame stretching, and so on. Due to a positive feedback coupling established between the upstream flow and the burning velocity, the velocity of combustion wave increases exponentially in time as \( U_{\text{fl}} = \theta U_{0} \exp\left(\alpha u_{0} t / D\right) \), where \( \alpha \) is a numerical factor of the order of unity [30–32].

During this initial stage of the exponential increase of the flame velocity, the accelerating flame acts as a piston producing compression waves in the unreacted gas, which steepen into the shock waves at the coordinate \( x = x_{sh} \) far ahead of the flame front (located at \( x = x_{f} \) [30–32] at the distance about \( x_{sh} - x_{f} = (5 + 7)n \) from the flame front. Correspondingly thickness of the boundary layer can be estimated as \( \delta_{l} \sim (x_{sh} - x_{f})/\sqrt{Re} = (5 + 7)\delta/\sqrt{Re} \), where Re is the Reynolds number for the upstream flow. Theoretical estimate for the boundary layer thickness is \( \delta = 0.3 \sim 0.4 \) mm. From the numerical calculations the boundary layer thickness was found to be 0.4 mm near the walls and about 0.5 mm in the corners.

During the second stage the rate of the flame acceleration decreases and the flame velocity–time dependence can be approximated as

\[
U_{\text{fl}} = \theta U_{0} \left[ 1 + \beta \left( t / t_{1} \right)^{n} \right],
\]

where \( n \) is in the range \( 0 < n < 1 \). It was shown [30] that for a piston moving with the velocity–time dependence (18) the Riemann solution \( u(x, t) \) for a simple wave is multi-valued everywhere for any values of \( 0 < n < 1 \), and the compression wave produced by the flame steepens into the shock directly on the surface of the flame (see Fig. 2). Fig. 4 shows the corresponding time evolution of the combustion wave computed for 3D and 2D channels of the same width \( D = 10 \) mm. The exponential increase of the flame velocities in both cases is shown by dashed lines in Fig. 4, while further velocity time can be approximated by function of type (18).

Contrary to a stationary flame, the flow with the accelerating flame is not isobaric. In the latter case pressure is growing at about the same rate as the flame velocity. From the time when the compression waves steepen into the shock close to the flame front, the unreacted mixture of considerably higher density compressed in the shock starts entering the flame front and produces a narrow pressure peak on the scale of the flame width. The corresponding computed pressure and temperature profiles for 3D and 2D cases are shown in Fig. 5a and b, correspondingly. After the flame was accelerated up to the local sound speed the shocks and the pressure peaks do not run away from the reaction zone where they were formed and the pressure peak is localized directly in the reaction zone.

While during the first stage the flame acceleration is related to the stretching of the flame front within a boundary layer, during the second stage further fast acceleration of the flame is due to its coupling with the shock wave formed at the flame front. Consequently, there are two feedback mechanisms leading to the development of the high flame speed. One is driven by the increased temperature, and hence reactivity of the mixture due to the shock, and the other by the increased density and hence amount of reacting fuel entering the flame front. A higher flame speed creates a higher gas velocity ahead of the flame. Consequently, the amplitude of the pressure peaks at the flame front continues growing due to the combustion of larger amount of compressed mixture entering the reaction zone during the second stage. Eventually, the pressure peak becomes strong enough to affect reactions. The increase of the pressure enhances reaction rate and the heat release in the reaction zone creating a positive feedback coupling between the pressure pulse and the heat released in the reaction causing additional flame acceleration.

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It results in more violent increase of the pressure peak, which finally steepens into the shock strong enough for formation of a detonation wave. Duration of the last stage of actual transition to detonation was estimated \[30\] as \( t_1 = 1300 \mu s \), which is consistent with the result of numerical simulations.

Note, that for 3D case the run-up distance and duration of the flame propagating before the transition to detonation are about three times shorter compared to 2D channel of the same width. The pre-detonation time estimated as time when the pressure reaches its maximum, and when the strong shock arises on the flame tip, overcomes the sonic barrier and forms a detonation behind its front, is 0.55 ms for 3D case and 1.35 ms for 2D case. It should be noted also, that temperature non-uniformities if any ahead of the flame can not produce a detonation through the Zeldovich gradient mechanism.

5. Schlieren and shadowgraphy visualization of DDT and its interpretation using 3D computations

Since the first attempts to understand the origin of DDT in channels the schlieren photography method was used in experimental studies. Schlieren photography is widely used in wide diversity of scientific areas, in biology, physics, chemistry etc. see e.g. \[49\]. It is one of the most informative method for studying combustion processes and high-speed flows involving shocks where the gradients in the refractive index are large, because the method is sensitive to the changes in a refractive index within the material and do not interfere with the flow. Contrary to a shadowgraph method, which measures the second derivative of density, in the schlieren method a knife-edge is placed at the focal point to block about half of the light beam. This results in a set of lighter and darker patches corresponding to positive and negative fluid density gradients in the direction normal to the knife-edge, so that the schlieren method measures the first derivative of density in the direction of the knife-edge, which controls contrast in light intensity distribution on the screen. This method revealed that one of the leading roles for the DDT phenomena belongs to the shock waves, which are forming close ahead the flame front just before the transition to detonation.

To capture the features of flame acceleration and the origins of detonation formation one needs accurately resolve both time and space scales which are far beyond the limits of the nowadays resolution of schlieren method. Unfortunately, even the best up to now temporary resolution of the cameras used in DDT experiments \[15,16,20–25\] is too low for feasible resolution, which would make possible to resolve the process of DDT in details needed for understanding the physics of DDT. In most cases one can recognize DDT using only two sequential snapshots. The first snapshot shows the flow pattern in the vicinity of the flame front. The second one shows already the detonation wave propagating at the background of the previous flow pattern (see e.g. \[24\]).

On the contrary, with nowadays computers development the available time and space resolution of the process using computer modeling is much higher than that can be obtained experimentally with schlieren method. It became much more feasible and can bring more detailed results about the DDT origin. Besides, 3D computer simulations provide us with three-dimensional images of the process not available with the schlieren technique, which in any case provides us only with 2D projection of the three dimensional flow, until holographic photos are not available for combustion experimental technique.

Typically the interpolation of the snapshots gives the information that the origin of detonation is located in the very vicinity of the flame front. This agrees well with the mechanism of detonation formation described in the previous sections. However, sometimes the snapshots give impression that the detonation was formed and propagating out from the region ahead the flame front. Oppenheim named such a scenario as “explosion in the explosion” and it was commonly associated with the concept of “hot spots” arising in the unreacted material at the points of triple shock intersections.
However, this is not the case because both schlieren and shadow photographs give a 2D projection of the original 3D pattern on the planar screen, which sometimes lead to misinterpretation of the process.

Let us consider how should the schlieren photos look like for the real gas-dynamic flow involving the flame and DDT presented in series of 3D images shown in Fig. 2. As an example Fig. 6 shows sequence of shadow photographs in the cross section XY of the flow on the first stage of flame acceleration presented in Fig. 2 at time instants $t = 200 \, \mu s$ and $300 \, \mu s$, correspondingly in Figs. 6a and b. The shadowgraphy visualization obtained experimentally [24] for the corresponding first stage of the flame acceleration is shown in the frame Fig. 6c (Fig. 5 of Ref. [24]). One can see that the flame reproduced by the shadowgraphy looks like a turbulent one which is usually named “turbulent flame brush”. However, as it can be observed from the 3D images of Fig. 2 either flame or flow is not turbulent until the detonation formation. The “turbulent” pattern here is a result of interference of light beams refracted on the different pieces of cellular flame surface. This issue shows us that the cellular laminar flame can be visualized and interpreted as a turbulent one using the techniques giving 2D projections of the 3D flow. And it may cause misunderstanding of the studying phenomena.

The shadow visualization of the flow on the second stage may cause similar misinterpretation. As an example Fig. 7 shows numerically obtained shadow photos using 3D simulations in the XY and XZ cross sections on the frames (a) and (b) correspondingly ($t = 487 \, \mu s$). The frame (c) in Fig. 7 is an experimentally obtained shadowgraphy for stoichiometric $H_2 - O_2$, $P = 0.75$ atm, $D = 5$ cm [24].

Fig. 8 shows numerically obtained shadow photos for the last stage of the transition to detonation. The pattern at time $t = 487 \, \mu s$, $492 \, \mu s$, and $495 \, \mu s$. Frames d) and e) are the experimentally obtained shadowgraphy for stoichiometric $H_2 - O_2$, $P = 0.75$ atm, $D = 5$ cm [24] with time resolution $\Delta t=100 \, \mu s$. 

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instant 487 ms (Fig. 8a) represents the end of the second stage and the patterns at time instants 492 ms (Fig. 8b) and 495 ms (Fig. 8c) show the detonation formation. The frames Fig. 8d and e represent the same phase of the process obtained experimentally in [24] with the time resolution Δ = 100 ms. Despite the distinctions between experimental and numerical setups (namely, in [24] the channel width was 5 cm and initial pressure of the stoichiometric H₂–O₂ mixture was 0.75 atm) one can see a good qualitative agreement of the flow patterns. The frame (d) in Fig. 8 corresponds to the frame (a), while the frame (e) shows already developed detonation wave as in the frame (c). The information about how the structure of the flame front is transformed into the detonation is lost and cannot be obtained at the experimental shadowgraphs. On the other hand the qualitative similarity of the flow patterns confirms that the process in natural experiment evolves via the mechanism similar to the described above.

The interpretation of the Oppenheim’s “explosion in the explosion” also can be obtained from analysis of the process shown on Fig. 2. Note first, that form Fig. 2 it is seen that the flame surface at the moment of detonation formation is multidimensional. It consists of several bulge tips that are advanced far ahead compare with neighboring flame bulges. These regions represent leading (tips) edges of the flame front where pressure pulses arise. On the contrary the shadow photos show projection of all planes intersecting the flame surface along the side walls of the channel. In the diagnostics plane one can observe the flame position and the shocks intersection points ahead of it, which can be more or less different depending on what cross section was taken (see e.g. Fig. 7 where the shadow visualization using XY and XZ planes are compared, Fig. 7a,b). These intersection points are the signals coming to the diagnostics plane out from the density gradients on the shock fronts radiated by the leading flame edges. There are no adequate conditions in such points to ignite detonation via local autoignition of the mixture, the detonation arises according to the mechanism described above in the reaction zone on the flame edge. In case of schlieren visualization with laser knife the pattern in the planar projection may show the detonation arising ahead the flame front (see e.g. Fig. 9) since the other part of the flow including the leading flame edge will be clouded by the laser knife. In this case it looks at the shadow photos as if detonation wave is formed ahead the flame front (See Fig. 9a). In fact as it is seen from 3D simulation, the phenomena of “explosion in the explosion” does not result out from the “hot spot” formation in the heated fuel–air mixture. It could be viewed as an artifact of the diagnostics caused by the lag between the leading edge of the flame where detonation arises and the remaining flame surface. Depending on how the schlieren or shadow photos were taken, the obtained image and interpretation of the one and the same phenomena can be quite different which can lead to misinterpretation of underlying physics of the phenomena. One can observe such a case obtaining full shadow photo (Fig. 8b) and compare it with the schlieren one (Fig. 9a).

6. Summary and conclusions

This work presents probably the most advanced and extensive direct numerical simulations, which allows to obtain high resolution 3D pattern of the flame acceleration and the transition from deflagration-to-detonation with account of a detailed chemical kinetics. 3D simulations provide us with 3D images of the accelerating flame and DDT, which in its turn makes it possible to get the correct interpretation of the experimentally obtained shadow and schlieren photos, and to resolve many confusions and erroneous conclusions about nature of the investigated phenomena. The performed 3D simulations support the mechanism of DDT proposed by the authors, which has been previously verified by 2D simulations. It should be noted that 2D simulations in general give a correct picture of hydrodynamic flow during the flame acceleration and DDT, as it is seen from the 2D cross sections in Fig. 2. The main difference between 2D case and 3D case is the different time scales of the process shown in Figs. 3–5.

In the present paper for the first time the patterns of schlieren and shadowgraph visualization of the flame acceleration and DDT were obtained using high resolution three-dimensional numerical modeling. Such implementation of 3D calculations makes it possible to avoid misinterpretation of the experimentally obtained schlieren and shadow photographs and was missed previously in the investigations devoted to transient gas-dynamic and combustion processes.

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