

# Numerical Investigation into Fast Deflagration and Its Transition to Detonation in Smooth Tube

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## Abstract

A high-resolution computational-fluid-dynamics (CFD) solver for the compressible Navier – Stokes problems with an overall kinetics of the hydrogen-oxygen chemical reaction is implemented which is applied to direct numerical simulation of propagation of fast deflagration, and its acceleration and transition to detonation in a 2D smooth tube filled by hydrogen-oxygen mixtures. The numerical results show that fast deflagration is a self-sustained combustion wave, and the pressure plays an important role to quickly transfer the heat produced during combustion to the unreacted mixture ahead of the flame. This work explains how to maintain and accelerate up the deflagration for its transition to detonation. The numerical solutions in this work are compared with experimental records. The comparisons show a good agreement between the numerical and experimental results.

## Mathematical Models and Numerical Methods

The basic equations governing the fast deflagration studied in this work are the compressible Navier - Stokes equations with chemical reactions that is controlled by the following chemical kinetics.

### Chemical Kinetics

A simplified one-step chemical kinetics introduced by Marinov et al [1] is employed:



To the above reaction there is only one production rate,

$$\dot{\omega} = A[\text{H}_2][\text{O}_2]^{0.5} e^{-\frac{E_a}{RT}} \quad (2)$$

$$\dot{\omega} = \begin{cases} A[\text{H}_2][\text{O}_2]_0 - \phi([\text{H}_2]_0 - [\text{H}_2])^{0.5} e^{-\frac{E_a}{RT}} & [\text{O}_2]_0 \geq \phi([\text{H}_2]_0 - [\text{H}_2]) \\ 0 & [\text{O}_2]_0 < \phi([\text{H}_2]_0 - [\text{H}_2]) \end{cases} \quad (3)$$

where  $\phi$  denotes the stoichiometric oxygen-hydrogen ratio that equals 0.5 in the above kinetics, and  $[\text{O}_2]_0$  and  $[\text{H}_2]_0$  are the initial molar concentrations of oxygen and hydrogen, respectively. The kinetics model (3) only involves one unknown variable, i.e., fraction of hydrogen. As a result, computational cost is significantly reduced. In principle, the kinetics (3) can be used in the cases with any oxidiser – fuel ratios, that is, fuel-rich, stoichiometric or fuel-lean combustion. When combustion is stoichiometric, however, the kinetics above will be reduced into

$$\dot{\omega} = A\phi^{-0.5}[\text{H}_2]^{1.5} e^{-\frac{E_a}{RT}} \quad (4)$$

All the cases studied in this work are stoichiometric combustion and kinetics (4) is hence employed.

### Boundary and Initial Conditions and Numerical Solutions

The initial condition is a reflection of the initial physical state of the reactant mixture. It is assumed that the initial reactant is an ideal mixture of fuel and oxidizer, which is statically and uniformly filled in a computational domain. In order to ignite reactions, there initially exists a high temperature in a very small zone, for example, a small vicinity of solid wall. After computation starts, the high temperature in the ignition zone will initiate the chemical reaction and generate propagation of the combustion waves.

In the above equation,  $[\text{H}_2]$  and  $[\text{O}_2]$  denote the molar concentrations of hydrogen and oxygen,  $A$  and  $E_a$  are the pre-exponential constant and activation energy of hydrogen and their values are  $A = 1.8 \times 10^{13}$  (cm<sup>3</sup>/mol-s) and  $E_a = 1.465 \times 10^5$  (J/mol), respectively. In this model of kinetics one still needs to solve two components for hydrogen and oxygen, respectively. Since the studied combustion is well premixed of fuel and oxidizer, it can be assumed that the ratio of the concentrations of hydrogen and oxygen is constant in computational domains without chemical reaction. In the reaction zone, ratio of the assuming rates of fuel and oxidiser is constant. Having these assumptions, the equation (2) becomes

There are three kinds of the boundary conditions in this work, inlet, wall and outlet boundary conditions. The inlet and outlet boundary conditions are implemented using the character relationship of the hyperbolic problem corresponding to the Navier – Stokes equations [2], so that the errors from the boundary conditions are reduced to the minimal level. The wall boundary condition for the flows is no-slip boundary condition, and for energy equation and mass transfer are adiabatic and no-mass-exchanging boundary conditions. The application of the no-slip wall boundary conditions allow to study the wall effect which is one of the important differences of this work and the work of [2].

The numerical method used in this work is finite volume method. The accuracy of finite volume method mainly depends upon flux calculation on the interface between two connected control volumes. The flux calculation involves three routines – reconstruction of the solution within the associated control volume, solution of the Riemann problem corresponding to the Euler equations and flux calculation for transport processes. The purpose of the solution reconstruction is to construct the distributed values on the interface of two control volumes from the averaged values over control volumes. In this work, a high resolution scheme, third order WENO scheme, is implemented in our in-house code [3]. After the solutions reconstruction, the Riemann problems will be solved by Liou-Steffen (AUSM) flux-vector splitting method [4]. Calculations to transport processes require to know the gradients of the solutions, which is computed by two

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methods, least squares method and Green-Gauss formula. To guarantee the total variation diminishing condition, SUPERBEE limiter [5] is adopted. After the spatial discretization, a set of ordinary differential equations is generated. A Runge – Kutta scheme of three levels is used to integrate the ordinary differential equations [6].

### Set-up of Numerical Computations

The fast deflagration and its transition to detonation studied in this work happen in a 2D smooth tube filled by hydrogen-oxygen mixture. The tube has a closed end and an open end, and is of the dimension of 5mm×200mm. In order to carry out the numerical computations, the computational domain is meshed uniformly by two sizes of finite volumes, which are 0.025mm×0.025mm and 0.05mm×0.05mm, respectively, so as to check mesh-independence of the numerical solutions. A typical flame thickness is approximately 0.5mm. Hence the resolutions of the two types of meshes ensure there are respectively 20 and 10 nodes in the flame zone. In fact, the numerical tests showed that the differences of the results produced by the two types of meshes are minor and therefore resolution of the mesh with the finite volume of 0.05mm×0.05mm is fine enough to produce accurate numerical solutions.

As mentioned in Section 2.3, initially, the reactant mixture is uniformly filled in the tube. The mixture is comprised of hydrogen, oxygen and inert gases such as nitrogen and argon. Their initial concentrations are case-dependent. Near the closed end wall it is assumed that there is a very thin layer or a very small point zone of high temperature which will initiate the chemical reaction. The high temperature may be generated by a fast deposit of the energy from an external source [2], or a shock wave reflection on the wall. In order to simplify the computations, these detailed processes to form the small high temperature zones are not simulated in this work, but the results are directly employed.

On the tube walls and closed end no-slip boundary condition is imposed for the flow and adiabatic boundary condition for the thermodynamic processes and no - mass exchange boundary condition for the mass transfer processes. The open end of the tube is outlet, on which the outlet boundary condition is specified. The computational time step is controlled by the CFL number. In this work, it is taken to be in the range of  $1.8 \times 10^{-9} \sim 2.5 \times 10^{-9}$  second.

### Computational Results and Discussions

The numerical results found that when external ignition temperature or deposit energy is certain there is a minimal concentration of hydrogen by which a fast deflagration can be activated. The minimal concentration is more than the low flammability limit. With increase of the deposit energy, the minimal concentration will decrease. However, there exists an absolute minimal concentration of hydrogen below which the fast deflagration cannot be initialized whatever the deposit energy is. This minimal concentration is larger than the low flammability limit as well. During the period of simulations, these fast deflagrations are sustained themselves or accelerated. No processes from the external sources, e.g., an external flow velocity, are needed to maintain the fast wave propagations. First critical concentration is named after the minimal concentration.

In the tube length of this research, not all the initialized fast deflagration can transition to detonation. In order to realize deflagration-to-detonation transition (DDT), the concentration of hydrogen must exceed the first critical concentration mentioned above. These results hence suggest that there is a second critical concentration of fuel, only beyond which DDT can take place. Namely, the second

critical concentration is larger than the first one under the same conditions. It may be argued that any fast deflagration can be accelerated to detonation if the tube length is sufficiently long and hence the second concentration equals the first one. The argument may be true, however this work deals with a finitely long tube and the conclusions above should be true at least for the cases with finite tube length which is often useful for real practice. In addition, the computational results also show that the initial temperature of the mixture has a favorable influence for the speed of propagation. The higher the temperature, the more the speed of combustion waves and therefore the less the second critical concentration.

It should be pointed out that the computational results in this work does not observe that the ignited fast deflagration is slowed down or degenerated to the slow deflagration (laminar flame or low-speed turbulent flame). In other words, as long as a fast deflagration is set-up, it either propagates at a high speed continuously or is accelerated up to detonation. In summary of these observations, it appears to suggest that the fast deflagration is a separated mode of combustion waves from the low deflagration (laminar flame or low-speed turbulent flame) and also we have a general rule,

$$C_{\min}^{DDT} > C_{\min}^{FF} > C_{LFL} \quad (5)$$

where  $C_{\min}^{DDT}$ ,  $C_{\min}^{FF}$  and  $C_{LFL}$  represent the minimal concentration of hydrogen for DDT (second critical concentration), minimal concentration of hydrogen for fast deflagration (first critical concentration) and low flammability limit, respectively. It is noted that these computational results above are basically in agreement of the experiments [7].

Propagation of fast deflagrations can be divided into two stages, ignition stage and fully developed stage of fast deflagration. After the ignition, the deflagration will spread and accelerate. The ignition stage is ignition-manner-dependent. The ignition stage generally completes at the length of 5 ~ 10 tube diameters. In this work, the two ignition sources are employed which are near the closed end wall. At the end of the ignition stage the combustion waves ignited by the two methods grow up to the fully developed stage and the pattern of both combustion waves is getting similar. That implies that influence of the two ignition manners can be ignored in the fully developed stage. To the ignition by a point source, the flame goes through hemispheric flame, finger-shaped flame, and finally becomes a so-called "tulip flame" [8, 9]. Here a comparison of the numerically computational results with the experiments done by Liberman et al [10] is presented in Figure 1. The experiments are a series of shadow photographs of  $H_2 - O_2$  flame at the initial pressure of 0.2 bar, while the computational results illustrate the distributions of the local density normalized by the initial density in which the blue area has a value of 0.07 and the yellow is about 1.5. One can see that both developments are of a good agreement. The speed of combustion wave is increased in this stage. The experimental measurement [10, 11] found that the increase rate follows an exponential rule. Qualitatively it is consistent with the numerical computations. Bychkov et al [12, 13] theoretically studied the flame development in this stage and obtained an analytical expression for the flame speed, which supports the conclusion as well.

In the fully developed stage, the combustion wave is getting quasi-steady, although the compression waves induced by the flame are yet of a large unsteadiness. Figure 2, for instance, displays a typical pattern when the wave ignited by a

line source near the end wall of the tube. In this case, the unreacted mixture is comprised of the hydrogen with the molar concentration of 23% and the oxygen with the molar concentration of 11.5% and an inert gas. The ambient temperature is 300K and initial pressure is 1 atm. The density and pressure in Figure 2 are normalized by the initial density and pressure, respectively. This propagation mode of fast deflagration and the flame shape was experimentally observed in the early 1950s [8, 14, 15] and by the experiments done recently [10, 11] as well. If comparing the density distribution in Figure 2 (b) with the schlieren photographs of Figure 11 in Liberman et al work [11], one can see that they are of the same pattern: two separated flames attached on the top and bottom walls respectively and a series of compression waves and weak shock waves ahead of the flame. Also, many experimental measurements, e.g., [16], showed that the speed of the fast deflagration in this stage is almost constant, which is supported by the numerical computations in this work as well.

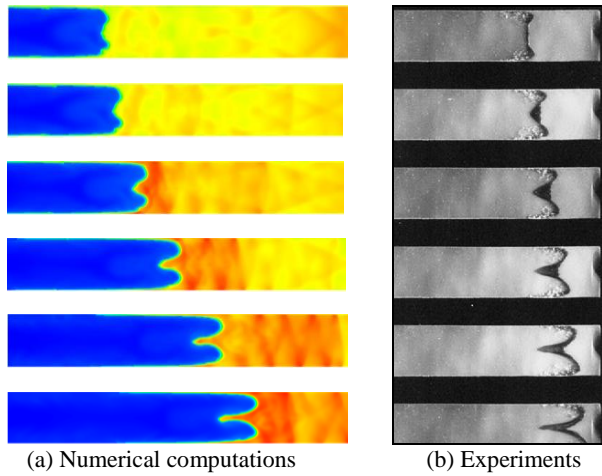


Figure 1 Comparison of the numerical results with the experiments done by Libermann et al [11].

Recently, Liu proposed a mechanism for DDT [2], which can be applied to explain the propagation of the fast deflagration as well. According to the mechanism, the propagation of fast deflagrations can be divided into two types of modes. One is acoustic mode and the other is convection mode. Propagation of the flame belongs to the convection mode and the corresponding compression waves are the acoustic mode. The wave of acoustic mode is produced by the wave of convection mode, however it affects movement of the wave of convection mode, for example, through transfer of the energy produced by the reactions. Theoretically, propagation of these two types of modes are different. In Figure 2 we can see that the wave of convection mode is quite stable that expresses a quasi-steady process, while the wave of acoustic mode has a strong unsteadiness. Just because of the unsteadiness, the energy produced by the reactions transfers ahead of the flame quickly to maintain a high speed of the combustion wave. For example, Figure 3 shows the temperature distribution ahead of the flame. The temperature of wave-form in Figure 3 is just produced by the pressure waves, which has a value of about 1.5 time initial temperature. Near the front of the flame the temperature is higher, since the intensity or amplitude of the wave of acoustic mode there is larger. This is the reason why the fast deflagration can propagate so fast without external sources. In the theoretical model of the low-speed deflagration, the waves of acoustic mode are filtered and therefore we cannot get a reasonable explanation to the propagation of fast deflagration from there.

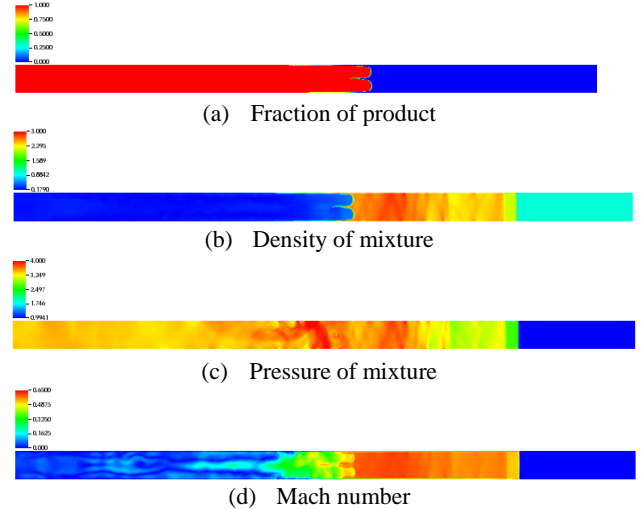


Figure 2 Distributions of physical quantities of a fast deflagration after the ignition by a line source on the end wall, in which the density in (b) and pressure (c) are normalized by the initial density and pressure, respectively



Figure 3 Temperature distribution ahead of the flame

If increasing the concentration of hydrogen to 28.5% but the ambient temperature and pressure keep same as the case in Figure 2, a periodically acoustic mode is produced ahead of the flame which forms a pattern of cellular structures. Figure 4 is the distribution of the mixture density, in which the time interval between two slides is 35  $\mu$ s. From Figure 4 it is seen that the movement speed of the leading edge of the flame is almost constant that equals about 315 m/s. To compare the numerical simulations with experimental observations, three schlieren photographs taken by Kuznetsov et al [17] are also showed in Figure 4. The numerical results are almost identical with the experimental records. The pressure variation is illustrated in Figure 5. One can see that the periodic mode with cellular structures is only in the front of the flame. From Figure 5 one also sees the formation and coalescing of the weak shock waves upstream away from the flame. All these processes are presumably a portent and preparation for a further acceleration of the fast deflagration. It should be pointed out that the periodic structures in Figure 4 and 5 can be produced in a 1D numerical simulation as well. For example, Figure 6 displays the profiles of pressure and temperature at three different time instants, which is obtained by solving 1D model of the tube with two open end.

In above section, the mechanism proposed by Liu [2] is applied to explain the propagation of fast deflagrations. According to that mechanism, the pressure wave of acoustic mode produced by the reactions is the basic reason for maintaining the fast propagation of the combustion wave. If the intensity of the acoustic mode wave or pressure wave ahead of the flame is not changed, the combustion wave will keep a constant speed in propagation. Nonetheless, when an acceleration of the fast deflagration happens, there must be a

significant change of the pressure wave ahead of the flame. The following numerical results will further verify this rule.

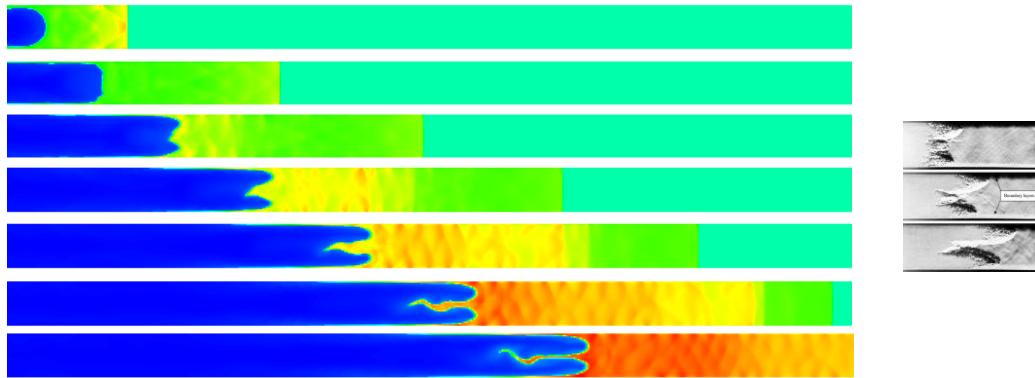


Figure 4 Distribution of the mixture density and comparison with the experimental observations [16]

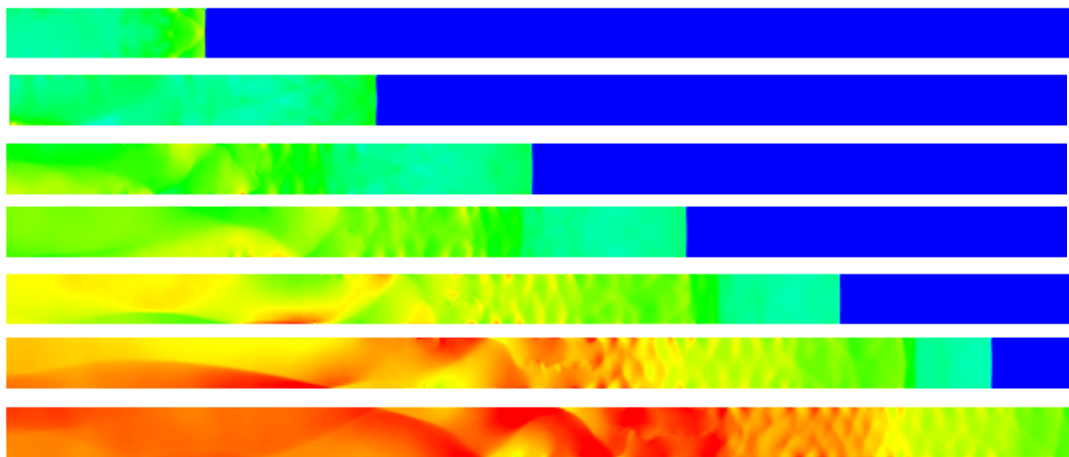


Figure 5 Distribution of the pressure in the same case as Figure 4

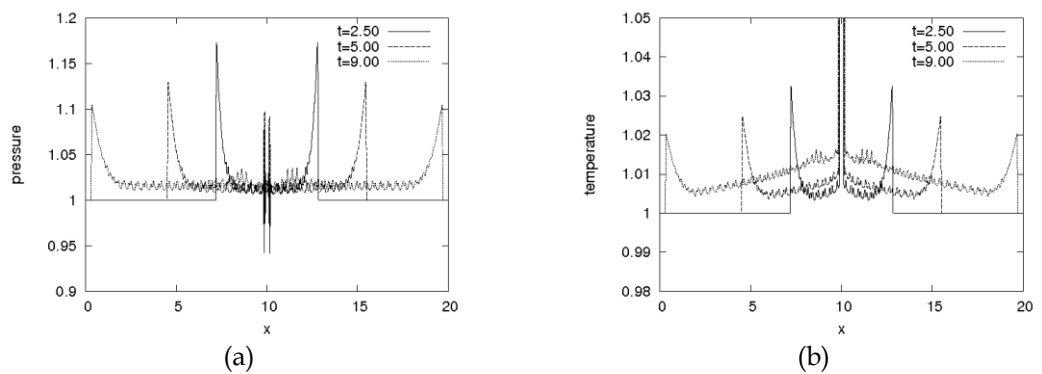


Figure 6 Profiles of pressure (a) and temperature (b) at three time instants

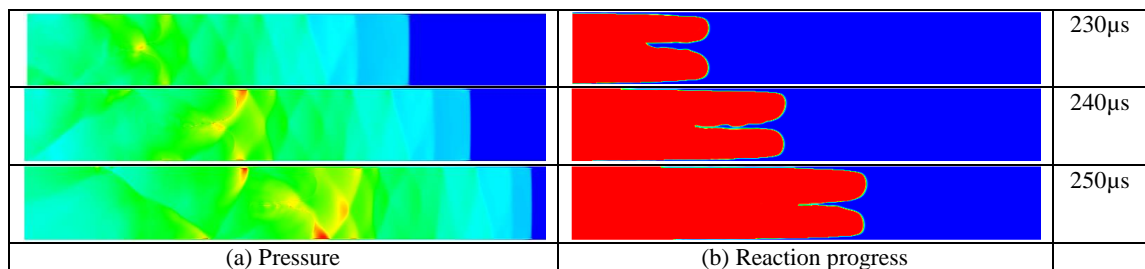


Figure 7 Evolution of pressure waves (a) and reaction progress (b) just before transition from deflagration to detonation

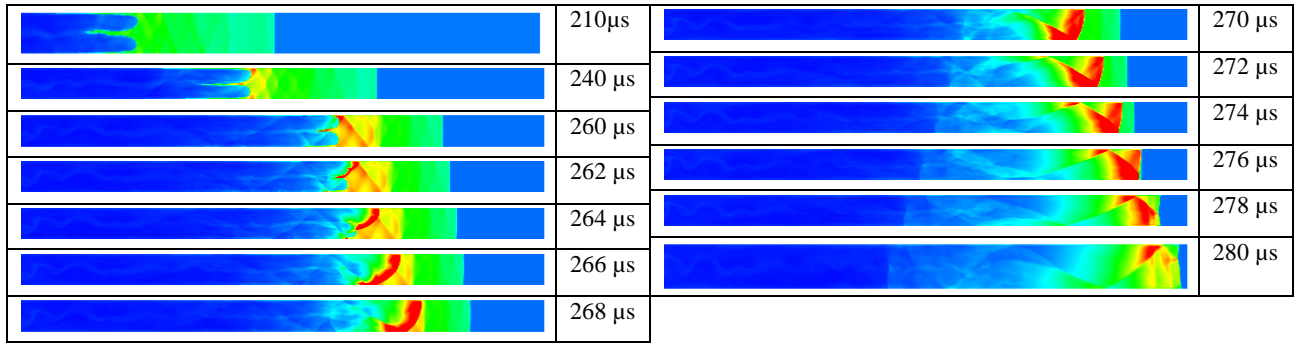


Figure 8 Distribution of the mixture density

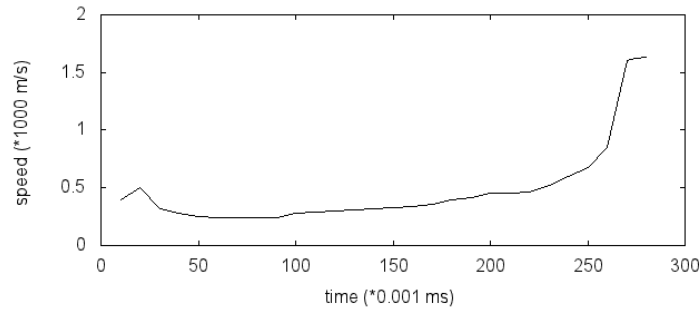


Figure 9 Speed of the combustion wave

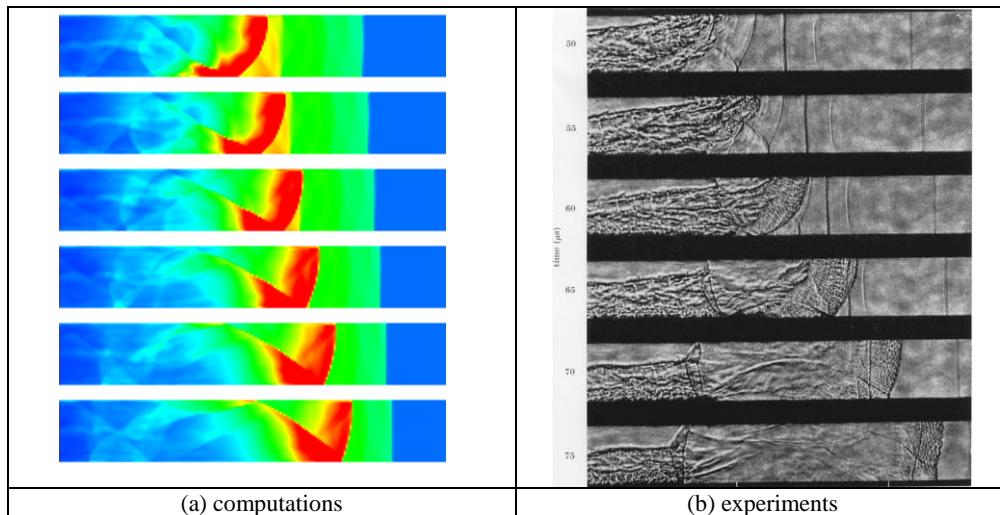


Figure 10 Comparison of numerical solutions and experiments [21].

Before presenting the results we should note two important points. The first one is that fast deflagration is a self-sustained combustion wave propagation, because it does not need an external source to maintain itself. This point has been proved by some previous research works [7, 10, 11, 16 – 18] and this work. The second point is the differences between the low-speed and fast deflagrations. The low-speed deflagration cannot produce overpressure but the fast deflagration does; the low-speed deflagration does not need to generate a big pressure wave to maintain itself but the fast deflagration needs. Because of having these attributes, the fast deflagration is often called "explosion", but it is not detonation. A further acceleration of the fast deflagration is possible for transition from deflagration to detonation. The transition to detonation from fast deflagration is therefore referred to as "explosion in the explosion". Now we move on

to present the numerical simulations on acceleration of the fast deflagration and its transition to detonation.

Since the length of the tube is finite, not all the quasi-steady fast deflagrations produced in this work can be accelerated up to detonation before the mixture in the tube is burned out. If raising the initial temperature in the mixture, however transition to detonation can early start. Accordingly, the initial temperature of the mixture is taken 450K in the following case study, while its initial pressure and concentration of hydrogen are 1 atm and 11%, respectively. After an evolution of quasi-steady stage (see Figure 9), the fast deflagration in this case study starts to speed up and transition to detonation. The detailed transition will be discussed in next section. Here we concerns development of the pressure wave ahead of the flame just before the transition, which is illustrated in Figure 7 (a). Three pairs of graphics on the pressure distributions and reaction progresses are showed in

Figure 7. They are at the time instants of 230 $\mu$ s, 240 $\mu$ s and 250 $\mu$ s, respectively (transition to detonation starts at 262  $\mu$ s). In Figure 7 (a), the red colour denotes 10 atm and the yellow about 7 atm. From Figure 7 (a) we see that the compression waves ahead of the flame start to form shock waves that are enhanced gradually. The original positions to form shock waves are mainly on the wall boundary layers. The speed of the flame, because of being deflagration, is less than that of the shock waves and separated from them, while the shock waves travel forwards away. Figure 7 (b) shows that in the zone of the shock waves there is no chemical reactions.

The density variations of the mixture in Figure 8 well demonstrate the whole processes of transition to detonation. One can see that the start point of the transition is from the top wall boundary layer at the instant of 262  $\mu$ s, where there is a strong shock wave. The initialized detonation quickly spreads along the flame front and there forms an area of new reactions which rapidly increases the heat released and enlarge and enhance the existing shock wave. Because of being stronger, this shock wave associated with the reactions travels the fastest and coalesces the shock waves generated previously, see Figure 8 at 264 $\mu$ s ~ 270 $\mu$ s. The coalescing of multi-shock waves further accelerates up the original shock wave or detonation so that it obtains a very sharp variation of its speed, see Figure 9. By the instant of 270 $\mu$ s, the first phase of the transition is done. In fact, in the first phase, the yellow area ahead of the flame (260 $\mu$ s ~ 270 $\mu$ s) can be viewed as a pre-heated zone. It is presumable in that zone the induction time gradient theory [19, 20] is applicable. If it is true, this work provides an explanation how the induction time gradient is built up, since this issue is still open at the moment.

The second phase of the detonation is to catch up and coalesce the leading shock wave and complete the transition from 270 $\mu$ s to 276 $\mu$ s. In the meanwhile, a little increase of the flame speed is generated, seeing Figure 9. In Figure 10 a comparison of the numerical simulations and experimental records [21] is displayed, from which one can see that both flame developments are almost identical.

### Conclusions

The numerical results shows that there exists a minimal concentration of hydrogen below which fast deflagration cannot be initiated. This minimal concentration, named after first critical concentration in this work, is larger than the low flammability limit of hydrogen. It is a function of the initial temperature and decreases with the temperature rising. In the finite length of tube, it is possible that the fast deflagration is secondarily accelerated so as to transition to detonation. In order to realise the transition, the concentration of hydrogen should be more than the first critical one. The minimal concentration of hydrogen that ensures realisation of deflagration-to-detonation transition is referred to as second critical concentration. These two critical concentrations like the flammability are the properties of the hydrogen-oxygen mixture, which will be useful in applications.

The numerical simulations also indicate that the fast deflagration is self-sustainable in propagation. Only when it is accelerated up, its propagating speed can be significantly changed, while in the other propagating time, its speed is almost unchanged. The acceleration of deflagration is a jump

process whose duration is very short. The mechanism proposed by Liu [2] can explain propagation, acceleration and transition of the fast deflagration. The numerically computational results are compared with the experimental observations. The comparisons show that the numerical solutions have a good agreement with the experiments.

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