Numerical Study of Shock-Flame Interaction and Deflagration-to Detonation Transition in H_2-O_2 mixtures Using a Detailed Chemical Reaction Model

A. D. Kiverin[1], M. F. Ivanov[1], M. A. Liberman[2, 3]

[1] Joint Institute for High Temperatures, Russian Academy of Science, Moscow, Russia
[2] Skobeltsyn Institute of Nuclear Physics, Moscow State University, Moscow, 119991 Russia
[3] Department of Physics and Astronomy, Uppsala University, Box 530, 751 21, Uppsala, Sweden

1 Introduction

The interaction of shock waves with the flame fronts is an important mechanism leading to flame acceleration, transition from deflagration to detonation (DDT), transition to turbulence. It results in distortion of the flame, the increase in the energy release rate, can lead to considerable flame acceleration and DDT and it is of great practical interest in the context of safety problem. There have been numerous of previous attempts to simulate the shock-flame interaction numerically using a simplified chemical model of a one-step exothermic reaction. However, a one-step reaction model cannot reproduce the main properties of the combustible mixture such as induction time in chain-branching kinetics, as well as an increase of the reaction rate. Taking into account considerable difference in the induction times obtained from detailed chemical models and from one-step models, the results of simulation using a one-step model must be considered with greatest discretion. It was shown [1] that the evolution to detonation from the temperature gradient is profoundly different for detailed chain branching kinetic models than for one-step kinetic models and that the steepest temperature gradient capable to initiate detonation is by orders of magnitude more shallower compared to that predicted from a one-step model for highly reactive mixture (H_2/O_2) and for slow reactive mixtures (methane/air). Use of reliable detailed chemical kinetic models is important for correct understanding of combustion phenomena since results obtained using chain-branching chemistry models are considerably different from that found for one-step chemistry. It is therefore important to investigate and understand the differences in the shock-flame interaction between chain-branching kinetics and the predictions from one-step models.

In this work we report selected results of high resolution two-dimensional numerical simulations with a detailed chemical kinetics of the series of comprehensive study of the interaction of a flame with an incident shock and then with a shock reflected from the endwall. The flame distortion by the shocks, the increase of the energy release rate in the system, and the transition from deflagration to detonation (DDT) caused by the shock-flame interaction are investigated.

Correspondence to: A.D. Kiverin <alexeykiverin@gmail.com>

2 Formulation of the problem, numerical method

The main focus of the present studies is to examine how the shock-flame interaction amplifies shocks and flame instabilities, generates a flame brush and leads to the transition to detonation in hydrogen-oxygen mixture. Emphasis is on comparing and contrasting the results of simulations using a detailed chemical kinetics with previous studies based on a one-step chemical kinetics. The high resolution simulations modeled a flame ignited near the left closed end and propagating to the right in the two-dimensional rectangular channel. A driven shock propagates from the right open end to the left. The initial velocity of the gas is set to zero everywhere ahead of the shock and the flame. We performed two series of simulations: for smooth slip adiabatic walls and for no-slip boundary conditions at the channel walls to expose clearly the features of the flame-shock interaction. In both cases the incident shock strength varied $M_{sh} = 1.2 \div 2.5$. Initial temperature and pressure were $T_0 = 298\text{K}$, $P_0 = 1\text{bar}$. We investigated effects of the shock-flame interaction examining the flame distortion by the incident and reflecting shocks, how the flame evolves after the interaction, how it modifies the energy release rate in the system, how the Richtmyer-Meshkov (RM) and Kelvine-Helmholtz (KH) instabilities grow and influence the development of the flame brush, and how the initial flame perturbations influence the growth rate of RM instability.

The computations solved the two-dimensional, time-dependent, reactive Navier-Stokes equations for compressible flow including the effects of viscosity, thermal conduction, molecular diffusion, real equation of state 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 and energy release [2, 3]. We used the real equations of state for the reactive species and combustion products with the temperature dependence of the specific heats, heat capacities and enthalpies of each species borrowed from the JANAF tables. The viscosity and thermal conductivity coefficients of the mixture were calculated using the Lennard-Jones potential. Coefficients of the thermal diffusivity conduction of i-th species $\kappa_i = \mu_i c_{pi} / \text{Pr}$ were expressed via the viscosity coefficient μ_i and the Prandtl number, $\text{Pr} = 0.75$. Details of the computational method were described and tested extensively in [2, 3, 4]. Its validation, convergence and resolution tests with the meshes up to 64 computational cells per flame width were presented in [4].

3 Shock-flame interaction

This section is devoted to the study of the flame instability development. The flame acceleration arises due to increase in flame velocity which for an initially laminar flame front is manifested as an increase in flame surface due to wrinkling of the flame front caused by the hydrodynamical instabilities.

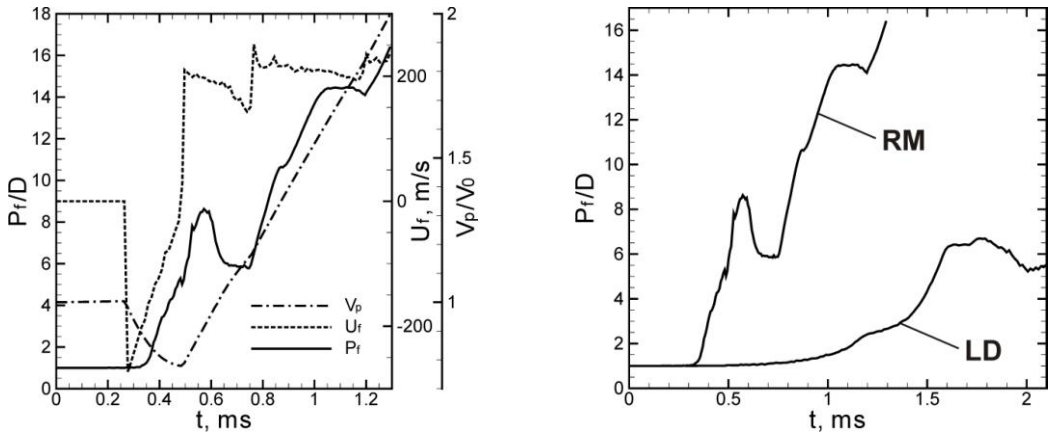

Figure 1. Growth of the flame front surface and the flame velocity resulted from the flame-shock interaction (left). Comparison of the flame surface growth rates in cases of free propagating flame and flame affected by the shock (right).

The perturbation resulting from the shock-flame interaction grows due to the Richtmyer-Meshkov (RM) instability and this leads to the additional increase in the flame surface and the burning rate. Development of the instabilities is analyzed accurately and clear scenario of the increase in flame surface and burning rate is formulated.

A series of simulations was performed to investigate the development of the RM instability resulting from the shock-flame interaction and how it influences the energy release rate depending on the amplitude of the initial flame front perturbation and strength of the incident shock. The flame accelerates due to the wrinkling of the flame front caused by the instabilities and consequently the increase of the flame surface. Depending on the strength of the incident shock there are different scenarios of the shock-flame interaction and the transition to detonation. Results of the simulations show a complex sequence of events: from the interactions of an incident shock with an initially laminar flame, development of the RM instability and wrinkled flame front and finally the emergence of a self-sustained detonation with typical detonations cells structure. The calculated evolution of the flame front surface and the flame velocity resulted from the flame-incident shock interaction is shown in the left image in figure 1. Here V_p is the volume of the burned products which defines location of the flame front relative to the endwall; P_f/D shows the increase of the flame surface, where P_f is the flame surface area and D is the channel width; $U_f=d(V_p/D)dt$ is the flame velocity. In order to isolate the impact of the RM instability, the flame front location in the right image of figure 1 are shown also for a flame propagating for the same conditions but without interaction with a shock. If the flame is allowed to grow with no shock interactions, the surface becomes slightly perturbed as the flame expands. The initial perturbations imposed on the flame front are small and barely seen at the startup conditions (stage 1 in figure 2). Later they are amplified either in the case of Landau-Darrieus (LD) instability development or in the case of the interaction with the incident and reflected shocks and with the flow generated by the flame. As the shock interacts with the flame, the RM instability on the large-scale is triggered by the overall curvature of the flame. The effect of these interactions is the increase of the surface area of the flame, and as a result the energy release in the system increases. The flame evolution in this case and in the case of LD instability development is shown in figure 2. In the left image of figure 2 one can observe development of the linear (2) and non-linear (3) stages of RM instability triggered by the interaction of the initially perturbed flame with the incident shock. It is important to note that non-linear stage develops under influence of the rarefaction wave which causes additional expansion of the flame (see corresponding time interval (3) in figure 1 where the rate of flame deceleration decreases).

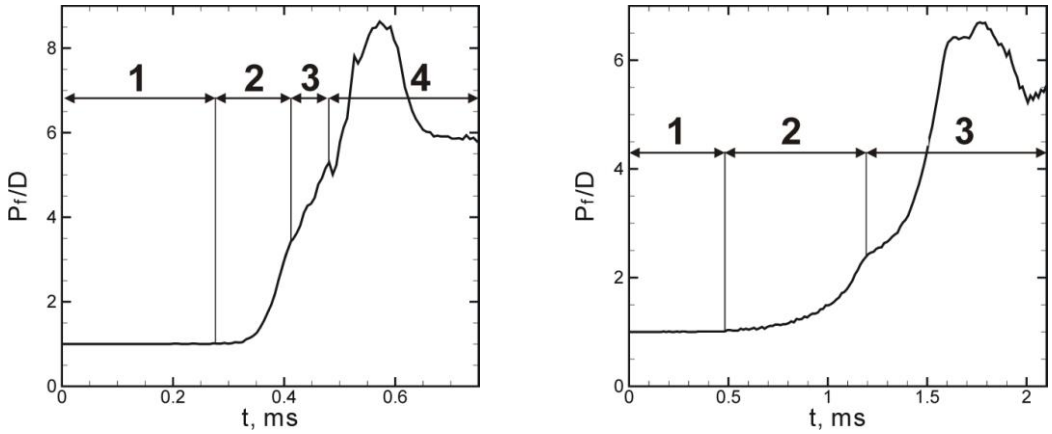

Figure 2. Development of RM (left) and LD (right) instabilities. 1 – stages of initial spectrum birth out from initial perturbation; 2 – linear stages of instabilities' development; 3 – non-linear stages of instabilities' development; 4 – further flame evolution.

Further development of the flame (stage 4) is caused by the interaction with the reflected shock and secondary shocks and corresponds to the development of secondary instabilities. In case when there is

no interaction with shock (right image of figure 2) the flame develops due to the LD instability of the flame front which evolves out from initial perturbations: linear stage of exponential growth (2) and non-linear stage of harmonics interaction which causes flame stabilization (3).

4 Deflagration to detonation transition

The shock-flame interaction amplifies shocks and the flame instabilities, generates a flame brush and leads to the transition to detonation. Depending on the strength of the incident shock there are different scenarios of the shock-flame interaction and the transition to detonation [5]. The simulations show that the interactions of shocks and flames can create the conditions under which deflagration-to-detonation transition may occur. As an example, we present here results for three regimes of DDT: 1) transition to detonation triggered by the shock reflected from the back wall with the Mach number of incident shock in the range M=1.5-2.5; 2) transition to detonation for the case of weak shocks, M=1.2-1.5, 3) the case of a strong incident shocks and transition to detonation in the incident shock, M≈2.5.

Figure 3 shows typical scenario and the flow structure during DDT which occurs when the incident shock wave of initial intensity M=1.8 first passes through the flame, reflects from the back wall and then re-catches and passes through the flame front.

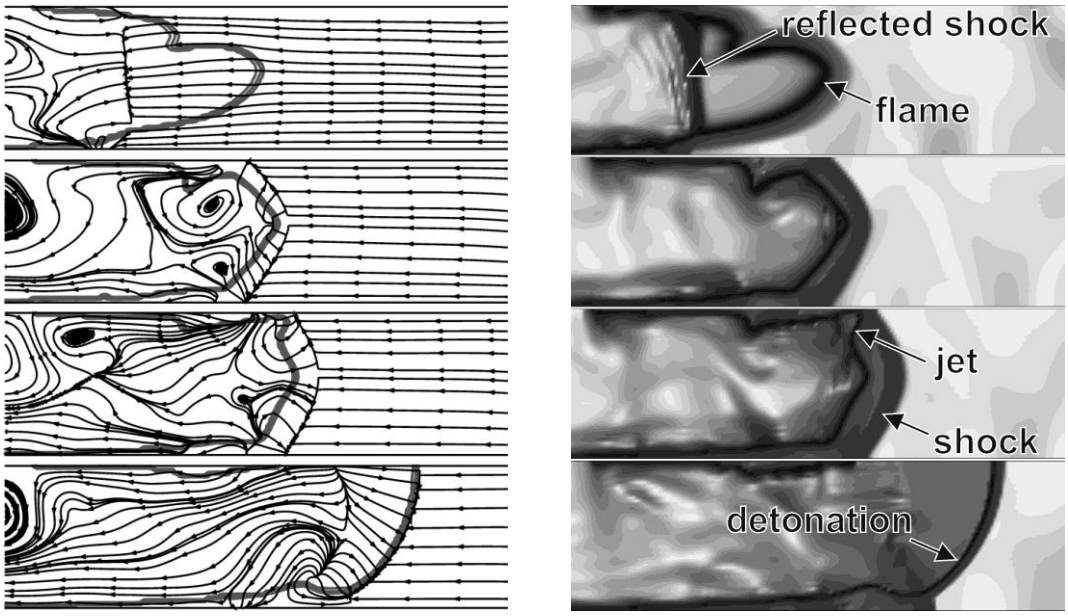

Figure 3. Structure of the flow (left) and transition to detonation (right) during shock-flame interaction for the shock Mach number M_{sh}=1.8.

The plots on the right in figure 3 show the details of the interaction of the reflected shock and the flame. After the shock is reflected from the back wall and passes through the flame a large scale vortex (swirl) develops behind the reflected shock (figure 3- right) as well as two vortices are developing near the walls when the reflected shock catches the right surface of the flame. It is likely that they are enhanced due to the flame-rarefaction wave interaction. When the shock emerges from the right side of the flame, it is refracted, triggers the RM instability, and the overall effect is the formation of a jet near the boundary wall. This causes a pressure peak propagating along the flame surface, which is coupled with the reaction zone and next will transition to detonation.

When intensity of incident shock waves is smaller, the flame is accelerated behind the reflected shock. The accelerated flame generates the pressure peak and transition to detonation according to the mechanism of DDT described in [2, 3].

Figure 4 shows the case of the flame interaction and transition to detonation for a strong shock wave, M=2.5. In this case one can observe the incident shock (1), the shock refracted on the flame

surface (2) and the shock reflected from the flame surface (3). As a result, a triple point of three shocks intersection is formed: (4) in figure 5. The pressure is maximal in the triple point and it is quickly (with supersonic speed) spreads along the flame surface simultaneously amplifying due to the positive feedback between the pressure and the enhanced reaction rate in the reaction zone. Frames in the figure show zoomed images of the triple point (4), the detonation (5), and the retonation wave (6). One should note that the mechanism of detonation formation remains similar in the variety of cases: the flame couples with the pressure wave and transforms into detonation due to the concurrent increase of the pressure and reaction rate.

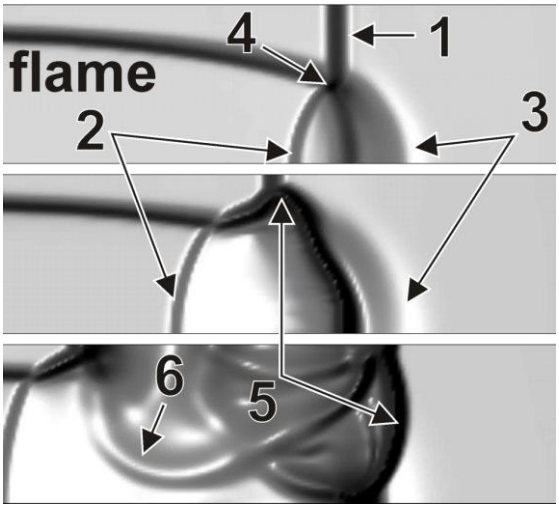

Figure 4. Formation of the triple point and transition to detonation for a strong incident shock wave.

5 Conclusions

The results of the present study show that numerical simulations of the shock-flame interaction with account of a detailed chemical kinetics are qualitatively different from those used a one-step chemical model. The conclusion is that the development of the RM instability and the resulting rate of the energy release are profoundly different from those obtained with a one-step chemical model. Results of the simulations, which use simplified one-step kinetic must be considered with greatest discretion, taking into account huge difference in the induction times of a one-step model and a detailed chemical schemes. The validity of the conclusion based on the one-step kinetics that the detonation arises due to the Zel'dovich gradient mechanism in a spatial gradient in chemical induction time formed in hot spots and the like is questionable. The mechanism of transition to detonation is the pressure peak localization at the flame front which is enhanced in time exponentially due to the positive feedback between the pressure peak and the reaction. This exponentially growing pressure pulse then steepens into a strong shock, which is coupled with the reaction zone, and triggers the transition to detonation. In the case of no-slip boundary conditions the overall picture of the flow and shock flame interaction is considerably complicated by the flame acceleration caused by the wall friction, the flame stretching along the wall in the boundary layer and development of KH instability.

References

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