Hydrodynamic Instability as a Mechanism for Deflagration-to-Detonation Transition

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The present work is concerned with identifying the basic mechanisms controlling the spontaneous transition from deflagrative to detonative combustion whose complete understanding remains elusive. In Zeldovich's foreword to Nettleton's monograph on gaseous detonation, when discussing the problem of transition, he wrote, "The role of the internal instability of the plane slow flame (Landau, Darrieus) is still not clear" [1].

The purpose of the present study is to gain a better insight into this question. To visualize the spatial picture of the transition a wave of premixed gas combustion spreading from the closed to the open end of a smooth-walled rectangular channel is studied by direct numerical simulation of the two-dimensional Navier-Stokes equations for a compressible reactive flow. A simplified chemical model based on a one-step, *n*-th order Arrhenius kinetics, controlled by the deficient reactant is employed. To single out the impact of the Darrieus-Landau instability, the gas flow is subjected to the free-slip and adiabatic boundary conditions, thereby eliminating possible influence of the momentum and heat losses, discussed in [2]. The simulations are performed on a parallel supercomputer, employing an adaptive mesh-refinement numerical code to ensure high resolution of the combustion waves as well as the shocks [3]. It is, for the first time, shown that in relatively wide channels ($70\div200$ flame widths, L_f) the Darrieus-Landau instability may bring on interaction of emitted and reflected shocks capable of nucleation of hot spots, ahead or within the folds of the corrugated flame, triggering an explosive transition from deflagrative to detonative combustion. The effect is found to be sensitive to the flame's normal speed, the reaction rate temperature- and pressure-dependences, favoring fast flames, high activation energies and high order reactions.

The emerging dynamical picture may be described as follows. After the ignition the flame speed rapidly increases from its normal value, corresponding to the associated open-space flame, to a markedly higher value, induced by the compressive preheating, due to the semi-confined geometry of the system. Upon this incipient stage, the flame is still planar and propagates at a nearly constant speed. Gradually, the high-speed planar flame looses its stability, developing slowly growing corrugations. Simultaneously, the flame speed undergoes progressive amplification, and in the course of time reaches and exceeds the ambient speed of sound. In addition to sustaining the leading shock, the evolving flame generates a cascade of oblique mild shocks reflected by the channel's walls.

Apart from the growth of the flame area, the flame acceleration may be caused by the positive feedback between the high-speed propagation of the corrugated flame and flame-generated compressive preheating of the unburned gas. The positive feedback mechanism enters the play when the heat liberated in the reaction zone exceeds that going into preheating of the unburned gas, the situation which may emerge in sufficiently fast burning mixtures [4]. At a certain stage, the fresh mixture ahead of the advancing flame falls into the proximity of the auto-ignition threshold, and becomes vulnerable even to mild temperature bulges (hot spots) permanently produced by the shuttling shocks. When the mixture becomes ripe enough, one of the hot spots triggers a localized explosion, initiating the rapid transition to detonation (Figs.1-3). The localized explosion occurs either between the flame brush and the leading shock, or in the interior of the flame fold. Under an unfavorable combination of parameters (slow flames) the autoignition threshold is never reached, rendering the transition unfeasible.

It may therefore be concluded that the Darrieus-Landau instability alone is definitely capable of triggering the transition. Yet, for many conventional explosives this would require an appropriate preconditioning (preheating, precompression), to make the flame-induced autoignition attainable. It is also found that the replacement of the free-slip by the more realistic no-slip boundary conditions (Fig.4), or by rough walls (Fig.5), facilitates the transition, by not only shortening the predetonation time and distance, but also by evoking the transition in situations where for smooth and free-slip walls it is ruled out. In the latter case the deflagration is triggered by a localized explosion in the near-wall mixture adjacent to the flame front.

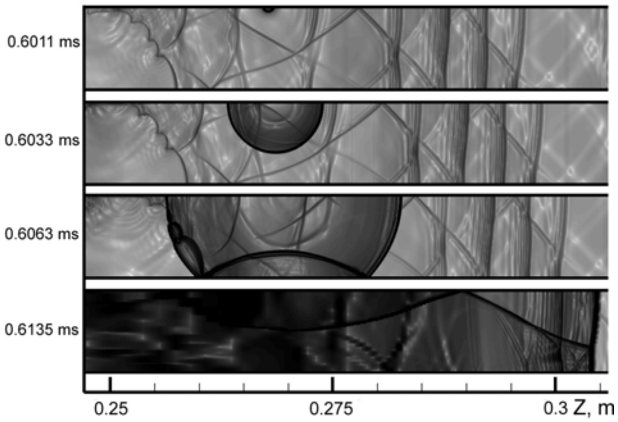

Figure 1.

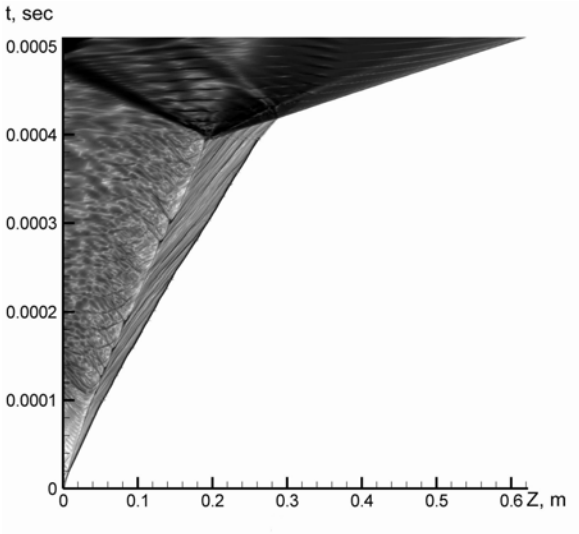

Figure 2.

Figure 1 depicts the modulus of the pressure gradient, $|\nabla P|$, at several consecutive instants of time. Conditions employed are specified as follows: the reaction order $n=2$; ambient temperature, pressure, and sound speed are $T_u = 300K$, $P_u = 1$ Atm, $a_u = 346 m/s$; adiabatic temperature of combustion products $T_b = 10T_u$; the flame's normal speed $U_f = 0.05a_u$; activation temperature $T_a = 4T_b$; channel width $D = 70L_f$; Prandtl number $\Pr = 0.5$; Lewis number $Le = 1$; specific heat ratio $\gamma = 1.4$. The transition is triggered by the explosion ahead of the flame front. Figure 2 shows the space-time record for the advancing flame, leading and secondary shocks, as well as detonation and retonation waves emerging upon the explosion, conditions are as for Fig. 1.

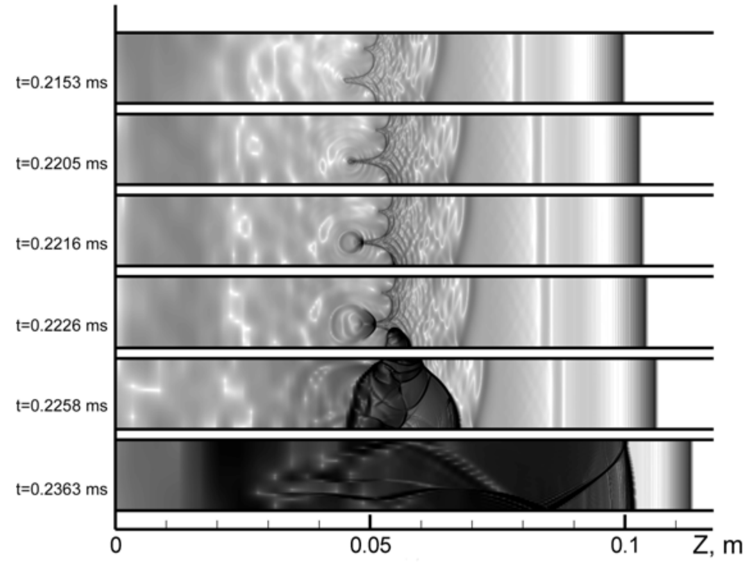

Figure 3.

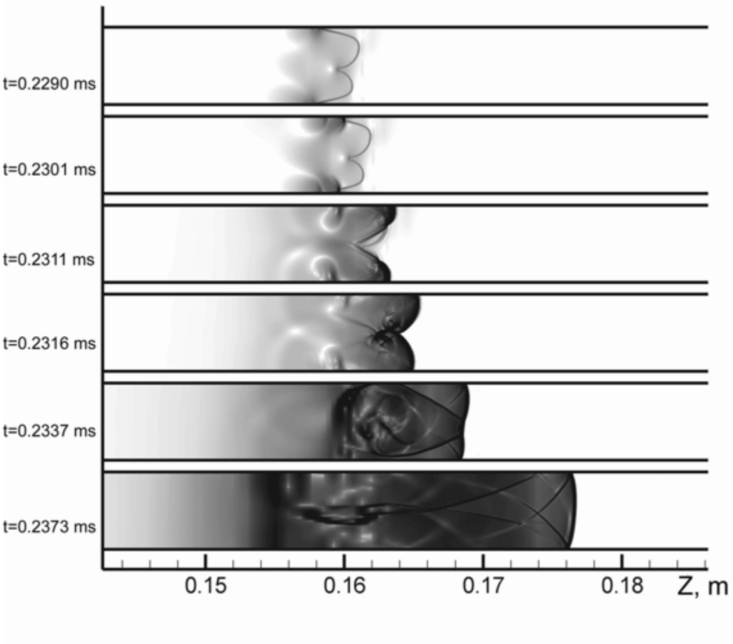

Figure 4.

Figure 3 shows the $|\nabla P|$- field for $n = 3,\ T_b = 8T_u,\ U_f = 0.04a_u,\ T_a = 4T_b,\ D = 140L_f$. Other conditions are as for Fig. 1. The transition is triggered by the explosion within the flame brush. Figure 4 shows the $|\nabla P|$- field for the smooth-walled channel with no-slip boundary conditions, $n = 3,\ T_b = 8T_u,\ U_f = 0.075a_u,\ T_a = 4T_b,\ D = 70L_f$. Other parameters are as for Fig. 1. Note that in this case, under the free-slip conditions the transition does not occur.

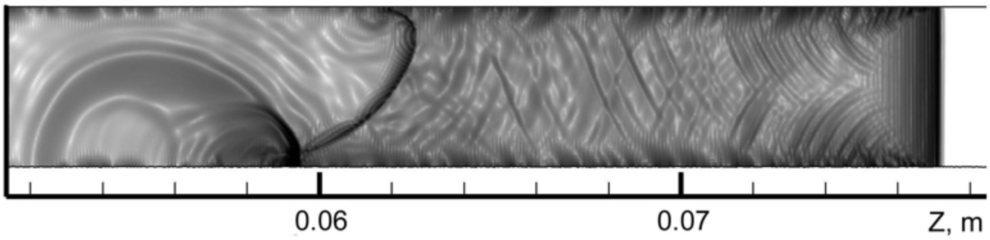

Figure 5.

Figure 5 shows the $|\nabla P|$- field for the rough-walled channel with free-slip boundary conditions. Other parameters are as for Fig. 1. In this situation, as one might anticipate, the transition is triggered near the wall and occurs much faster.

References

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