Numerical Simulations of Deflagration-to-Detonation Transition: The Role of Heat Losses

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1 Introduction

Spontaneous transition from deflagrative to detonative combustion is one of the major phenomena of premixed gas combustion whose first-principle understanding is still far from adequate. Turbulent combustion, experimentally observed and often considered to play a dominant role in the transition, cannot tell the whole story because turbulent burning velocities are still a factor of 10 or more too small to generate strong enough pressure waves. Recent theoretical findings based on the one-dimensional ZND-Fanno model [1] suggested that the transition is presumably triggered by the flow deceleration in the boundary layer, irrespective of whether the bulk flow is turbulent or not. The later numerical simulations in narrow channels [2-4], and experimental studies with capillaries [5] provided solid evidence that the transition may indeed take place in laminar flows.

The first numerical simulation of the transition in narrow channels was conducted under adiabatic conditions [2]. The impact of walls was accounted for through no-slip boundary conditions inducing resistance to the gas flow. The hydraulic resistance (friction) causes a gradual precompression and, hence, preheating of the fresh mixture adjacent to the advancing deflagration. After some induction period, this development leads to autoignition triggering an abrupt transition from deflagrative to detonative propagation. The detonation first develops in the boundary layer, where the impact of hydraulic resistance is stronger, and thereupon spreads over the channel's interior. The subsequent study of the problem [6] was aimed at elucidation of the impact of heat losses invariably present in realistic confined systems. The hydraulic resistance and heat losses exert opposite effects on the transition. The resistance raises the local temperature (through adiabatic compression) and thereby promotes autoignition. The heat loss tends to reverse this trend by reducing the temperature. In smooth channels, both mechanisms are of comparable influence. Therefore, one cannot be certain about the final outcome of the above competition. Experimentally, however, an often successful transition is an undeniable fact.
As has been shown in [6], with the channel walls maintained at the ambient temperature, and the reaction kinetics assumed monomolecular, the transition does not occur, at least within the parameter range explored. However, for the bimolecular kinetics (other conditions as in the monomolecular case), the transition proves readily feasible, with the predetonation distance somewhat above that of the adiabatic limit. Higher molecularity implies a higher sensitivity of the explosive mixture to the pressure change, which in these problems is quite significant.

The present study offers an extension of the previous one [6] over wider channels (100 flame-widths) and lower incipient flame velocities (Mach number = 0.045), closer to those of real-life explosives.

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2 Formulation and numerical results

To visualize the spatial picture of the transition, a wave of premixed gas combustion spreading from a closed to open end of the rectangular channel is studied by numerical simulations of the two-dimensional Navier-Stokes equations for a compressible reactive flow. The reaction rate is modeled by a singe-step Arrhenius kinetics. The latter is assumed to be of the first order with respect to the deficient reactant and of the second order with respect to the density, to account for the binary nature of chemical reactions taking place in real chemical systems. To avoid too large a disparity between the spatio-temporal scales involved and the numerical complications this entails, yet, helpfully, without too much detriment to the generic qualitative picture, the numerical simulations are conducted for somewhat reduced values of the scaled reaction energy N and the ratio a_p/u_p, compared to those typical of real-life explosives. Specifically we set $N = 4,\ \ a_p/u_p = 10,\ \ \sigma = 0.2,\ \ Le = 1,\ \ Pr = 1,\ \ \gamma = 1.3,\ \ d = 0.5 \div 10.$

Here $N = E/RT_p$, T_p is the adiabatic temperature of burned gas under constant pressure; a_p is the sonic velocity at $T = T_p$; u_p, velocity of the free-space deflagration relative to the burned gas; $\sigma = T_0/T_p$, were T_0 is the initial temperature of unburned gas; $\gamma = c_p/c_v$, where c_p, c_v specific heats; d is the scaled width of the channel in units of $(a_p/u_p)l_{th}$, where l_{th} is the flame width. The computational method used and its validation are described in [2]. The resolution tests are presented in [6].

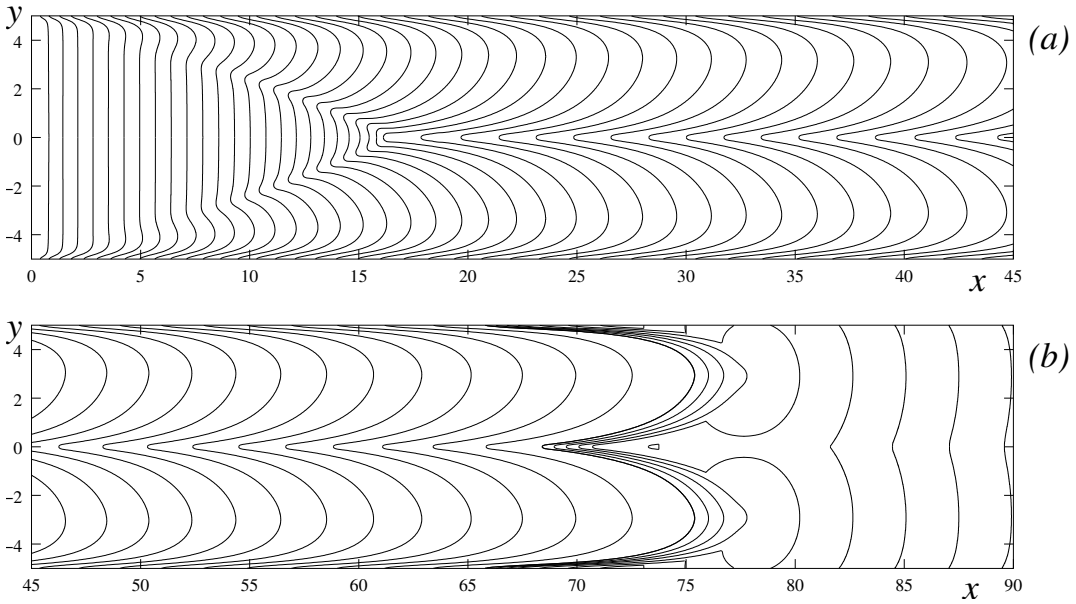

Figure 1: Temporal evolution of the reaction front. Scaled coordinates (x, y) are referred to 10 flame-widths. The solution shown corresponds to no-slip isotermal boundary conditions; $N = 4$, $Le = 1$, $Pr = 1$, $u_p/a_p = 10$, $\sigma = 0.2$, $\gamma = 1.3$, $d = 10$. Note the 5-fold reduction of the time-interval between the profiles above the autoignition point ($x > 75$).

Figure 1 depicts the reaction front profiles at several consecutive instants of time for the channel width $d = 10$ and isothermal boundary conditions. Similarly to the results reported in [6], shortly after the ignition, but when the details of the initiation are already 'forgotten', the flame assumes a U-shaped profile convex towards the fresh mixture and flattened near the center. Thereupon the flame develops two bulges near the channel walls. The bulges grow and eventually merge at the channel axis. The merging triggers a secondary shock clearly seen on the tonal picture (Fig. 2). The further evolution leads to a localized autoignition of the mixture adjacent to the leading edge of the 'tulip' flame, setting off the transition from deflagrative to detonative propagation. On Fig. 2 one can readily identify the evolving flame, leading shock, emergence of the detonation and retonation waves, as well as

transverse shocks induced by the shock-wall interaction. Note the islands of unburned gas formed near the wall immediately after the autoignition event (Fig. 1). Figure 3 plots the temporal evolution of the reaction wave velocity along the channel's axis calculated for several channel widths (d) at isothermal boundary conditions. As one would anticipate, the predetonation distance is longer for wider channels. The transition fails in sufficiently narrow channels ($d < d_{cr} = 0.6$) resulting in the total extinction rather than settling into the deflagrative mode. A similar observation has been reported in the recent experimental study of the transition in capillaries [5].

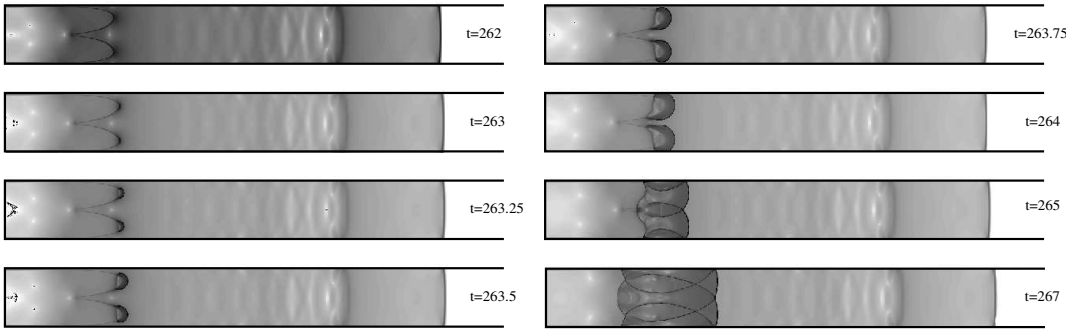

Figure 2: Pressure gradient norm at several consecutive instants of time (marked on the right). Stronger shading corresponds to higher pressure gradient. Conditions are identical to those of Fig. 1.

Note that $d_{cr} = 0.6$ is actually not a detonability limit. For the chosen parameter set one may well generate a steady self-sustained detonation at $d > 0.35$, provided the initiation hot spot is wide enough (direct initiation). Yet, under no-slip boundary conditions the steady deflagration does not seem feasible, at least in the parameter space explored.

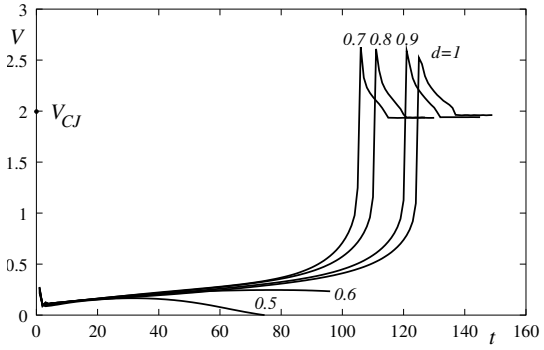

Figure 3: Reaction wave velocity V (scaled) versus time t (scaled) calculated for several channel widths, d. Other conditions are identical to those of Fig. 1. V_{CJ} corresponds to the Chapman-Jouguet detonation.

3 Concluding remarks

The results obtained are qualitatively similar to those of [6] for faster flames, reinforcing the argument in favor of the friction based concept of the transition. The inability of inducing a self-sustained deflagration may be attributed to the particular form and parameters of the reaction rate adopted. The numerous data on detonability vs. flammability limits in narrow tubes provide solid evidence that the long-lived deflagrative propagation is indeed feasible. The flammability limits are generally wider than the detonability limits. However at relatively low activation energies the situation may reverse [7], and

this seems to be the case in the present study. More research on this fundamental and intriguing question is needed.
Finally, we would like to report on a recently found alternative mechanism of the transition, unrelated to friction [4]. It transpires that in wide enough channels where, due to the Darrieus-Landau instability, the flame interface becomes wrinkled, the transition may be triggered by autoignition of the fresh mixture trapped within one of the flame folds. Under normal conditions this effect should be feasible in fast burning systems such as acetylene and hydrogen-fluorine mixtures where the normal flame-speed may raise as high as 20m/s. Yet, for many conventional explosives this would require an appropriate preconditioning (preheating, precompression) to make the flame-induced autoignition possible. The difficulty in reaching the autoignition in moderately fast burning mixtures perhaps explains why the transition is reluctant to occur in unconfined systems dealing with outward propagating 'free-space' flames.

Acknowledgments

These studies were supported by the U.S.-Israel Binational Science Foundation (Grant 200-2008), the Israel Science Foundation (Grant 350/05), the European Community Program RTN-HPRN-CT-2002-00274, the Swedish Natural Science Research Council (VR) under Contact E5106-1494/2006, and the Swedish Royal Academy of Sciences.
The authors thank Elaine Oran and Vadim Gamezo for helpful discussions.

References

[1] Brailovsky, I., and Sivashinsky G., 2000. Hydraulic resistance as a mechanism for deflagration-to-detonation transition. *Combustion Flame*, vol. 122:492-499.

[2] Kagan,L., and Sivashinsky, G.I., 2003. The transition from deflagration to detonation in thin channels. *Combustion Flame*, vol. 134:389-397.

[3] Oran, E.S., and Gamezo, V.N., 2005, Flame acceleration and detonation transition in narrow tubes. *Proc.* 20^{th} *ICDERS*, Montreal, Canada (CD).

[4] Liberman, M.A., Sivashinsky, G.I., Valiev, D.H., and Eriksson, L.-E., 2006, Numerical simulation of deflagration-to-detonation transition: the role of hydrodynamic instability. *Int. J. Tran. Phenomena*, vol. 8:253-277.

[5] Wu, M.-H.,Burke,M.P., Son,S.F., and Yetter,R.A. 2006 Flame acceleration and the transition to detonation of stoichiometric ethylene/oxygen in microscale tubes. *Proc. Combust. Inst.* vol. 31, to appear.

[6] Kagan,L., Valiev,D., Liberman,M., Gamezo V., Oran E., and Sivashinsky, G. 2006. Effect of hydraulic resistance and heat losses on the deflagration-to-detonation transition. *Proc. 5th Int. Colloq. Pulsed & Continuous Detonation*, Moscow, Russia, to appear

[7] Bykov, V., Goldfarb, I., Gol'dshtein, V., Kagan, L., and Sivashinsky, G. 2004. Effect of hydraulic resistance and heat losses on detonability and flammability limits. *Combustion Theory Modelling*, vol. 8:413-424.