Computational study of detonation-wave propagation in narrow channels

Ashwin Chinnayya and Abdellah Hadjadj
CORIA, CNRS UMR 6614, INSA & University of Rouen
76801 Saint Etienne du Rouvray Cedex, France

1 Introduction

Progress toward the miniaturization of increasingly advanced micro- and nano-electromechanical systems has highlighted the need for a better knowledge of the design of such devices. In the field of energy and power, as the systems are scaled down the thermal efficiency of conventional propellant devices is seriously degraded due to significant heat losses which can cause the combustion extinction. A promising technique is to use shock or detonation waves in gaseous media to enhance the chemical reaction rates [2]. In addition to the classical safety issues, possible applications [18] of micro-detonations refer to energy production, propulsion or actuation [14], [8], or to the predetonator of a pulsed detonation engine. For energetic materials, microscale applications may include detonation interaction with microstructure [16].
From a theoretical point of view and following the ZND model [9], a detonation is a self-sustaining process and a rapid regime of burning, where strong shock waves raises abruptly the thermodynamic state, so that the initiation of the chemical decomposition turns the gaseous reactants into products. This combustion process leads to an equilibrium state downstream of the shock, while the released energy and the induced pressure drop sustain the leading shock front. From experimental point of view, it has been shown that the viscous effects may strongly affect the propagation of the detonation wave when the length scale of the tube is reduced. The finite thickness of the reaction zone renders the latter sensitive to the dissipative nature of the boundary layer, meaning that the diffusive transport phenomena cannot be neglected any more. This yields a decrease of the detonation velocity compared to the one inferred by the Chapman-Jouguet theory.
In terms of instabilities, it is well known that most explosive mixtures are unstable. They provide a key mechanism for the self-propagation of detonation. These instabilities are multidimensional, exhibiting a complex shock structure, with longitudinal as well as the transverse waves and Mach stems. As a consequence, the leading shock is subjected to rapid deceleration and acceleration. These instabilities are particularly present when the temperature dependence of the chemical reaction rate is high. In this case, quenching behind the incident shock can occur. However, the multiple shock interactions provide hot spots, starting points of local re-ignitions and micro-explosions [1]. Moreover, as a consequence of vorticity-generating mechanisms, the turbulence can enhance the mixing in the reaction zone and the global chemical decomposition rate as well [10]. Therefore, the mechanism of propagation of these unstable detonations cannot be explained solely by only the ZND mechanism [3]. In addition, the shock front appears highly wrinkled and the cellular pattern shows a wide spectrum of length scales [1], [15].
In the case of stable detonations, as the activation energy is lowered, the cellular pattern pertains if the heat reaction is high enough [6], [9]. It becomes more regular with weaker transverse waves and exhibits the diamond-like structure. Even in the absence of thermal sensitivity of chemical-kinetic, Clavin in his

Correspondence to: Ashwin.Chinnayya@coria.fr

review paper [5] has shown theoretically that an initial one-dimensional front is unstable against multi-dimensional disturbances. Indeed, the deflection of the streamlines across the wrinkled shock perturbs the heat-release rate distribution and longitudinal instabilities are generated, which in a feedback loop, support the leading shock instabilities. This pure "hydrodynamic instability" is increased with heat release and is reinforced by the sensitivity of the heat-release rate of temperature.

In terms of detonation velocity deficit, several mechanisms proposed by different authors are reviewed in Lee [10] and Camargo et al. [3]. Zel'dovich [19] was most probably the first to point out that the wall momentum and heat losses were non-negligible with scale reduction. He included friction as drag forces and heat losses in a one-dimensional formalism. On the other hand, Zhang and Lee [20] concluded that energy dissipation, due to friction, is the main cause of velocity deficit [20] whereas Manson and Guénoche [11] proposed another phenomenological mechanism to account for the velocity deficit. They assume that chemical reactions are inhibited or significantly modified in a viscous fluid layer adjacent to the walls. Two distinguished zones in the flow could then be identified: the potential core of the flow, where the released energy will sustain the detonation front and the boundary layer. In their model, the authors have considered different heats of reaction in the boundary layer and the potential core of the flow. Practically, the energy release was then modified in the Hugoniot equation by a fraction proportional to the section of the potential flow. Also, it was noted that the sonic surface could not be strictly a plane surface, specially near wall region. It turns out that both studies lead to the fact that the velocity deficit depends linearly on the inverse of the tube diameter. An improved model was proposed by Fay [7], where the two-dimensional boundary layer effects were accounted for the propagation of the detonation wave. The velocity deficit is explained by the development of the boundary layer downstream of the leading shock. In this model, in a reference coordinate system attached to the shock, the wall moves at the same velocity than the upstream flow. Due to the boundary layer growth, this velocity increase will diffuse into the subsonic zone of the potential core flow. The negative displacement causes flow divergence. The flow was then considered to be a one-dimensional flow in a slowly enlarging channel whose cross-sectional area was proportional to the turbulent boundary layer thickness. The shematic illustration of the flow divergence is given in Figure 1. In comparing the results of Fay's model with

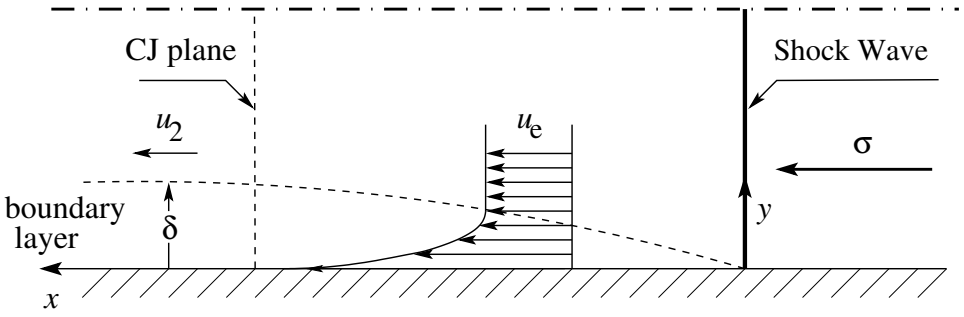

Figure 1: Shematic illustration of the flow divergence [7].

the experimental data, Camargo et al. [3] have shown that within the uncertainty of chemical kinetics, the best agreement was obtained for stable detonations, i.e. for mixtures whose propagation mechanism follows the ZND model.

The work presented in this paper deals with the study of stable detonation in narrow channels, in the case of absence of thermal sensitivity of chemical kinetic. The scale reduction induces a velocity deficit of the detonation front and will damp the hydrodynamic instabilities as well as transverse waves, which eventually lead to the disappearance of the cellular pattern. The current study focuses on the analysis of the mean structure of the reaction zone that extends from the shock front to the sonic surface underneath this limit of disappearance. The Master equation is derived from the Navier-Stokes reactive model and the generalized Chapman-Jouguet sonicity and thermicity conditions are presented and compared

to the numerical results. The relative contribution of the different dissipative effects are evaluated. It is also shown that the structure of the downstream subsonic pocket is correlated to the development of the boundary layer. Finally, the differences with the phenomenological mechanisms proposed in the literature are highlighted.

2 Numerical Results and Discussion

In this study, the two-dimensional multi-species Navier-Stokes reactive equations are used. The set of equations is solved using a high-order shock-capturing scheme, base on Mapped-WENO5 method for the convective fluxes and a 4^{th} order compact scheme for the discretization of the diffusive fluxes. The details of the numerical method, the thermodynamics (perfect Gas Law and Janaf) and the mixture transport properties can be found in [4]. The thermodynamic and transport properties of the working fluid have been chosen to be that of a stoichiometric propane/oxygen, whose reactivity depends linearly on the pressure [12].
The propagation of detonation waves in 2D narrow channels is investigated. The initial pressure and temperature are $3kPa$ and $300K$, respectively. In the following, we denote Δ as the thickness within the ZND reaction zone where the fuel mass fraction reaches 1% of its initial value. H is the height of the channel. The ZND profiles of all variables are used as initial conditions at one end of the channel. After a transient, where the detonation velocity decreases, it stabilizes to a constant value. The subsonic pocket is found to be self-similar. The structure of the detonation is then analyzed from the numerical results.

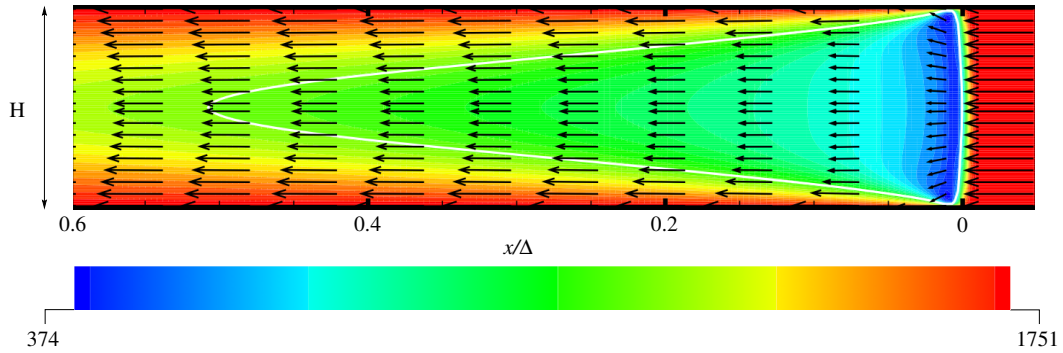

Figure 2: Longitudinal velocity flowfield in the shock frame. Sonic line in white.

The longitudinal velocity flowfield in a reference coordinate system attached to the shock is depicted in Figure 2. In this case, the height is $H = \Delta/8 = H_{ref}$. After the passage of the leading shock, a boundary layer will develop. The no-slip boundary implies that the velocity at the solid wall is equal to the shock velocity. Then, near the boundary, the flow is supersonic whereas it is subsonic in the core of the flow downstream the shock. The transition between these two regimes is done through the sonic line in white. The velocity jump will diffuse from the walls. Thus the flow is accelerated not only by the energy release but also by the momentum diffusion coming from the walls. One can see that the subsonic zone leans against the detonation front, which is almost planar. The upper edge of the sonic envelope is located at the intersection between the base of the shock and the beginning of the boundary layer. Their relative evolution is examined in the following.

Figure 3 represents the position of the subsonic boundary, the viscous layer thickness, the displacement thickness as function of a normalized distance from the shock. The flow can be divided into three parts:

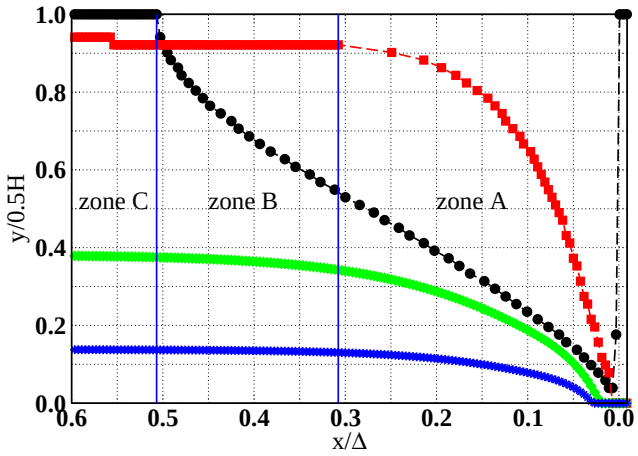

Figure 3: Subsonic pocket (black dots •). Boundary layer thickness (red squares ■). Displacement thickness (green diamonds ♦). Momentum thickness (blue stars ⋆).

zone A in which the boundary layer is developing, zone B where the boundary layer no longer evolves and which is located inside the subsonic zone. The zone C corresponds to the supersonic flow. The development of the boundary layer coincides with the development of the downstream subsonic region. From Figures 2 and 3, one can see many similarities with the mechanism proposed by Fay [7] on Figure 1, except for the sonic surface. Moreover, chemical decomposition also takes place in the supersonic region near wall boundaries, which implies that less energy is available to support the detonation front, as Manson and Guénoche [11] suggested.
The Master equation can be derived from the Navier-Stokes reactive equations. It reads

$$\mathcal{H} + \mathcal{P}_{visq} = (\gamma - 1)\left(-\dot{q} + \Phi + \dot{q}_{th} + \dot{q}_{diff}\right) \tag{1}$$

where in the local Frenet basis $(\vec{l}, \vec{n})$, $\mathcal{H} = \rho\left(c^2 - \|\vec{u}\|^2\right)\dfrac{\partial \|\vec{u}\|}{\partial l} + \rho c^2 \|\vec{u}\| \dfrac{\partial \theta}{\partial n}$, θ deviation angle of the streamlines. $\mathcal{P}_{visq}$ is related to the power of the viscous stress, $\dot{q}_{th}$ the thermal flux, $\dot{q}_{diff}$ the species diffusion, $\dot{q}$ the released energy, Φ the viscous dissipation rate function. There is a singularity when the Mach number is one, i.e. the sonicity condition. The thermicity condition then easily follows. The Figure 4 represents the values taken from the different terms of this energetic balance. They have been normalized by the maximal value taken by $\mathcal{P}_{visq}$. Near the leading shock, the contribution of the species diffusive flux and the thermal flux are negligible. Thus, the development of viscous boundary layer is clearly responsible for the location of the sonic line. When one moves away from the shock, all the contributions of the Master equation decrease. At the end of subsonic zone, the viscous dissipation rate and the species diffusive flux become negligible. However, the thermal flux cannot be neglected anymore as its contribution is of the same order of magnitude that $\mathcal{H}$. The thermal flux is thereby important in determining the end sonic location.

The structure of the detonation front has been studied for a given height. The study also intends to examine the influence of the intensity of dissipative effects on detonation. The height of the channel is varied and in addition to the previous case, five heights have been considered : $4H_{ref}$, $3H_{ref}$, $2H_{ref}$, $H_{ref}/2$, $H_{ref}/4$. The Figure 5 represents the normalized mean detonation velocity as function of the inverse normalized height. The velocity decreases as height is decreased. Figure 6 depicts the triple points trajectories for the different heights investigated. As the dissipative effects decrease, the transverse instabilities reappear again. Indeed, the reactive mixture has an approximate polytropic coefficient of 1.2, and a reduced heat of reaction of 60. Erpenbeck [6] has shown that for a detonation overdrive of

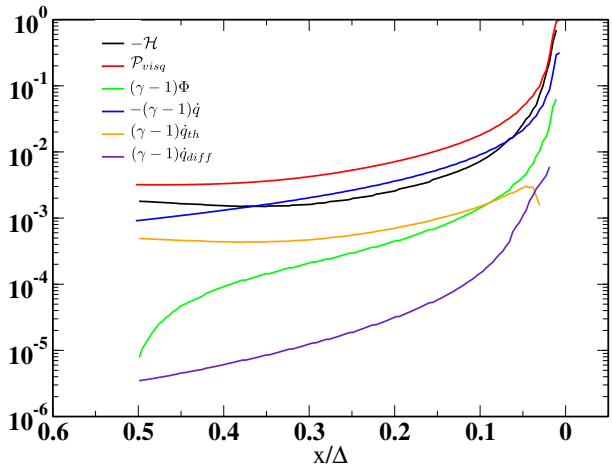

Figure 4: Balance of the different contributions of the Master equation on the sonic line.

1, transverse instabilities appear in the case of absence of thermal sensitivity of chemical-kinetic. The numerical results clearly demonstrate that transverse instabilities are damped with the increase of dissipative effects. The multidimensional time-averaged structure of the subsonic reactive region and its adjoining flow of a detonable mixture with higher reaction sensitivity could then be analysed, following Radulescu *et al.* [13], which would give higher physical insight about the "turbulent structure of gaseous detonations" [10, 15, 17].

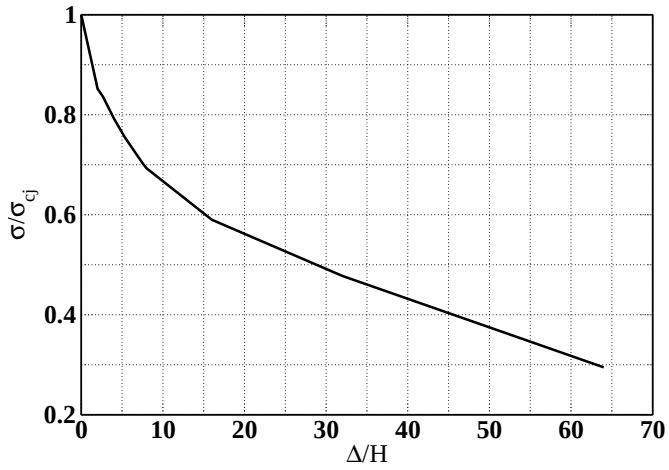

Figure 5: Mean detonation velocity.

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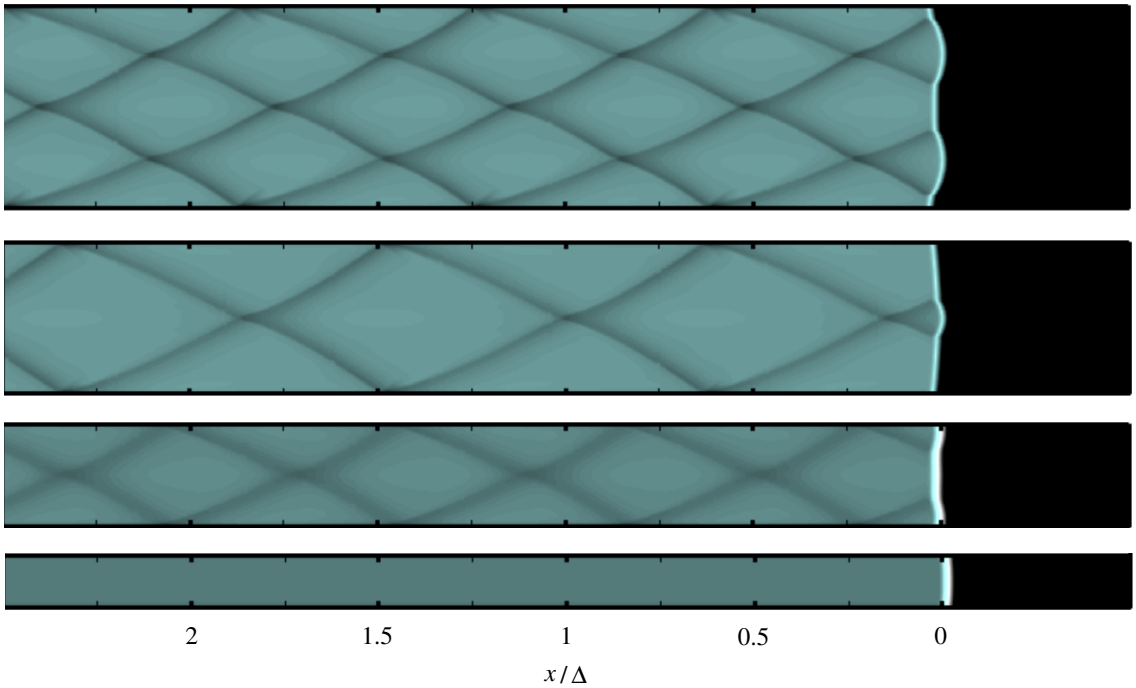

Figure 6: Triple point trajectories for different channel heights. From top to bottom: $H = 4H_{ref}$, $H = 3H_{ref}$, $H = H_{ref}$.

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