Numerical Simulations of Mildly Unstable Gaseous Detonations in Small Channels

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1 Introduction

Detonation is a complex phenomenon that consists of a shock wave coupled to reaction zone moving at a high-speed velocity. It has issues in many engineering sciences such as safety and explosion, aerospace propulsion systems (pulse-, rotating- and oblique-detonation engines). Detonation wave propagating in a narrow channel filled with a reactive mixture exhibits different flow features and hydrodynamics instabilities with boundary layers effects. The flow resistance can lead to a detonation velocity deficit compared to the ideal Chapman-Jouguet detonation velocity and can eventually cause the failure of the detonation. Detonation are unstable for most known gaseous combustible mixtures. These multidimensional instabilities provide an essential mechanism for detonation propagation. Different mechanisms were proposed to explain the velocity deficit. Zel'dovich [1] proposed an analytical model based on a one-dimensional formalism in which drag forces and heat losses are considered as the mechanisms that lead to the velocity deficit. Manson and Guénoche [2], on the other hand, considered that the chemical reaction are inhibited in a thin viscous layer near the wall due to heat losses. In their model, the detonation propagation is only sustained by the chemical energy released in the core of the channel. For Fay [3], the boundary-layer development behind the shock wave leads to a mass diffusion from the core of the channel to the wall. This diffusion leads in turn to the velocity deficit of the detonation front. Camargo *et al.* [4] pointed out that the boundary-layer development have an effect that is identical to that of a curved detonation front.

The goals of the present work are to investigate the structure of gaseous detonation waves propagating in a thin rectangular channel and to characterize the sonic surface and the viscous boundary layer growing behind the detonation front.

2 Numerical Model and Computational Setup

The dynamics of the compressible medium is described by two-dimensional unsteady reactive Navier-Stokes equations with variable thermodynamics properties and reactive multi-species transport equa-

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tions. The system of equations is written in the following conservation form

$$\frac{\partial U}{\partial t} + \frac{\partial}{\partial x}\left[F(U) - F_v(U)\right] + \frac{\partial}{\partial y}\left[G(U) - G_v(U)\right] = S(U) \tag{1}$$

where U is the vector of conservatives variables, and $F(U)$ and $G(U)$ are the convective fluxes in x and y directions, respectively. $S(U)$ is the vector of chemical source terms.

$$U = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \\ \rho_1 \\ \vdots \\ \rho_{\mathcal{N}_{sp}} \end{bmatrix}, \; F(U) = \begin{bmatrix} \rho u \\ \rho u^2 + P \\ \rho uv \\ (\rho E + P)u \\ \rho_1 u \\ \vdots \\ \rho_{\mathcal{N}_{sp}} u \end{bmatrix}, \; G(U) = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + P \\ (\rho E + P)v \\ \rho_1 v \\ \vdots \\ \rho_{\mathcal{N}_{sp}} v \end{bmatrix}, \; S(U) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \mathcal{W}_1\dot{\omega}_1 \\ \vdots \\ \mathcal{W}_{\mathcal{N}_{sp}}\dot{\omega}_{\mathcal{N}_{sp}} \end{bmatrix}$$

ρ, ρ_k, P, e, $E = e + (u^2 + v^2)/2$, $\mathcal{W}_k$ and $\dot{\omega}_k$ are the density, the k^{th} species-density, the pressure, the internal and the total energy, the molar mass and the chemical source term of the the k^{th} species, respectively. $\mathcal{N}_{sp}$ is the total number of species. The diffusive fluxes $F_v(U)$ and $G_v(U)$ are

$$F_v(U) = \begin{bmatrix} 0 \\ \tau_{xx} \\ \tau_{yx} \\ q_x \\ \mathcal{J}_{x,1} \\ \vdots \\ \mathcal{J}_{x,\mathcal{N}_{sp}} \end{bmatrix}, \quad G_v(U) = \begin{bmatrix} 0 \\ \tau_{xy} \\ \tau_{yy} \\ q_y \\ \mathcal{J}_{y,1} \\ \vdots \\ \mathcal{J}_{y,\mathcal{N}_{sp}} \end{bmatrix}$$

The diffusive flux in the species conservation law $\mathcal{J}_{x,k}$ and $\mathcal{J}_{y,k}$ are given by the Fick law. The viscous stress tensor and the dissipative fluxes are represented by τ and q, respectively. Details on how these parameters are computed can be found in A. Chaudhuri *et al.* [5]. The system of Eqs. 1 is solved using a fifth-order shock-capturing scheme, based on WENO5-Mapped method for the convective fluxes and a fourth-order compact scheme for the discretization of the diffusive fluxes. The details of the numerical method, the thermodynamics (perfect Gas Law and JANAF) as well as the mixture transport properties can be found in A. Chaudhuri *et al.* [6]. A uniform Cartesian mesh is used. The simulation were performed in a fixed reference frame with the implementation of a moving multi-blocks strategy. Thus the region of the domain which was discarded was far from the limiting characteristic, which would correspond to the sonic surface in the stable case.

The initial pressure and temperature are $P_0 = 3$ kPa and $T_0 = 300$ K, respectively. The thermodynamic and transport properties of the working fluid have been chosen as a stoichiometric propane/oxygen mixture. A single step has been used for the chemical mechanism: $\mathcal{F} + \mathcal{O} \longrightarrow \mathcal{P}$. A total of 9 chemical species is involved. The fuel and oxidant are respectively $\mathcal{F} \equiv \mathrm{C_3H_8}$ and $\mathcal{O} \equiv 5\mathrm{O_2}$. The detonation products consist of a mixture of gaseous components $\mathcal{P} \equiv 1.047\mathrm{CO_2} + 1.953\mathrm{CO} + 2.63\mathrm{H_2O} + 1.12\mathrm{OH} + 0.587\mathrm{H_2} + 0.86\mathrm{O_2} + 0.4478\mathrm{H} + 0.487\mathrm{O}$. The chemical composition is taken similar to the one given by the Chapman-Jouguet equilibrium state using the software GASEQ or as in S.Trélat [7], at initial conditions of 1 bar and 300 K. In this case, the reduced chemical energy $Q_r/\mathcal{R}_u T_0$ is equal to 78.5 [8]. The chemical source term for $\mathcal{F}$ is $\dot{\omega}_\mathcal{F} = -[\mathcal{F}]/\tau_\mathcal{F}$. The chemical time scale is $\tau_\mathcal{F} = B\exp(E_a/\mathcal{R}T)/[\mathrm{O_2}]$. In what follows, we denote Δ as the distance from the shock within the ZND reaction zone, where the fuel mass fraction reaches 1% of its initial value. The pre-exponential

factor B has been calibrated so that $\Delta = 1.068\,\mathrm{mm}$. Δ depends linearly on the inverse of the pressure and Δ is equal to the findings of Schultz and Shepherd [8]. The hydrodynamic structure of propane-oxygen detonation exhibit very high turbulent features, which is due to its complex reaction zone [9]. However, as the chemistry has been simplified, the modes of longitudinal instabilities cannot be present. H is the height of the channel. Initially, left and right flow conditions are imposed.

In the left part, a one-dimensional ZND solution is imposed, while a uniform state of a gas mixture at rest in initial conditions P_0 and T_0 is assumed. With regards to boundary conditions, a no-slip adiabatic condition is imposed on solid walls, and a symmetric conditions are set on the symmetry axis of the domain. Open-boundary conditions are fixed at the left and right boundaries. Owing to the symmetry of the flow, only half- channel is computed.

3 Results and discussion

In this section, simulations using three different activation energies ($E_a/\mathcal{R}T_0 = 0$, 10 and 20) with three different channel widths (H_{ref}, $2H_{ref}$ and $4H_{ref}$, with $H_{ref} = \Delta/8 = 0.1335\,\mathrm{mm}$) are carried out to investigate the structure of a detonation wave and its associated boundary layer. $B \times 10^{-8}$ is equal to 15 , 7.4 and 3.2 when $E_a/\mathcal{R}T_0$ is equal to 0, 10 and 20, respectively.

Stable detonation ($H = H_{ref}$ and $E_a/\mathcal{R}T_0 = 0$) When the width of the channel is set to $H = H_{ref}$ and the activation energy is equal to zero, the detonation front exhibits no triple-point (see Figure. 1). This configuration will be referred to us stable detonation wave. After a transient time, the detonation velocity stabilizes at $1752\ \mathrm{m/s}$ which corresponds to a velocity deficit of 25.51% compared to the CJ case. At the same time, the flow becomes "self-similar" i.e. the velocity profiles at different positions collapse using a suitable x-scale factor. The structure of the detonation front is then analyzed in the following section.

The longitudinal flow velocity in the shock-attached frame is shown in Figure 1. The velocity vectors are also plotted at different sections of the channel and the distance from the leading shock is scaled by Δ. Through the shock, the gas velocity is reduced and the flow passes from supersonic to subsonic regime. The continuous release of the chemical energy in the flow leads to the gas expansion and the flow acceleration, especially at the core of the channel. Moreover, in the shock-attached frame, the no-slip boundary implies that the wall velocity is equal to the shock speed. Thus, near the wall the flow is supersonic while it is subsonic at the core of the channel. The transition between these two flow regimes is done trough the sonic line which is the white line in Figure 1. Thus in the shock-attached frame, the flow is accelerated by two means: the chemical energy released in the flow and the wall momentum transfer which accelerate the gas near the wall to match the wall velocity. Moreover, the results indicated that the CJ surface is not planar as suggested by Manson and Guénoche [2] and Manzhalei [10]. The sonic locus meets the centerline of the channel at approximately $0.5\ \Delta$.

Figure 1 illustrates also that the flow is deviated just downstream the front which has a slight curvature. Indeed, due to the high velocities in the vicinity of the wall, the streamlines are deviated towards it. Close inspection of Figure 1 using one-dimensional vertical cuts at streamlines deviation position (see Figure 2) shows that the pressure is much higher closest to the walls and decreases at the core of the channel. The density has a similar trend. Therefore, the density is higher at the wall than at the core of the channel leading thereby to an apparent sink of mass going from the core flow into the channel walls. This effect leads in turn to a divergence of the flow behind the shock front. For the flow to head for the walls, the shock front curves. The latter reacts to this apparent divergence by curving near the wall to direct the flow radially into walls [11].

The flow expansion due to the flow divergence will slow the rate of chemical energy released. Thus more energy is released downstream the sonic surface and does not support anymore the detonation front. From this analysis it's clear that the viscous boundary layer growth can be important in detonation propagation.

It is worthwhile to characterize the viscous boundary layer which is mainly responsible for the velocity deficit observed. x is the distance from the shock. As the sonic locus matches the centerline of the channel at a Reynolds number of $Re_x = 400$ and as events happening behind the sonic surface are supposed to do not have an influence on the propagation of the detonation front, the study will focus only on the portion of the boundary layer bounded by the sonic surface. The skin-friction coefficient $C_f(x) = 2\tau_{\text{wall}}/(\rho u^2)_\infty$,where $\tau_{\text{wall}} = (\mu\frac{\partial u}{\partial y})_{\text{wall}}$ and ∞ refer to the center of the channel, can be approximated by $C_f(x) \approx 17.1\ Re_x^{-1.07}$.

Unstable detonation ($H = 2\,H_{ref}$, $H = 4\,H_{ref}$, $E_a/\mathcal{R}T_0 = 0$, 10 and 20) In order to investigate the influence of the boundary-layer growth and the influence of the activation energy parameter on the structure of the detonation wave, two heights $H = 2\,H_{ref}$ and $H = 4\,H_{ref}$ are considered. For each height, the activation energy $E_a/\mathcal{R}T_0$ is set to 0, 10 and 20 respectively. When H increases, the viscous effects are reduced. The instabilities of the front appear again and lead to the formation of a cellular detonation wave as shown in Figure 3 showing the pressure history for $H = 4\,H_{ref}$ calculated for $E_a/\mathcal{R}T_0 = 0$, 10 and 20. The red tracks give the trajectories of the triple points that form the cellular regular structure. The results are presented in the frame $x - \sigma_1\,t$ with $\sigma_1 = 1100\,\mathrm{m/s}$ which skews a bit the cellular structure from a losange form to a square-like shape. When the activation energy increases, the trajectory of the triple points becomes more marked and transverse waves and the detonation front exhibits one cell in the transverse direction.
The results are then averaged as in Sow *et al.* [13]. The skin-coefficient friction C_f and the displacement thickness δ^*, which is the distance by which the external stationary field is displaced outwards as a consequence of the increase in velocity in the boundary layer in the shock-attached frame, are than studied (see Tables 1 and 2) in order to characterize the boundary layer growth. Our simulations show that the power of the skin-friction coefficient is around -1 which is greater than the value of -0.5 predicted by the laminar theory. Moreover, the displacement thickness scales as in $Re^{-\alpha}$, $\alpha \approx 0.5 - 0.65$ which is far from the value of -0.2 suggested by Fay for turbulent-boundary layer. The slight increase of α when the activation energy increases is probably due to the amplification of the transverse waves.

4 Summary

We have simulated detonation wave propagation in thin channels filed with a working fluid which thermodynamics and transport properties are that of a stoichiometric C_3H_8/O_2 mixture using a reduced chemical mechanism by means of a WENO-mapped scheme. The computed results show that the viscous boundary layer has globally a dependence in $Re^{-0.6}$. This result seems consistent with the observations of Damazo *et al.* [12] which indicate that the boundary layer downstream the detonation front have a laminar behavior.

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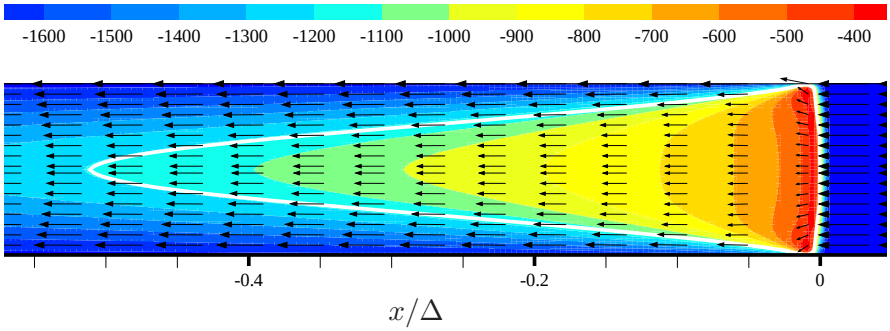

Figure 1: Longitudinal velocity $[\mathrm{m/s}]$ flow field in the shock-attached frame. The white line indicates the sonic condition. $E_a = 0$, $L = L_{ref}$, $H = H_{ref}$.

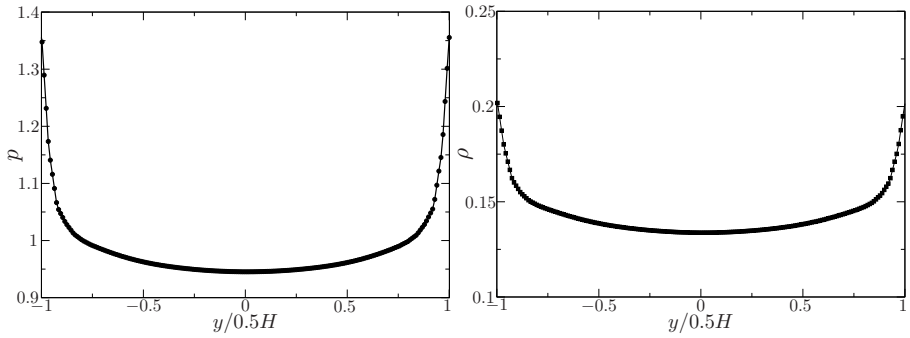

Figure 2: One-dimensional vertical plots of the flow field at $x = 0$. a) Pressure [bar] as a function of normalized coordinate. b) Density $[\mathrm{kg/m^3}]$ as a function of normalized coordinate. $E_a = 0$, $L = L_{ref}$ et $H = H_{ref}$.

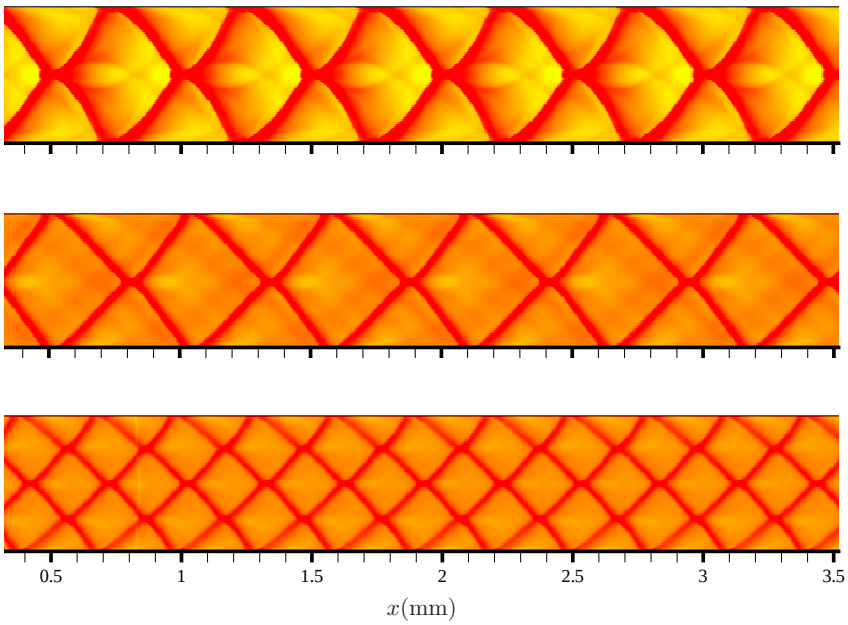

Figure 3: Maximum pressure histories for various activation energies. From the bottom to the top: $E_a = 0$, $E_a/\mathcal{R}T_0 = 10$ and $E_a/\mathcal{R}T_0 = 20$. $L = L_{ref}$, $H = 4H_{ref}$.

	$E_a/\mathcal{R}T_0 = 0$	$E_a/\mathcal{R}T_0 = 10$	$E_a/\mathcal{R}T_0 = 20$
$2\,H_{ref}$	$27.47Re_x^{-1.077}$	$37.04Re_x^{-1.11}$	$37.22Re_x^{-1.12}$
$4\,H_{ref}$	$12.2Re_x^{-0.897}$	$16.5Re_x^{-0.938}$	$18.7Re_x^{-0.961}$

Table 1: Skin-friction coefficients C_f.

	$E_a/\mathcal{R}T_0 = 0$	$E_a/\mathcal{R}T_0 = 10$	$E_a/\mathcal{R}T_0 = 20$
$2\,H_{ref}$	$0.93Re_x^{-0.47}$	$1.65Re_x^{-0.56}$	$1.45Re_x^{-0.53}$
$4\,H_{ref}$	$1.9Re_x^{-0.561}$	$2.2Re_x^{-0.580}$	$4.0Re_x^{-0.653}$

Table 2: Displacement thickness δ^*/x.

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