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NUMERICAL STUDY OF THE INFLUENCE OF DISSIPATIVE EFFECTS ON THE PROPAGATION OF DETONATION WAVES IN NARROW CHANNELS

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Abstract. A numerical study of the propagation of propane/oxygen detonation waves is conducted in the context of narrow shock tubes undergoing strong confinement effects. To deal with shock waves, chemical reactions, heat and viscous stresses, a high-order Navier-Stokes solver based on WENO scheme, coupled with the Strang's splitting method, is used in the framework of multi-species reacting mixtures. Results show that the development of viscous and thermal boundary layers behind the shock wave tends to decrease the speed of the detonation wave compared to the Chapman-Jouguet detonation velocity, σ_{CJ} . More specifically, the boundary layer effects lead to changes in the reaction zone, by reducing the amount of energy behind the leading shock front and decrease the propagation velocity, which finally causes large velocity fluctuations. A scenario, based on the energy deficit in the boundary layer, is proposed to explain the cause of the attenuation of the detonation velocity. This energy loss, which represent a fraction of the total energy, is trapped in the vicinity of the walls and does not contribute to drive the shock front.

1 Introduction

MEMS/NEMS (Mico/Nano Electro-Mechanical Systems) have become a growing and prosperous field for research and development in science and technology nowadays. An important problem in the development of MEMS is the design of devices that are able to produce mechanical work from chemical heat release, *i.e.* the micro-engines. At miniaturization level, the time scales associated with heat-loss are reduced dramatically while the characteristic time scales for heat release stay virtually independent of scale. Thus, the efficiency of conventional devices such as internal combustion engines and gas turbines is seriously degraded when they are scaled to small sizes. One possibility to overcome this difficulty is to accelerate the heat release using shock-induced (or shock-assisted) combustion. However, this technique requires a deeper insight into the mechanisms governing microscale shock waves and detonation with friction and heat transfer at walls. Recent studies [2, 14, 15] have shown that the viscosity and heat losses play a key role in the attenuation of the shock speed as well as the shock intensity in the long-time evolution, demonstrating the transition from a hyperbolic behavior towards a diffusive regime. More specifically, regarding the propagation of detonation waves in narrow shock tubes, Haloua et al. [7], for instance, investigated experimentally unstable gaseous detonation of stoichiometric propane/oxygen mixtures, diluted or not with argon or helium in a shock tube of 38 mm diameter. By varying the initial pressure from 1 to 0.003 bar, four modes of propagation were clearly identified: stable detonation, stuttering mode, galloping mode, and fast flame. The last mode corresponds to the slowest one which is dominated by the dissipative effects. Also, Zel'dovich et al. [20] performed one-dimensional detonation studies including friction and thermal losses in rough tubes. By decreasing the tube diameter, a reduction of detonation velocity is observed, confirming earlier findings [18]. On the other hand, in the coordinates associated with the detonation front, the excess of mass through the boundary layer was taken into account in Fay [4] by assuming an effective increase in the tube area. The sonic line was then determined by solving a reacting-flow model in a slowly divergent flow. Manson and Guénoche [11] postulated that chemical reactions were inhibited or significantly modified in a layer adjacent to the tube walls behind the detonation front. The classical detonation equations were then modified by assuming different heats of reaction in the boundary layer and the potential core of the flow. Also, they noted that the CJ surface retains its usual meaning throughout the entire section, except in near-wall regions. Therefore, the shock front receives less energy compared to the ideal case, leading to a velocity deficit of the shock front and sometimes to an extinction of the detonation, if the boundary layer becomes sufficiently large.

In spite of many studies on the subject, the mechanisms of detonation waves propagation and attenuation in narrow tubes are quite complex, and fundamental knowledge of flow physics in presence of strong shocks interacting with chemical reactions, viscosity and heat release is still needed. Additionally, due to strong flow unsteadiness at very small scales, a direct insight into these processes needs to be clarified in the light of high-fidelity numerical simulations. Subsequently, the recent progress made in computer science and numerical methods allows the use of robust and accurate solvers based on high-order shock-capturing methods to solve complex compressible flows in presence of stiff gradients confined within very thin reaction zones. The present work uses a fifth-order WENO scheme coupled with the Strang's splitting method to numerically study the detonation propagation and attenuation in narrow channels including viscous effects. The objective is to shade more physical insight for the considered problem. The paper is organized as follows. In section 2, the mathematical model as well as the numerical methods are briefly described. Then, results are presented in section 3 starting with one-dimensional inviscid and viscous computations. The objective is to assess the performance of the methods and to partially validate the proposed methodology. Then, subsection 4 is devoted to the study of two-dimensional propane/oxygen detonation waves in a narrow channel. The comparison between inviscid and viscous detonations are provided, leading to the conclusion given in section 5.

2 Mathematical and numerical methods

Even though small-scale channels are considered with moderate Mach numbers, the corresponding Reynolds numbers can reach relatively high values due to high pressures caused by the detonation waves. Therefore, the continuum approach (low Knudsen numbers, $K_n \sim M/R_e < 10^{-3}$) is still valid, allowing thereby the use of Navier-Stokes equations for the numerical simulations of this problem. In this study, a one-dimensional formulation is first used (for simplicity), in which viscosity and heat transfers are integrated as source terms in the momentum and energy equations, respectively. Then, two-dimensional computations are conducted using fully compressible NS equations, where the viscosity of the mixture is calculated via the Wilke law [19], and the thermal conductivity is obtained using the Ferziger's expression [5]. The molecular diffusion coefficient of each species is evaluated with mixture law provided by [3]. The gas is supposed to be thermodynamically perfect and obeys to the perfect gas law. The specific heats at constant pressure for each species are described by the JANAF Tables [10]. In both formulations, the chemical reactions are modeled using a single step irreversible mechanism.

The numerical strategy developed in this study includes a variety of modern high-order low-dissipation shock-capturing schemes (WENO-5 [9] and Mapped WENO [8]) and the Strang's splitting method [17] in order to couple the chemical source terms with the NS solver. A Quasi-Steady-State-Approximation [12] is chosen to integrate the source terms. Note that for the 1D solver, the numerical fluxes are evaluated with an HLLC (Harten, Lax, van Leer with restored contact discontinuity) solver [1], whereas a fifth-order Mapped WENO [8] is used to evaluate the characteristic fluxes in a 2D case. For both cases, a third-order TVD Runge-Kutta method is used for time advancement.

3 Results and discussion

Following the classical ZND (Zel'dovich, Von Neumann, Döring) theory, a detonation front consists of a shock wave followed by a reaction zone of finite length. In the ideal case, the detonation front travels at a constant speed, which is determined by the Chapman-Jouguet (CJ) state as a locus of tangency of the Rayleigh line and the reactive Hugoniot curve. In real cases and due to boundary layer effects, the reaction zone is affected by friction and heat losses, which tend to dissipate the energy and thereby reduce the velocity of the detonation wave.

3.1 1D detonation

This section deals with one-dimensional computations of detonation. In the first part of this section, the inviscid configuration will be presented. Then in the second part, viscous effects as well as thermal losses will be accounted for by means of the Zel'dovich model [20].

3.1.1 Inviscid vs. viscous detonation

The working fluid is a propane/oxygen mixture in stoichiometric proportions. As said previously, the kinetic mechanism used is based on a single irreversible reaction. The composition of the eight main products $(H_2O, CO_2, CO, O_2, OH, H, O, H_2)$ is the same as at the equilibrium CJ state [6]. The configuration is a reactive shock tube, in which we are mainly interested in the detonation wave self-similarity propagation. In the low-pressure chamber, the fresh gases are at rest, under thermodynamic conditions of 1 bar and 300 K. The left part of the tube contains the same mixture moving from the left to the right at 1500 m.s⁻¹ under 10 bar and 3000 K. The length of the domain is 3 cm. The computational domain is made of 20000 cells. CFL number is fixed to 0.4.

In the left side of the tube, a constant-volume combustion is taking place, continuously raising pressure and temperature. Simultaneously, an incident shock wave travels through the fresh gases, where reactions take place. The outcome is that the pressure waves, coming from the heat release and the strengthening driver pressure gas will catch up the incident shock front. The overdriven detonation wave that follows, will stabilize close to its theoretical value. On physical insight, no chemical reactions should occur within the unavoidable numerical shock wave thickness. So, to be able to capture the correct pressure jump across the shock, a shock sensor has been designed [13]. Doing so, the chemical energy is only released in the reaction zone and is available to sustain the detonation wave near its theoretical value.

The numerical results at 2 μ s are shown in Fig. 1. The pressure profile is depicted in Fig. 1a. The overall numerical strategy allows us to capture the Neumann spike, which is comparable to the theoretical Von Neumann state obtained from [16]. In Fig. 1b, the products and reactants mass fraction profiles are shown. We can see that the propane is consumed through the reaction zone of length 32.5 μ m, which is stuck to the detonation

front, and that products are formed. At the end of the reaction zone, the products tend to their equilibrium state.



Figure 1: Pressure profile (in bar) with - - - : Neumann state (left) and species mass fraction distribution (right).

The chemical induction time $\tau_1 = 15 \times 10^{-8} [O_2]^{-1}$ used for this computation has been calibrated so that the reaction zone length in the inviscid case varies as the inverse of the initial pressure of the mixture as found in [16]. In the computation, with decreasing pressure, the length of the tube is increased in order to get stabilized numerical detonation waves. The reaction zone is defined as the distance between the shock front and the place where the mass fraction of propane is equal to 1% of its initial value. Fig. 2a shows that the reaction zone Δ evolves as the inverse of the initial pressure, as in the work of Schultz and Shepherd [16] for non-diluted stoichiometric propane-oxygen mixtures. In the same way, the decrease of initial pressure of mixture leads to a slight decrease of the detonation velocity as depicted in the inviscid case of Fig. 2b.

As the detonation propagates through a narrow tube, wall effects become predominant with the decrease of diameter or pressure. Indeed, viscous boundary layer develops behind the detonation front. Due to the induced friction, the detonation front is slowed down. Furthermore, it is expected that the thermal losses extracts some of the chemical heat released into the reaction zone, decreasing further the detonation velocity. The Zel'dovich model consists of the reactive Euler equations, in which the dissipative effects are accounted for by inclusion of a drag force and heat losses respectively in the momentum and energy equations. The reactive mixture is the same as in the previous subsection. The diameter will be fixed at D = 38 mm. And the wall effects will be studied through the initial pressure decrease. The drag force or friction term is modeled as a pressure loss $-\psi\rho|u|u/(2D)$, with ρ , u and ψ are respectively the density of fluid, its local velocity and the friction coefficient. The latter equals to $64 R_e^{-1}$ when the local Reynolds number based on the tube diameter D is below 2500. This friction coefficient is written as $0.316 R_e^{-1/4}$



Figure 2: a) Thickness of Reaction Zone Δ (mm) vs. Initial Pressure P_0 (bar) - b) Detonation Velocity σ (km.s⁻¹) vs. Initial Pressure P_0 (bar).

when the Reynolds number is increased from 2500 to 10^5 . The initial pressure is varied from 1 bar to 100 Pa.

In Fig. 2b, the numerical results obtained with the chemical induction time τ_1 are represented by the curve with squares. It shows that viscosity begins to decelerate the detonation wave velocity compared to the inviscid case represented by the curve with circles when the pressure is less than 200 Pa. This means that at high pressures, chemical time scale clearly controls the wave propagation through the tube. Indeed, the chemical time scale is $\tau_{chem} = \Delta/(\sigma - u_{CJ})$, with Δ , σ and u_{CJ} respectively the reaction zone length, the detonation speed and the fluid velocity at CJ state in the inviscid case. The viscous time scale can be defined from the momentum equation as $\tau_{visc} = 2D/(\psi u_{CJ})$. The ratio of chemical and viscous time scales τ_{chem}/τ_{visc} can be shown to vary now from 10^{-5} to 10^{-2} when the upstream pressure is decreased within the studied range. This is clearly highlighted when the chemical time scale is increased. By multiplying τ_1 by 100 to obtained τ_2 and keeping viscous time scale unchanged, the detonation velocity is drastically reduced as shown by the curve with diamonds in Fig. 2b. The order of magnitude of the ratio between the chemical and viscous time scales is now varied from 10^{-3} to 1. In this case, there is a competition between both time scales.

In order to study the influence of both viscosity and heat transfer on the detonation wave propagation, calculations with similar initial conditions as in viscous case with τ_2 have been carried out. The expression $4\lambda(T_w - T)/D^2$ models the energy source term coming from the thermal losses through the wall, where λ is the thermal conductivity of the mixture and $T_w = 250$ K is the wall temperature. The results depicted on curve with up triangles in Fig. 2b shows that the influence of the thermal losses seem to be negligible in the attenuation of detonation wave propagation. By making a similar time scales analysis as previously between the viscous and thermal time scales, the obtained ratio varies from 10^{-4} to 10^{-1} .

However, it can be noted that the detonation wave speed obtained in the previous simulations are greater that those of Haloua et *al.* [7]. That is probably due to the fact that the experimental data exhibit a multidimensional detonation structure that cannot be completely captured by a 1D model where the chemical reactions occur in the same way on each section of the tube. Therefore, in order to highlight these phenomenon, two-dimensional detonation computations have been performed.

4 2D detonation

This section is devoted to the study of two-dimensional detonations of stoichiometric propane/oxygen mixtures in a narrow channel. After the passage of the detonation front, there is a velocity jump. A boundary layer then develops near the walls in the downstream flow and after a certain distance from the shock front location, the thickness of the boundary layer is of the same order of magnitude than the diameter of the tube. This is specifically true for low diameter tubes. In order to bring out how this confinement affects the structure of the detonation, viscous computations with adiabatic walls have been made in a tube with 79 mm length and 0.267 mm half-height. The initial pressure is 3kPa and the initial temperature is 300 K.

A ZND profile has been used for initialization. The latter has been duplicated along the height of the tube. The meshs' size is such that there is 128 points in the reaction zone for the conditions mentioned above. The cartesian grid is $N_x \times N_y = 9472 \times 95$. The latter grid has been chosen after a grid convergence study. The initial reaction zone of 1.068 mm length is perturbed by a pocket of unburnt gases. The combustion of this pocket generates compression waves that perturb the leading shock front. The instabilities of the initial planar shock will lead to transverse structures. The simulations have been pursued until mature detonation structure. It means that the detonation velocity at the centerline of the channel is constant in time average (cf. Fig. 3) and that the detonation structure is self-similar. From this figure, in the inviscid case, the detonation front propagates at mean constant velocity, 2.4275 km.s⁻¹ which corresponds to a little increase of 0.24 % compared to the one-dimensional ZND inviscid calculation and at 2.1119 km.s⁻¹ in the viscous case, which corresponds to a decrease of 13 % compared to the two-dimensional inviscid result. Fig. 3 also reveals oscillations of the detonation velocity at frequency f, which is about the same in both cases.

After attainment of a mature detonation structure, intersection of oblique shocks and reflection with walls will give rise to triple point-shock interactions as depicted in Fig. 4. This figure represents the numerical schlieren based on pressure at 28 μ s. The locus where the interactions mentioned above occur are triple points, where the fluid pressure and density are highest. Their trajectories have been monitored by recording the local maximum of the pressure gradient in time. Detonation cells are then formed, as shown in Fig. 5. In the viscous case, these cells have 0.6722 mm length and 0.2868 mm width. It is interesting to note that the length of the detonation cells is approximately equal to

the averaged detonation wave velocity divided by the frequency f.



Figure 3: Detonation velocity, σ (km.s⁻¹) take at centerline vs time (µs).



Figure 5: Triples points trajectories in viscous case.

The oscillations of the detonation velocity can be explained by the periodic passage of the triple point at the centerline of the channel. The sudden increase in detonation velocity corresponds to the triple shocks reflections, while the low-velocity excursions correspond to the incident shock propagation.

Fig. 6 depicts the mass fraction gradient of propane at the top and the mass fraction gradient of OH at the bottom for different times. The mass fraction are expressed here as Y_k/Y_k^0 , with Y_k^0 the initial mass fraction. The local Mach number relative to the time average detonation velocity σ is $M_r = (\sigma - u)/c$. The sonic locus where $M_r = 1$ is in white line. The subsonic region lies between the shock front and the sonic locus. Its topology is different from the picture given by [11]. The supersonic region lies everywhere else. It can be seen that the subsonic region is self-similar.



Figure 6: a) Gradient of Propane mass fraction at 26.5 μ s - b) Gradient of OH mass fraction at 30.5 μ s .

All pressure waves generated from heat release in the subsonic zone will catch up the detonation front. Therefore, all energy released by the chemical reactions in the reaction zone is available to sustain the shock propagation. The reaction zone lies beyond the subsonic region. Some propane is still present within the boundary layers. Thus a non-negligible part of chemical reactions occur outside the subsonic region. This can explain the detonation velocity decrease as shown in Fig. 3. It is remarkable that at the centerline of the channel, the relative Mach number is sonic when the propane is almost burnt. The length of the subsonic reaction zone is taken as the distance between the detonation front and the sonic locus at the centerline. Due to the development of the boundary layer in downstream flow, the fluid is slowed down near the walls and the length of the subsonic reaction zone is thus increased compared to the inviscid case, respectively of 1.324 mm and 1.23 mm. The chemical energy released near the walls is not available to sustain the detonation front but rather to heat the walls which are adiabatic. This results in the

attenuation of the detonation accross the shock.

5 Conclusions

In this study, computations of detonation waves propagating in narrow channels have been performed using high-order numerical schemes. The numerical methodology proposed in this study, which includes a fifth-order WENO schemes with the Strang's splitting method, has been first validated through a one-dimensional inviscid ZND detonation. The obtained results agree well with those found in the literature. Two sets of numerical simulations have been carried out. The one-dimensional viscous simulations revealed that the detonation wave propagation is attenuated at very low initial pressures or when the chemical time scale is of the same order of magnitude as the viscous time scale. The order of magnitude of the thermal time scale does not seem to be low enough to affect the wave speed and explain the velocity deficit observed in the experiments. Additionally, two dimensional computations have been conducted to highlight the detonation waves attenuation, in term of velocity deficit, undergoing strong confinement effects. The attenuation of the detonation is attributed to the fact that a part of the chemical energy is released in the boundary layer and did not contribute to sustain the shock front. Moreover, it has been shown that the reaction length is increased in the viscous case compared to the inviscid one. Finally, one should notice that since the current computations have been done with adiabatic walls, further studies with isothermal boundary conditions and heat losses are needed.

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