Dynamics of Detonations with Constant Mass Divergence

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1 Introduction

It is well known that real detonations exhibit a complex three-dimensional cellular structure [1]. There is a growing experimental evidence that the cellular structure of detonations promotes its propagation in the presence of losses. For instance, when a detonation propagates from a tube into an unconfined volume, triple points can cause a local re-ignition on the shock front and therefore maintain the detonation [2].

While unsteady limit problems like detonation diffraction are more difficult to model, steady problems can yield more insight by comparing experiments with models set with various testing hypotheses. The main loss mechanism in steadily propagating detonations is the global mass divergence experienced by the reacting gases in the structure. Detonation propagation in narrow channels [3–5] is governed by the divergence of reacting gases into the boundary layers. In weakly confined tubes [6], the gases in the reaction zone diverge. Likewise, the reacting gases diverge laterally in porous wall tubes [7, 8]. The authors of these previous studies attempted to compare their experiments to a quasi-1D ZND model with mass divergence. They generally found fair agreement for stable mixtures, while the agreement was much poorer for unstable detonations, characterized by complex reaction zone structures. In the latter case, quasi-1D model was found to significantly overestimate the detonation limits. The authors took this as an indication of the role of the three-dimensional cellular structure in controlling the limits of detonations with mass divergence [3, 4, 7, 8].

It is difficult to estimate the precise amount of mass divergence in narrow channels and porous wall tubes. In narrow channels, knowledge of the boundary layer structure is required to estimate the global mass divergence. Likewise, for porous wall tubes, an estimate for the radial mass divergence is difficult. Furthermore, the front is not uniformly curved, making the validity of a quasi-1D nozzle flow with uniform divergence questionable. There is thus a need for experiments with a controllable amount of mass divergence, such that meaningful comparison with quasi-1D and multi-dimensional models can simulations can be made.

In the present study, the mass divergence is controlled by a diverging channel geometry that keeps the global rate of mass divergence constant. Recognizing that a quasi-1D motion of a fluid in a channel with variable cross section $A(r)$ has only a source in the mass equation of the form:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial r} = -\rho u \left(\frac{d(lnA)}{dr} \right) \tag{1}$$

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we consider a channel geometry with a constant logarithmic derivative $K = d(lnA)/dr$, i.e., a channel with an exponentially shaped wall. This provides a constant mass divergence at any cross section of the channel. In this manner, a quasi-steady state with constant loss can be achieved. The dynamics of detonations in a characteristic weakly unstable unstable ($2C_2H_2 + 5O_2 + 21Ar$) and a highly unstable ($C_3H_8 + 5O_2$) are monitored. Comparison is then made with the predictions based on quasi-1D models with area divergence and with multi-dimensional simulations.

2 Experiments

The experiments were performed in a rectangular channel, 3.5-m-long thin rectangular channel, 203-mm-tall and 19-mm-wide. The last meter of the channel was equipped with glass windows allowing to visualize the flow evolution by via high-speed large scale shadowgraphy. The experiments were performed in $2C_2H_2 + 5O_2 + 21Ar$ and $C_3H_8 + 5O_2$ are monitored. The gases were mixed in a separate vessel and left to mix for a minimum of 24 hours before an experiment. Varying the initial pressure, p_0, of the test mixture permitted us to control the reactivity of the mixture. Ignition of the mixtures was achieved with a high voltage capacitor discharge through a spark-gap, with a nominal spark energy of 100 J. In some experiments, a ($C_2H_4 + 3O_2$) driver was used in the first section of the shock tube.

As explained in the introduction, a diverging section was used with a constant logarithmic derivative of the cross-sectional area. Accordingly, a long (1m long and $K = 2.302\ m^{-1}$) and a short (0.5 m long and $K = 4.605\ m^{-1}$) exponential ramp have been designed to make the diverging channels. Two different ramps were used in order to correct the experiments from boundary layer losses inherent in a thin channel geometry. The mixture sensitivity was monitored by changing the initial pressure. Experiments were performed for decreasing pressures until a self-supported detonation wave can no longer be established in the diverging section. On this basis, experiments have been performed for the acetylene mixture on a wide range of initial pressures from 18.9 Kpa to 4.1 Kpa on the large and small ramps. In the same fashion, the propane mixture has been tested at a range of 13.8 Kpa to 2.75 Kpa of initial pressures on both ramps.

Figure 1 shows select composite shadowgraphs illustrating the dynamics of the curved detonations in the diverging section of the channel. Figures 1 (a), (b) and (c) show the detonation wave in acetylene-oxygen-argon at initial pressures of 13.8, 4.8 and 4.1 Kpa propagating in the diverging area. Also figures 1 (d), (e) and (f) show the detonation wave in propane-oxygen at initial pressures of 10.3, 3.45 and 2.75 Kpa. At sufficiently high pressures (Figs. 1 (a) and (d)), both mixtures display curved detonation fronts with a fine cellular structure.

By decreasing the sensitivity of the mixture at lower pressures, the divergence plays a more important role. A much enlarged cellular structure is apparent in both mixtures, as can be seen in (Figs. 1 (b) and (e)). In the weakly unstable detonation, transverse detonations along the path of the triple points are observed until the limit, shown for example in Fig. 1 (b). In the more unstable mixture, the transverse waves appear as non-reactive near the limit, shown in Fig. 1 (f). Instead complex shear flow with finely textured un-reacted pockets are observed.

In order to quantitatively investigate the dynamics, velocity measurements have been performed for the detonation front along the top wall in each experiment. It found that the detonation maintains a constant speed. This value is reported for each experiment in Figs. 2 (a) and 2 (b) for the acetylene and propane mixtures, respectively. At each pressure, the non-dimensional rate of mass divergence is $K_{eff}\Delta_i$, where Δ_i is the ZND induction length for that particular mixture from kinetic simulations and K_{eff} is the effective rate of mass divergence due to both the ramp expansion and losses to boundary layers. The

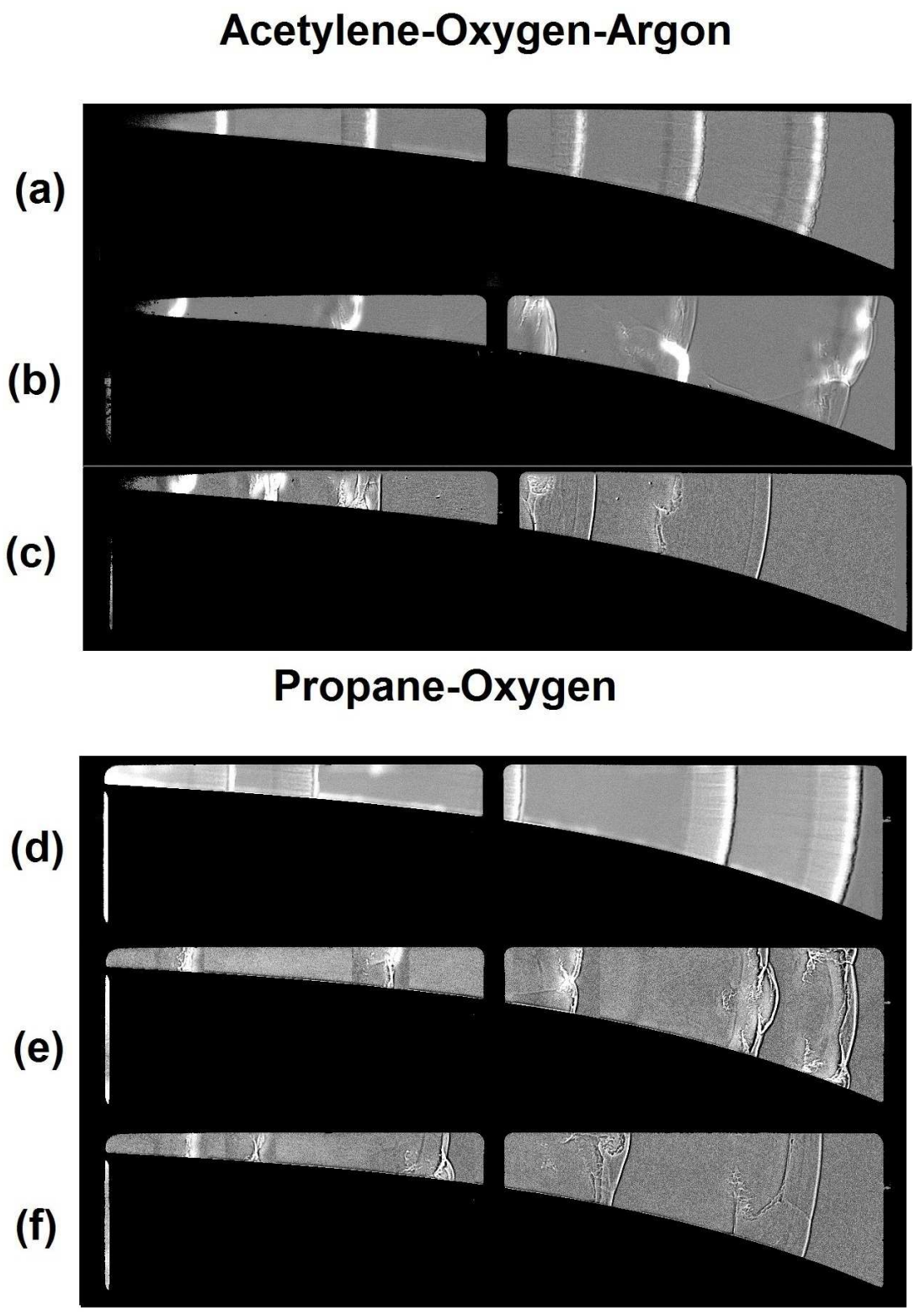

Figure 1: Detonation structure at sequential time frames for acetylene mixture at (a) 13.8 Kpa (b) 4.8 Kpa (c) 4.1 Kpa and propane mixture at (d) 10.3 Kpa (e) 3.45 Kpa and (f) 2.75 Kpa psi

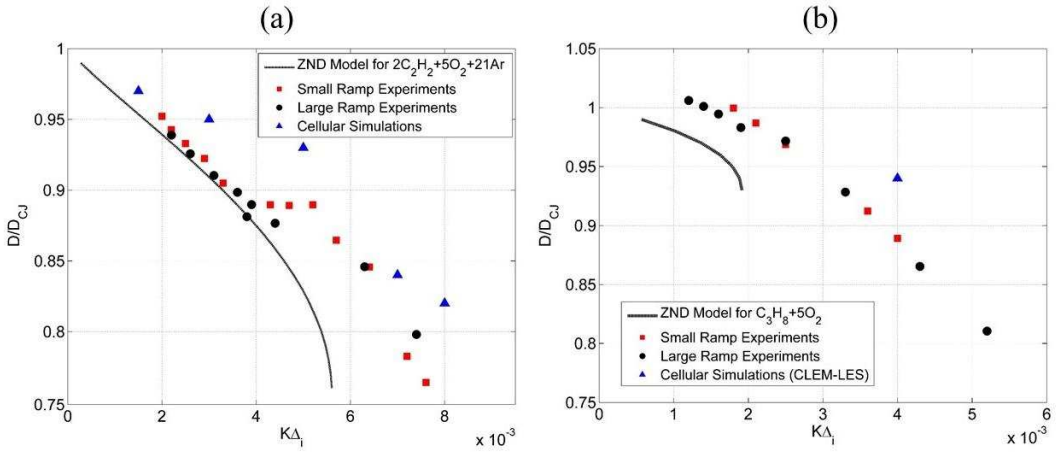

Figure 2: $D - K\Delta_i$ relations for (a) acetylene and (b) propane mixtures

systematic effect due to boundary layers was estimated by comparing the experiments performed in the two channels with different divergence and assuming that there is a unique relation between velocity deficit and curvature. The obtained relationship between wave speed and total divergence is shown in Figures 2 (a) and 2 (b) for the acetylene and propane mixtures. Note that the results obtained for the small and large ramps overlap for a given mixture by construction used to estimate the boundary losses.

The results shown in Fig. 2 illustrate that the velocity deficit increases with the rate of mass divergence. Both mixtures have approximately the same behavior, with maximum velocity deficits of approximately 20%. The limiting maximum mass divergence $K\Delta_i$ beyond which detonations are quenched is also similar for both mixtures, approximately 0.008 for the acetylene mixture and 0.005 for the propane mixture.

3 Comparison with a quasi-1D model with mass divergence

In order to get further insight into the role of mass divergence on the detonation dynamics observed experimentally, we first compared the experiments with an estimate of the velocity deficit obtained from a quasi-one-dimensional model with lateral mass divergence (figure 3) Since the ZND model neglects the existence of the cellular dynamics, this comparison would permit to assess the role of the cellular structure on the dynamics.

The ZND structure with mass divergence is given by [9]

$$\frac{dp}{dt} = -\rho v^2 \frac{(\dot{\sigma} - v\alpha)}{\eta} \quad , \quad \frac{d\rho}{dt} = -\rho \frac{(\dot{\sigma} - vM^2\alpha)}{\eta} \tag{2}$$

$$\frac{dv}{dt} = v \frac{(\dot{\sigma} - v\alpha)}{\eta} \quad , \quad \frac{d\lambda}{dt} = -A\ \lambda\ e^{\frac{-E_a}{RT}} \tag{3}$$

where v, λ and A denote the velocity in the shock attached frame, progress variable for reactions and pre-exponential factor in the one-step chemistry respectively. α denotes the area divergence of the stream tube shown in figure 3 and is represented by $(\frac{1}{A'}\frac{dA'}{dx})$. Also $\dot{\sigma}$ denotes the thermicity representing the effective rate of energy release expressed by [9]

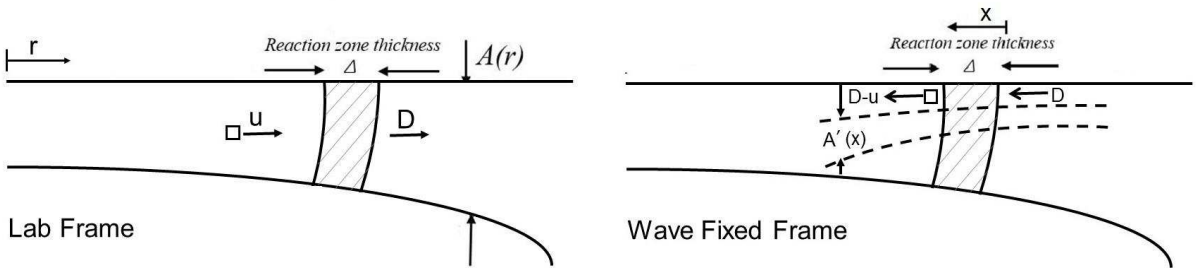

Figure 3: A curved detonation wave and quasi-one-dimensional flow behind it in the wave fixed frame

$$\dot{\sigma} = \frac{(\gamma - 1)Q\frac{d\lambda}{dt}}{c^2} \quad where \quad \eta = 1 - M^2 \quad and \quad M = \frac{v}{c} \tag{4}$$

and c, M and η denote the sound speed, Mach number and sonic parameter. Also for small-curvature quasi-steady waves the variation of the stream tube area $A'(x)$ behind the leading shock is related to the area divergence rate of the channel by

$$\frac{1}{A'}\frac{dA'}{dx} = \frac{1}{A}\frac{dA}{dr}\left(\frac{D}{v(x)} - 1\right) \tag{5}$$

where D is the detonation velocity.

The thermo-chemical parameters for each mixture were extracted from chemical equilibrium and constant volume ignition calculations following the procedure outlined in [8]. For a given rate of mass divergence, the corresponding wave velocity was found by integrating the equations above from the shock towards the burned state and seeking the solution satisfying the generalized CJ condition [10–12].

The results obtained are shown in figure 2 for both mixtures. For the weakly unstable mixture, the model predicts surprisingly well the velocity deficit less than 10%. At higher velocity deficit, the detonations with larger rates of mass divergence can propagate than predicted by the model. The predicted limiting value of the mass divergence is lower than the experimental one by 25 %.

For the more unstable propane mixture, there is a much more substantial difference between the experiments and the model prediction. The experimental velocity is systematically larger than predicted for a given mass divergence. The predicted limiting value of the mass divergence is lower than the experimental one by 60 %, while maximum velocity deficit is also much larger in the experiment. These large discrepancies, and the fact that the losses are over-predicted by the quasi-1D model indicates that the cellular structure plays a more important role. This indicates the inadequacy of the steady ZND model, which neglects cellular instabilities, to capture the failure mechanism in unstable mixtures.

4 Comparison with cellular simulations

In order to gain more insight on the role of the cellular structure on detonations with global mass divergence, we have performed numerical simulations of the cellular structure. The simulations were performed using the MG code developed by Mantis Numerics Ltd., which features a second order accurate Godunov solver to treat convective terms [13]. For the acetylene mixture, the Euler equations,

supplemented by a one-step Arrhenius reaction model, were solved for several pressures using a resolution of 16 grid cells per half reaction length. For propane, the compressible LEM-LES (CLEM-LES) strategy [14] is adopted for $p_o = 0.6$ psi using a base resolution of 1 cell per half reaction length. The CLEM-LES model is a grid-within-a-grid approach that has been adopted from the Linear Eddy Model for Large Eddy Simulation [15], but designed to treat both highly compressible and reactive flows. Further details can be found in [14, 16]. The results of the simulations are also included in the figure 2. It can be seen that for the acetylene mixture, there is a relatively good agreement between the experiments and the numerical simulations. These observation indicate that the failure mechanism in the weakly unstable mixtures in the experiments is consistent with the limits of curved ZND detonations, where the existence of cellular structure is neglected. Near failure, the cellular simulation results are found in good agreement with the experimental results for velocity deficits, but differ from the predictions based on the quasi-one-dimensional model. This illustrates that the cellular structure plays a sensible role near failure even for this mixture, usually considered as an ideal detonation with negligible role of cellular structure.

For the unstable mixture, we have not attempted to conduct inviscid calculations, owing to the intrinsic difficulties associated with numerical diffusion in highly unstable detonations [17]. Instead, the preliminary CLEM-LES results recover well the experimental velocity deficit. This result suggests that the burning mechanism permitting the wave to remain self-sustained well beyond the limit predicted by a quasi-one-dimensional model is well recovered by the turbulent model, consistent with the findings of Maxwell et al. [14].

5 Conclusions

In this work, the influence of cellular structure on the dynamics of detonations in diverging geometries was investigated. In this regard, experiments on mixtures with stable and unstable cellular structure were performed. Through experiments, dynamics of detonations in a diverging geometry was studied. Experimental results were also compared with the ZND model predictions and cellular detonations simulations. The results showed that the dynamics of the stable mixture was relatively close to what predicted by the ZND theory. However, the experimental velocity deficit and loss rate for extinction of unstable mixture were significantly different with ZND predictions for unstable mixture. Such results indicate the inadequacy of ZND model for prediction of detonations dynamics in unstable mixtures.

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