Acoustic timescale characterization of unreacted pockets in unstable detonation waves

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1 Introduction

Volumes of unreacted fluid surrounded by combustion products are observed in unstable cellular detonations [1–3]. These pockets of unreacted gas form behind the slip line after being preheated by the incident shock and have the shape of a "tongue." When the transverse wave collides with another transverse wave or a channel wall, the tongue is pinched off to form an isolated pocket of unreacted fluid [1, 3].

Radulescu *et al.* [1] suggest that diffusive phenomena plays an important role in the consumption of these pockets and that their consumption helps sustain the detonation wave. Kiyanda and Higgins [3] further demonstrate the turbulent flame front reaction is limited to the burnt/unburnt gas interface using simultaneous Schlieren and self-luminous images. The results also suggest that when transverse waves impact walls or other transverse waves, localized auto-ignition may occur inside the unreacted pockets. However, it is unclear whether these fast reactions produce compression waves that may interact with the lead detonation front.

Regele *et al.* [4] performed numerical simulations of one-dimensional detonation initiation and found that the ratio of the heat release time to acoustic time of a localized hot spot characterizes the pressure response in the surrounding fluid. This behavior is consistent with the asymptotic analyses predicted by Kassoy [5]. Kurtz and Regele [6] expand upon this characterization and show that by varying the heat release to acoustic timescale of a hot spot by only two orders of magnitude the ensuing thermomechanical response varies from weak compression/acoustic waves to strong shock wave emission.

The objective of this work is to use the timescale analysis approach to characterize and predict the potential magnitude of compression waves generated from the turbulent reaction that occurs at a pocket's interface and from the homogeneous reactions that are observed in experimental data [1–3]. This analysis may help explain some of the sources of the very irregular cellular structure observed in unstable detonation waves. The approach will be to measure the unreacted pocket size and reaction duration from experimental Schlieren and self-luminous images. The acoustic timescale will be estimated and the ratio of the reaction to acoustic timescales will be calculated. Simple 1-D numerical simulations will be performed to estimate the magnitude of compression waves that may be created from the calculated timescale ratios.

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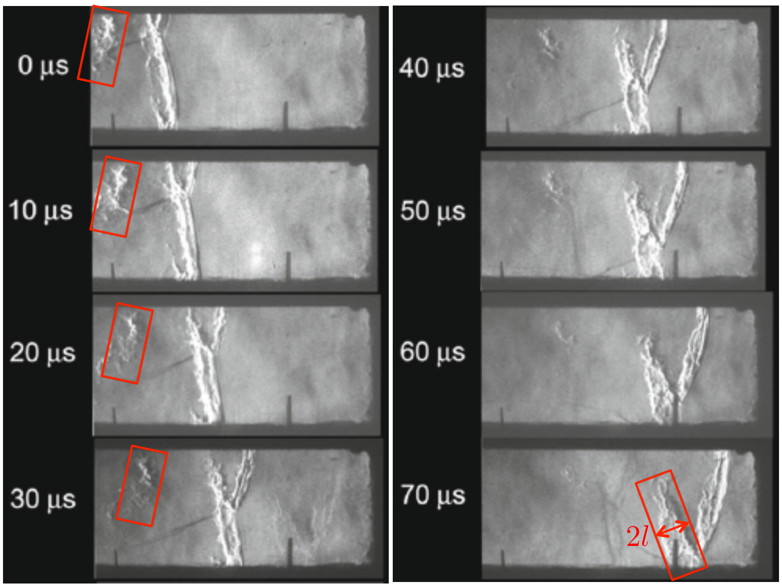


Figure 1: Figure 5 of Kiyanda and Kiggins, 2013 [3]. Unreacted pocket reaction in an unstable detonation wave propagation. It takes roughly $50\,\mu$s for most of the pocket to be consumed.

2 Experimental Pocket Reaction Analysis

2.1 Surface Reaction

Figure 1 shows the Schlieren image sequence for a single-headed unstable detonation wave in a reactive mixture of stoichiometric CH_4-O_2 at a pressure $p_0 = 3.4\,\mathrm{kPa}$. It takes roughly $70\,\mu$s for the transverse wave to propagate from the top of the channel to the bottom. Once the transverse wave reaches the bottom the wave reflects off the wall and the unreacted pocket of fuel is isolated from the main reaction front. As annotated in the figure, we define the length scale of the pocket to be half the width. The frame $t = 70\,\mu$s indicates the beginning of the reaction of the isolated pocket and mirrors the reaction that had occured previously in frames 0 to $40\,\mu$s. Thus, as reported in Ref. [3], it takes roughly $50\,\mu$s for a pocket to react so that the pocket reaction time is $t_r = 50\,\mu$s.

Based upon the height of the domain, we can estimate the width of the pocket to be $w = 16\,\mathrm{mm}$ so that the characteristic length scale is $l = w/2 = 8.0\,\mathrm{mm}$. The acoustic timescale of this pocket can then be evaluated be dividing by the speed of sound inside the pocket. The results [3] indicate the unreacted pocket temperature is roughly $T = 1000\,\mathrm{K}$. With a stoichiometric mixture of CH_4 and O_2 at this temperature the specific heat ratio and gas constant are calculated to be $\gamma = 1.18$ and $R = 311.8\,\mathrm{J/kg \cdot K}$, respectively. With a sound speed of $a_0 = 606\,\mathrm{m/s}$, the acoustic timescale is estimated to be $t_a = l/a_0 = 13\,\mu$s.

The ratio of the reaction time to acoustic time is then evaluated to be $t_r/t_a = 3.8$. The previous analysis by Kurtz and Regele [6] focused on limiting extremes where the reaction to acoustic timescale ratios were 0.1, 1, and 10. The timescale ratio $t_r/t_a = 3.8$ for the unreacted pocket observed in the unstable detonation in Fig. 1 is in between the case that creates a strong compression wave and the case that reacts in a nearly isobaric fashion. It can be anticipated that the reaction of the unreacted pocket does facilitate some increase in pressure. The magnitude of this pressure rise is evaluated in the Section 3.

A similar analysis can be performed for the unstable detonation wave presented in Bhattacharjee's thesis [7] where the same reactive mixture and initial conditions are used, but the initial pressure is

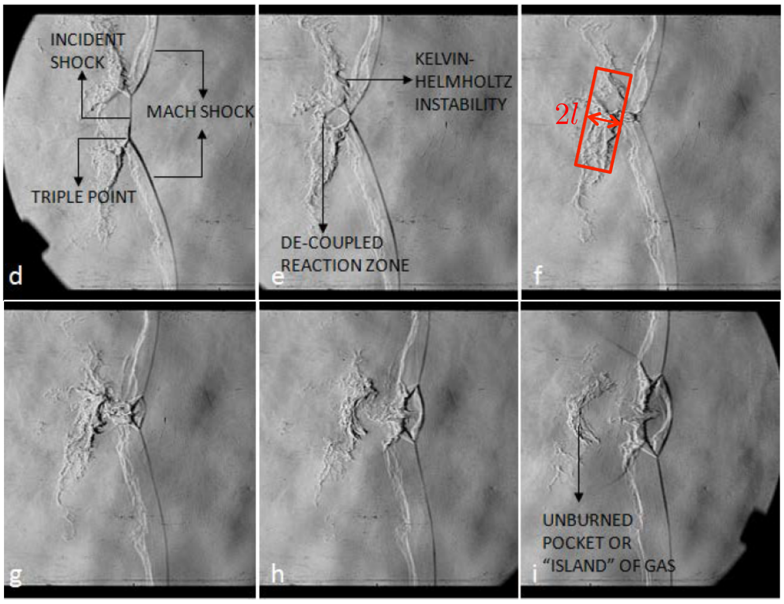


Figure 2: Portions of Fig. 3.1 and 3.2 from Bhattacharjee's thesis [7]. In this case, the unreacted pocket is created when two transverse waves meet and pinch off an unreacted pocket of width $w = 2l$ =19.2 mm.

$p_0 = 3.5\,\mathrm{kPa}$. The width of the unreacted pocket in frame (f) is 19.2 mm, which gives a characteristic length $l = 9.6$ mm. If the unreacted pocket temperature is assumed to be the same as in Ref. [3] $T_0 = 1000$ K, the sound speed is the same and the acoustic timescale is $t_a = l/a_0 = 16\,\mu$s. The reaction is observed to occur over roughly 5 frames, with each frame being $11.53\,\mu$s, to give a reaction time $t_r = 57.7\,\mu$s. The ratio of the reaction to acoustic timescale is calculated to be $t_r/t_a = 3.6$. The greatest uncertainty stems from the assessment of the reaction time since it is unclear when the pocket is fully reacted. Some residual reactants are still left after five frames, but after six frames any remaining reactant is negligible.

The unreacted pocket reaction times in these two cases are within 7% of the mean of these two values, which suggests that these pocket sizes may be somewhat regular. However, other transverse wave collisions have been shown to produce unreacted pockets much larger than these and have been suggested to be a source of the irregularity observed in the detonation cell structure [3]. The uncertainty in the reaction time is significant enough that only one significant figure is used. Thus, in both of these cases the time scale ratio can be approximated as $t_r/t_a \approx 4$.

2.2 Pocket Auto-ignition Reaction

The behavior observed in the previous section shows how an unreacted pocket is consumed through reaction at the turbulent surface. Rapid reactions have been observed to occur immediately following the collision of two transverse waves [2] or after transverse waves impact the channel wall [3].

Figure 3 shows a sequence of Schlieren images from Ref. [3] as a transverse wave propagates downward and impacts the wall at the $20\,\mu$s frame. Displayed to the right of this frame is a self-luminous image that captures where the reaction is occurring. At this frame the reflected transverse wave has not entered the unreacted pocket material yet. At the $30\,\mu$s frame the Schlieren image shows that the shock has entered the pocket region. At the $40\,\mu$s frame the transverse shock has propagated all the way through the pocket and the Mach stem has formed along the bottom wall. The self-luminous image in the

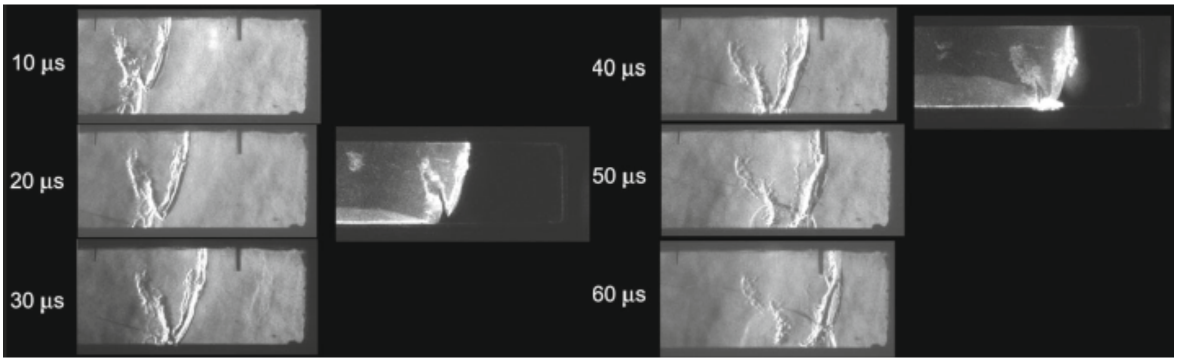
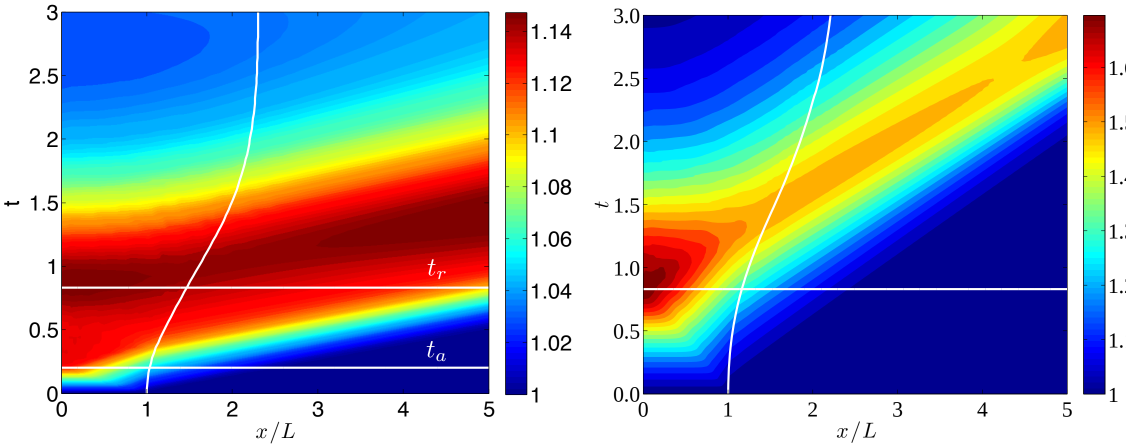


Figure 3: Figure 6 from Kiyanda and Higgins, 2013 [3]. Transverse shock reflection from the lower wall causes a large temperature increase in the unreacted pocket and facilitates auto-ignition at a rate fast enough to create a compression wave.

$40\,\mu$s frame shows a bright region homogeneously distributed within the unreacted pocket behind the transverse wave, which suggests auto-ignition may be occurring in the material.

In frames $50\,\mu$s and $60\,\mu$s, the Schlieren images suggest that compression waves originate from the reaction region. As performed in the previous section, a similar timescale analysis can be performed for this reaction event. It is unclear from the Schlieren image what the proper length scale should be. The self-luminous image gives a good indication of the size of the localized hot spot reaction. The hot spot height from the bottom of the channel is measured to be $l = 6$ mm. Clearly the temperature inside the pocket will increase as the transverse shock is transmitted through it. However, with only single digit accuracy, the speed of sound will not change dramatically. Thus, the acoustic timescale is estimated to be $t_a = 10\,\mu$s. It is unclear how long the reaction lasts without additional self-luminous images. However, based upon the Schlieren and self-luminous images, the reaction is estimated to begin sometime between the 30 and $40\,\mu$s frames and ends sometime between the 40 and $50\,\mu$s frames, which gives a reaction time of roughly $t_r = 10\,\mu$s. The ratio of the reaction to acoustic time becomes $t_r/t_a = 1$. Previous timescale analyses [4, 6] show that for this timescale ratio, the reaction of this fluid volume will produce compression waves with pressure amplitude on the order of the post-combustion pressure for a constant volume reaction, which is consistent with the density gradients observed in the Schlieren images in frames 50 and $60\,\mu$s.

This localized explosion from transverse wave collision has been observed in other work as well [2]. One of the issues with the image sequence in Fig. 3 is the lack of temporal resolution ($\Delta t = 10\,\mu$s) to obtain a more precise measurement of the reaction duration. Austin [2] captured the collision of transverse waves using Schlieren images with a $1.6\,\mu$s frame speed. No self-luminous images are present in this work so it is difficult to clearly show the localized auto-ignition created by the wave collision. However, two sets of density discontinuities are emitted from within what appears to be the collision area, which suggests a reaction may have occurred to produce compression waves. Unfortunately, it is unclear what the length scale of the localized hot spot region is in order to measure the acoustic timescale. The reaction length scale is estimated to be $l = 1$ mm, which gives a timescale ratio $t_r/t_a = 1$. This timescale suggests strong compression waves would be emitted from the reaction region, which is consistent with the Schlieren images.



(a) Tubulent flame surface reaction $t_r/t_a = 4$

(b) Auto-ignition timescale $t_r/t_a = 1$

Figure 4: x-t diagrams of normalized pressure p/p_0 for the timescale ratios for a turbulent flame and auto-ignition.

3 Numerical Analysis

In order to estimate the potential amplitude of compression waves emitted by the pocket surface reaction and localized auto-ignition, 1-D numerical simulations using the reactive Euler equations are performed for a pocket of unburned reactants at constant temperature surrounded by combustion products. For brevity, the auto-ignition from a region of unreacted fluid and the ensuing thermomechanical response is assumed to provide a rough estimate of the compression waves that may be generated from both the turbulent flame front and the auto-ignition events. A more detailed investigation of a retreating reaction front is the subject of future work.

The numerical approach is consistent with that in Ref. [4]. The computational domain is set up in the same way as that performed in Kurtz and Regele [6] for the plateau only case with the surrounding region at a post-combustion temperature. A pocket with an initial non-dimensional temperature $T = 5$ is used and pocket sizes are chosen such that the ratio of the reaction time to acoustic time $t_r/t_a = 4$ and 1. These two ratios correspond to the turbulent flame and auto-ignition reactions, respectively.

The non-dimensional reaction parameters use a heat of reaction $q = 42$, pre-exponential factor $B = 10$, activation energy $E_a = 17$, and specific heat ratio $\gamma = 1.2$. The equations are solved using the adaptive wavelet-collocation method and the grid resolution is increased until the ignition time varies by less than 0.1%.

Figure 4 shows x-t contours of the pressure normalized by the initial pressure p/p_0. The x-axis is normalized by the pocket size L so that the pocket edge is located at $x/L = 1$ in both cases, but case (a) is four times smaller than case (b). In both cases, a compression wave is created as the reaction commences and pushes the surrounding fluid away from the pocket. The compression wave amplitude in the $t_r/t_a = 4$ case is $p/p_0 = 1.14$ (14% pressure rise), whereas the $t_r/t_a = 1$ case has a pressure rise $p/p_0 = 1.5$. Therefore, the pocket reaction with a timescale ratio $t_r/t_a = 1$ produces a significantly stronger compression wave than the $t_r/t_a = 4$ case, which suggests that the auto-ignition reaction observed above is more likely to produce comression waves that may be visible in a Schlieren image. Furthermore, the small pressure rise in the $t_r/t_a = 4$ case rises by only 14%, which suggests that it may be difficult to observe compression waves emitted from the turbulent flame front.

4 Conclusions

The reaction of unreacted pockets in unstable detonation waves are analyzed by looking at the reaction times that occur from surface reactions and after transverse wave collisions. In the absence of wave collision, the pockets react primarily at the surface. The fuel burns in a more homogeneous fashion in cases where transverse wave collision leads to a rapid consumption of fuel. For both types of reaction, the ratio of the heat release to acoustic timescale of the pocket or reaction region is used to assess the propensity to create compression waves, which may propagate upstream to the detonation front.

The timescale ratio calculated from the reaction of the turbulent flame at the burnt/unburnt gas interface of the unreacted pockets is approximately 4. Numerical analysis of this type of reaction shows that only a mild a pressure rise of 14% can be expected from this type of reaction. While finite compression waves will be created, it may be difficult to observe them experimentally since the density gradient is much less than the other surrounding structures.

When transverse waves collide or impact the channel wall, a homogeneous reaction of a portion of the unreacted pocket occurs. The size of the reaction region and time associated with these reactions produces reaction to acoustic timescale ratios near unity. Numerical simulations of this type of localized pocket reaction show that the emitted compression wave has a pressure rise of 50%.

It is still difficult to accurately quantify these timescale ratios. In order to perform this analysis more accurately, temporal resolution on the order of $1\,\mu$s is needed for both Schlieren and self-luminous images simultaneously.

References

[1] M. I. Radulescu, G. J. Sharpe, C. K. Law, and J. H. S. Lee, "The hydrodynamic structure of unstable cellular detonations," *Journal of Fluid Mechanics*, vol. 580, p. 31, May 2007. [Online]. Available: http://www.journals.cambridge.org/abstract_S0022112007005046

[2] J. M. Austin, "The Role of Instability in Gaseous Detonation," Ph.D. dissertation, California Institute of Technology, 2003.

[3] C. B. Kiyanda and A. J. Higgins, "Photographic investigation into the mechanism of combustion in irregular detonation waves," *Shock Waves*, vol. 23, no. 2, pp. 115–130, Oct. 2013. [Online]. Available: http://link.springer.com/10.1007/s00193-012-0413-8

[4] J. D. Regele, D. R. Kassoy, and O. V. Vasilyev, "Effects of high activation energies on acoustic timescale detonation initiation," *Combustion Theory and Modelling*, vol. 16, no. 4, pp. 650–678, Jan. 2012. [Online]. Available: http://www.tandfonline.com/doi/abs/10.1080/13647830.2011.647090

[5] D. R. Kassoy, "The response of a compressible gas to extremely rapid transient, spatially resolved energy addition: an asymptotic formulation," *Journal of Engineering Mathematics*, vol. 68, no. 3-4, pp. 249–262, Aug. 2010. [Online]. Available: http://www.springerlink.com/index/10.1007/s10665-010-9402-z

[6] M. D. Kurtz and J. D. Regele, "Acoustic timescale characterisation of a one-dimensional model hot spot," *Combustion Theory and Modelling*, vol. 18, no. 4-5, pp. 532–551, Jul. 2014. [Online]. Available: http://www.tandfonline.com/doi/abs/10.1080/13647830.2014.934922

[7] R. R. Bhattacharjee, "Experimental Investigation of Detonation Re-initiation Mechanisms Following a Mach Reflection of a Quenched Detonation," Ph.D. dissertation, University of Ottawa, 2013.