Detonation Diffraction in Regular and Irregular Mixtures

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Diffraction of a gaseous detonation has been widely studied [1-7] in the context of both applications and as a scientific experiment that provides insight into the interaction between the combustion processes at the wavefront and the fluid motion induced by the diffraction process. For detonation propagation in tubes and channels, it is firmly established that there are reasonably well-defined critical conditions $(e.q., \text{diameter } d_c)$ that separate failure (sub-critical) and successful detonation transition (super-critical) when diffracting into a larger volume. However, there is no fundamental theory for the prediction of the critical quantities like d_c . The empirical correlation $d_c \approx 13\lambda$ holds for many common fuel-oxygen or -air mixtures [8] but breaks down for mixtures with a large amount of argon dilution. Critical tube diameters of up to 30 λ were measured [3] for stoichiometric C₂H₂-O₂ mixtures with 80% Ar dilution. This effect appears to be linked to systematic differences in the regularity of the instability pattern on the detonation front with variations in the mixture composition [9] in fully developed detonations. Recently, we [10, 11] have proposed that the effective normalized activation energies θ ($\theta = E_a/RT_{ps}$) can be used as a figure of merit to characterize the degree of cellular regularity in propagating detonation. Lee [12] has proposed that the mechanisms of detonation failure are qualitatively different in mixtures with regular and irregular cellular structure and that this is linked to the different roles of transverse waves in the combustion process.

The objective of the present study is to obtain detailed measurements that can be used to provide quantitative data to test the various theories about detonation diffraction and speculations about the role of transverse waves in mixtures with very different degrees of cellular regularity. To do this, we use laser schlieren photography, multiple-exposure chemiluminescence imaging and, for the first time in a diffraction experiment, planar laser-induced fluorescence (PLIF) of the OH radical, Fig. 1. The reaction front velocity was obtained from the multiple exposure chemiluminescence images. The mixtures studied were H₂-N₂O ($\theta = 9.5$) which has an irregular cellular structure, and up to 70% Ar-diluted H₂-O₂ ($\theta = 4.5$), which has a very regular cellular structure. Instead of characterizing the mixtures by cell width, a poorly defined quantity in irregular mixtures, we have used the calculated induction zone length Δ at Chapman Jouguet (CJ) conditions. In terms of this, the critical diameters are $d_c \approx 530\Delta$ for $\theta = 4.5$ and $d_c \approx 230\Delta$ for $\theta = 9.5$.

The detonation diffraction facility consists of a 1.5 m long tube with a circular cross section and an inner diameter d of 38 mm joined through a sharp 90° corner to a 0.8 m long, 150 mm square test section. The tube is equipped at the ignition end with a 305 mm long Shchelkin spiral and spark plug. Pressure histories were



Figure 1: Simultaneously obtained experimental images of sub-critical experiments: a) schlieren, b) PLIF of OH-radical, c) multiple exposure chemiluminescence. 0.5 H₂ + 0.5 N₂O (θ = 9.5), P₀=45 kPa. Image heights from left: schlieren 110 mm, cropped schlieren 80 mm, overlay 80 mm, PLIF 70 mm, chemiluminescence 109 mm. The detonation is traveling from left to right.

recorded by six pressure transducers equally spaced in the tube and test section. The detonation velocity in the tube prior to the diffraction was measured to be within 1.5 % of the calculated CJ value U_{CJ} .

The PLIF images show the details of the OH front geometry in the diffraction process, Fig 2b and e. In the sub-critical case, saw-tooth-like geometries in the OH front are observed where the shock wave decoupled from the reaction front [13]. These are remnants of key-stone shaped features characteristic of cellular structure present on the fully developed detonation prior to reaching the abrupt area change. These structures appear to be passively convected in the decoupled region. In the critical case, the key-stone structures are regenerated at the front when the re-ignition event takes place. In the super-critical regime, the structure is persistent and actively evolving during the diffraction process.

The differences between the mixtures are most striking in the sub-critical and critical regime. In the critical regime, the coupling between shock and reaction front persists significantly longer for $\theta = 4.5$ than for $\theta = 9.5$. This is clearly evident on the overlay of simultaneously obtained schlieren and PLIF images, Fig. 2c and f. For the sub-critical H₂-O₂-Ar mixtures, the leading shock is strongly distorted from circular and the reaction front was attached to the lead shock up to 2.3 tube diameters (d) from the tube end plate. The reaction front velocity on the tube axis remained above 0.8 U_{CJ} until approximately 1.5 d. For the sub-critical H₂-N₂O mixtures, the reaction front decoupled rapidly over the whole outline, leading to a self-similar, nearly circular shock shape shortly after the detonation exited the tube. The reaction front velocity decreased to approximately 0.6 U_{CJ} after a distance of 1.1 d. This rapid decay in reaction front velocity can be attributed to the higher activation energy of the H₂-N₂O mixture, which leads to larger changes in the induction time for small changes in the lead shock strength.

We have performed a simplified analysis of the sub-critical regime comparing the



 $0.22 \text{ H}_2 + 0.11 \text{ O}_2 + 0.67 \text{ Ar}, P_0 = 100 \text{ kPa}, \theta = 4.5, \text{ shot } 202.$



schlieren image PLIF image false color overlay

Figure 2: Observations for sub-critical experimental outcome in the critical regime. The detonation is traveling from left to right. (a) and (b) schlieren image height 150 mm height. (b) and (d) are the simultaneously obtained corresponding OH PLIF images, (c) and (f) are false color overlays as indicated by boxed region in schlieren images.

residence time of a fluid element at the OH front with the induction time of that fluid element. This indicates that the decoupling of shock and reaction front is due to the rapid increase in induction time relative to residence time as the wave decays and creates an unsteady expansion of the flow. The saw-tooth geometries of the OH front are convected with the post shock flow field but the energy release rate is small in these regions although a transition to diffusive combustion may be taking place on the time scale of our observations. In the super-critical regime, re-ignition events and resulting transverse detonations are observed in both mixture types. The three-dimensional structure of transverse detonation was revealed using stereoscopic imaging. The high-luminosity region was reconstructed to clearly show the location of the transverse detonation just below the shock surface.

In conclusion, we have quantitatively documented the differences in the diffraction process in mixtures with regular ($\theta = 4.5$) and irregular ($\theta = 9.5$) detonation instabilities. Our measurements of reaction front geometry and velocity can be used to make quantitative tests of models for the role of transverse waves and turbulence in the combustion process in detonation waves.

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