Detonation Initiation Regimes of Shock-Flame Complexes in Fuel Blends of Hydrogen and Methane

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1 Introduction

The growing adoption of hydrogen as a fuel source across various applications has elevated safety concerns, particularly in its use as a component of hydrogen-natural gas blends. These blends are gaining prominence for their potential to reduce carbon emissions; however, significant knowledge gaps persist regarding the dynamics of flame acceleration and the transition from deflagration to detonation in such mixtures. A key question of our research is to answer the question of how much hydrogen content addition to natural gas in pipelines would be considered safe.

Of particular safety concern is to better understand deflagration-to-detonation transition (DDT), which consists of two key phases: flame acceleration and detonation onset. During these phases, the flame velocity approaches the Chapman-Jouguet (CJ) deflagration speed before transitioning to detonation. Experimental and numerical studies have explored the pre-DDT regime by examining self-sustained detonation waves interacting with perforated plates or obstacles, generating choked shock-flame complexes characterized by velocities near the CJ deflagration state [1–3].

The run-up distance (L_{DDT}) has been studied extensively and linked to mixture properties and geometric parameters. Veser et al. [1] defined L_{DDT} as the point where the flame tip velocity achieves 95% of the choked flame speed. They proposed a correlation for hydrocarbon mixtures with orifice plates, incorporating parameters such as laminar burning velocity, expansion ratio, sound speed, and tube geometry, including blockage ratio (BR) and radius. Similarly, Silvestrini et al. [2] proposed a correlation for smooth and obstacle-laden tubes, defining L_{DDT} as the distance at which the flame velocity reaches 0.5DCJ in hydrogen and other hydrocarbon mixtures. Mehr and Ciccarelli [3] extended it to pure hydrogen-oxygen/air mixtures, defining L_{DDT} as the distance from ignition to the first detonation re-initiation. Their work included correlations for stoichiometric hydrogen-oxygen mixtures at $p_0 \leq 45$ kPa with BR=75%. Saif et al. [4] investigated hydrocarbon-oxygen mixtures, relating L_{DDT}—from the choked flame complex to detonation onset—to detonation cell size and instability parameter χ. These works collectively illuminate L_{DDT} under varied conditions.

On the other hand, numerical studies primarily examined detonation initiation of shock-flame complex arrangements in methane-oxygen mixtures using one-step models [5–7]. In particular, turbulence closure, via. the linear eddy model approach [5] or through high resolution Navier-Stokes modelling [7], was found useful to capture the detonation re-initiation timing, however the methods do not lend themselves well to performing a full parametric study due to the added overhead. Moreover, the application of one-step combustion models generally fails to account for the sensitivity of reaction rates to abrupt flow changes, such as behind transverse shocks, thus leading to unphysical flow evolutions during the re-initiation process. While detailed chemistry mechanisms address this aspect, they incur significant

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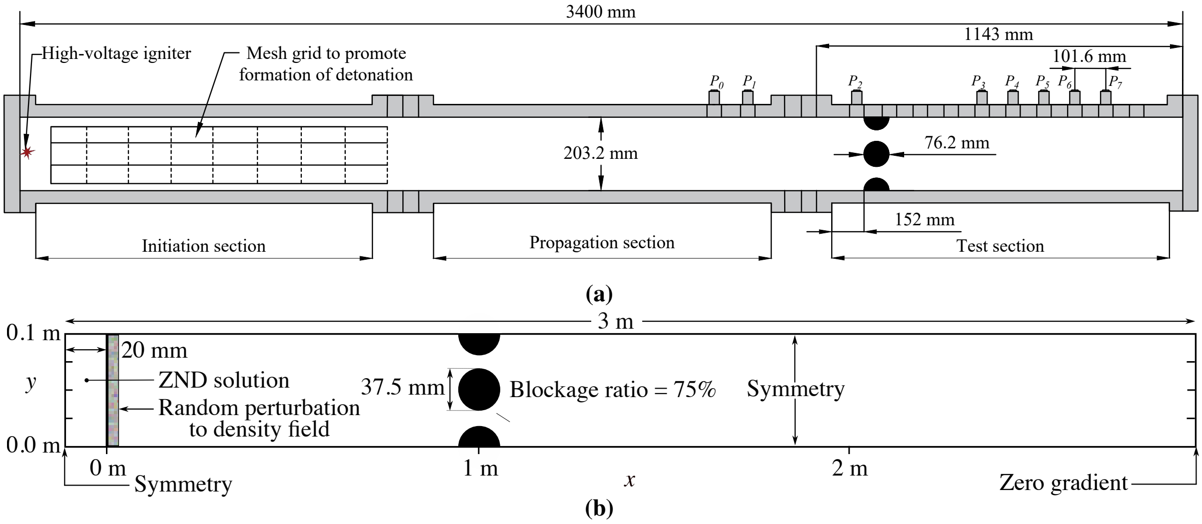
computational costs. To balance accuracy and efficiency, Zhu et al. [8] developed a four-species, four-step reaction mechanism, simplifying kinetics while retaining essential physics. Recent studies have applied this model in inviscid Euler simulations to investigate detonation phenomena, including quenching and re-initiation by reactive transverse waves [9, 10].

Despite significant progress, the transition of choked flames to detonation in hydrogen or hydrogen-methane blends remains largely unexplored. This study addresses the gap by investigating the DDT process in hydrogen-natural gas blends through a combined experimental and numerical approach. Experimentally, the final stage of the transition, where fast flames in hydrogen-methane mixtures evolve into detonations, is examined using an experimental setup similar to Saif et al. [4]. Numerically, a global four-step combustion model [10] is employed to overcome the limitations of simpler approaches and provide precise insights into flame acceleration, detonation limits, and the critical conditions for DDT. By combining experimental and numerical methods, this study seeks to advance understanding of DDT dynamics in hydrogen-natural gas mixtures, enhancing safety in the storage, transport, and utilization of hydrogen-based fuels.

2 Experimental Setup

The experiments were conducted in a 3400-mm-long shock tube with a cross-section of 203.2 mm by 19.1 mm, as shown in Fig. 1a. The tube was filled with a premixed gas mixture of interest and ignited at the end wall using a high-voltage ignition system. The apparatus consisted of three sections: the first section contained a mesh grid to promote turbulent flow and facilitate detonation initiation, while the second section allowed the wave to propagate and reach a self-sustained state. The detonation velocity in this section was confirmed to match the computed Chapman–Jouguet (CJ) velocity under the same initial conditions, using two PCB pressure transducers mounted on the top wall.

In the final section, the detonation wave interacted with a column of obstacles with the blockage ratio of 75%, forming a shock-flame complex. Visual observations were captured using a large-scale shadowgraph system and a high-resolution Z-type Schlieren system, with exposure times set to 460 ns. The frame resolutions were 1280 × 272 px for the shadowgraphs and 380 × 250 px for the Schlieren imagery, with inter-frame times of 27.09 μs and 11.53 μs, respectively. Six pressure sensors along the top wall of the final section recorded pressure data to provide detailed insights into the detonation dynamics.



(a)

(b)

Figure 1: Schematic of a) experimental and b) numerical set-up

3 Numerical Modeling

In our study, we investigated the dynamics using a two-dimensional reactive Euler approach [9], and also attempt a relatively simple turbulent combustion closure approach through the partially stirred reactor (PaSR) approach of Kartha et al. [11]. In the Euler method, diffusion terms were driven by numerical diffusion generated by the employed finite-volume scheme facilitating deflagrative burning on reaction surfaces. While the specific details regarding the 4-step combustion modelling approach, and its calibration, are detailed elsewhere [8, 10], we refer to our specific implementation challenges to the blended fuels of interest in another abstract submitted to this conference series [12]. For this study, we consider the following chemical reactions and the fuel blend ratio (FBR) formula for the fuel blends of interest:

$$\begin{aligned} & a \cdot (\mathrm{CH_4} + 2 \cdot \mathrm{O_2}) + b \cdot (\mathrm{H_2} + 0.5 \cdot \mathrm{O_2}) && \to R0, R1 \\ & \to a \cdot \mathrm{CO_2} + (2a + b) \cdot \mathrm{H_2O} && \to P1 \qquad (1) \\ & \rightleftharpoons a \cdot \mathrm{CO} + (4a + 2b) \cdot \mathrm{H} + (a + (2a + b)) \cdot \mathrm{O} && \to P2 \end{aligned}$$

$$\text{Fuel Blend Ratio, FBR} = \frac{X_{\mathrm{H_2}}}{X_{\mathrm{H_2}} + X_{\mathrm{CH_4}}}, \qquad (2)$$

where a and b are the proportions of methane and hydrogen in the fuel, while $X_{\mathrm{H_2}}$ and $X_{\mathrm{CH_4}}$ denote their respective mole fractions in the mixture.

The numerical domain considered was a two-dimensional channel measuring 3 m × 100 mm, as shown in Fig. 1b. The channel includes a column of obstacles configured in two arrangements: one with five cylinders and another with two cylinders, both featuring a blockage ratio of 75%. A Zeldovich–von Neumann–Döring (ZND) detonation is initialized at $x = 0$ m, propagating toward the right. The left boundary extends to $x = -20$ mm to encompass the initial structure. To generate the initial cellular wave structure, a density perturbation is applied ahead of the detonation front. The cylinder array begins at $x = 1$ m, allowing the detonation wave to stabilize to within 3% of the Chapman–Jouguet (CJ) velocity before encountering the obstacles.

Boundary conditions include zero-gradient on the right and symmetry along all other surfaces, including the obstacle boundaries. All simulations are initialized at a uniform temperature of $T_0 = 300$ K, with varying initial pressures. Adaptive mesh refinement (AMR) [13] is applied to resolve fine details in regions of interest. The base grid resolution is 10 mm, refined to a minimum of 78 μm in critical zones. Further details regarding the numerical implementation are available in Floring et al. [9].

4 Results and Discussion

Figures 2a and 2b illustrate the time evolution of the choked shock-flame complex in experiments, contrasting unsuccessful and successful detonation cases for a fuel blend ratio (FBR) of 90%. To conserve space, shadowgraphs are provided exclusively for this FBR. The results demonstrate that, after diffraction, the flame closely follows the leading shock, maintaining a coherent shock-flame structure. In the unsuccessful case, the shock-flame complex fails to re-initiate detonation within the test section, even after multiple shock reflections. Conversely, in the successful case, detonation reformation occurs within fewer than three shock reflections off the channel walls. Specifically, when the Mach stem or triple point reflects off the bottom wall, the compressed gas behind the leading shock induces a localized explosion, ultimately triggering detonation.

The experimental run-up distance, defined as the length required for the choked shock-flame complex to re-initiate detonation after diffraction, is presented in Fig. 2c for fuel blend ratios of 0%, 33%, 60%, and 90%. The parameter γ_{ps}, representing the specific heat capacity ratio behind the leading shock wave, reveals a notable dependence of DDT lengths on gas mixture properties. The graph shows that, low-γ gas mixtures exhibit longer run-up distances, while high-γ mixtures re-initiate detonation more readily. When γ_{ps} is above 1.25, approximately corresponding to a 50% FBR, a distinct go/no-go behavior emerges: detonations quenched by the obstacle either fail to re-initiate or re-establish immediately. This may also due to the reason that, hydrogen-dominated mixtures exhibit strong chain branching reactions, making them highly sensitive to local conditions and potentially more susceptible to quenching. This is

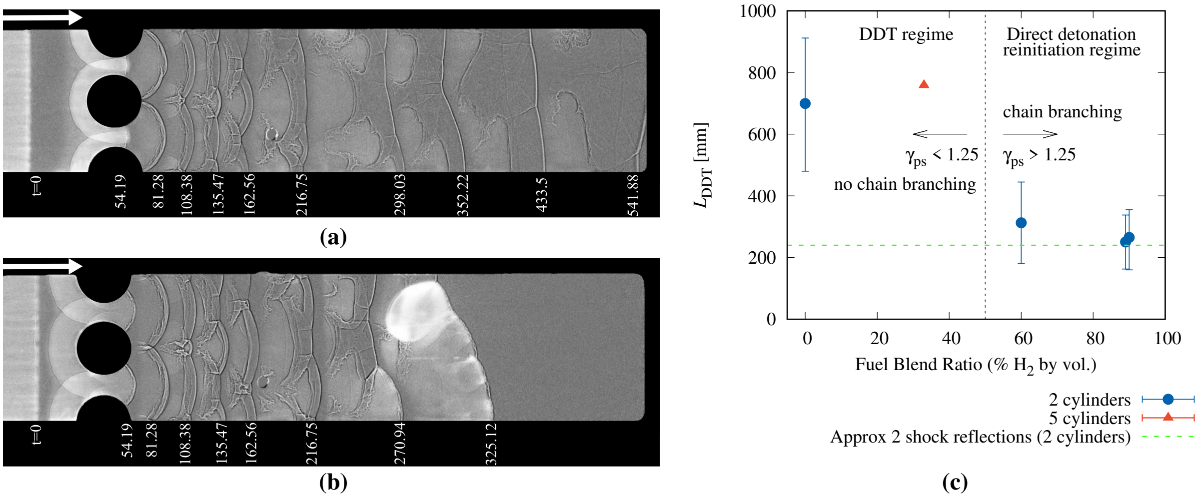
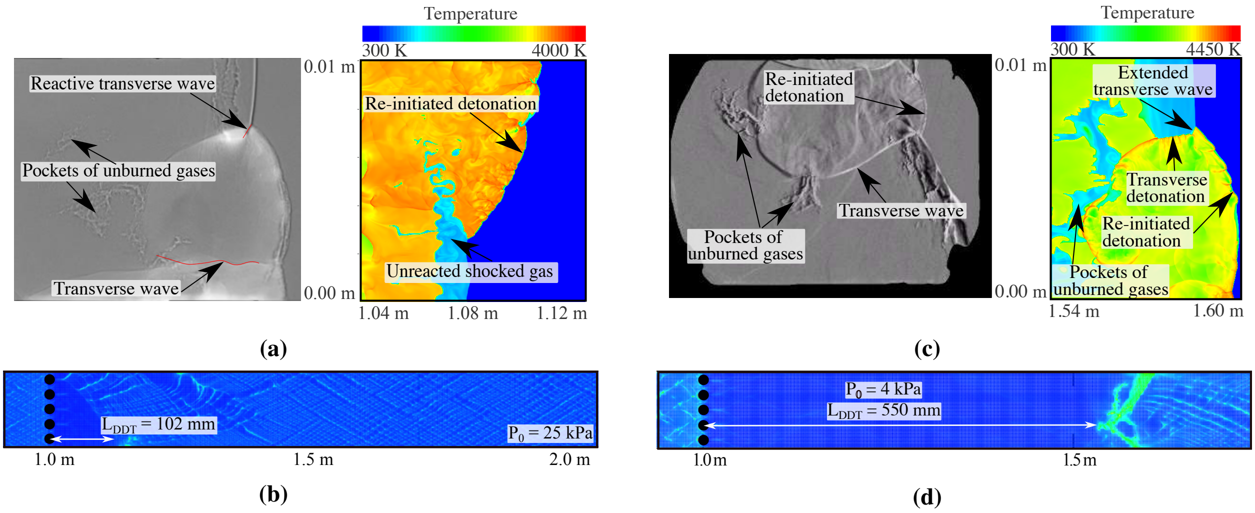


Figure 2: Shadowgraphs for FBR of 90% at two different initial pressures: a) $p_0 = 12.96$ kPa (failed DDT), b) $p_0 = 13.03$ kPa (successful DDT), and c) experimental L_{DDT} vs. blend ratios.

in accordance with the findings of Yang et al. [14] who found that the transmitted shocks propagating at 65-80% of the Chapman-Jouguet (CJ) detonation velocity produced post-shock temperatures within the chain-branching crossover ignition limit of hydrogen, leading to autoignition and subsequent detonation re-initiation. Furthermore, Maley [15] suggested that detonation re-initiation is influenced by the isentropic exponent (γ), as it governs the formation of hydrodynamic jets. They proposed that in hydrogen mixtures, high-γ suppresses strong jets behind Mach shocks, limiting turbulent mixing and preventing re-amplification of quenched detonations. However, they have shown that hydrocarbon-oxygen detonations, including CH_4 and other hydrocarbons, can re-initiate after significant distances, with turbulence tightly coupled to the leading shock.

In general, the Euler modelling approach has been instrumental in elucidating the re-initiation process, revealing that shock reflections generate localized explosions, which propagate as transverse reactive waves to re-establish detonation. Figures 3a, 3c, and 4a compare experimental results with numerical simulations for 0%, 33%, and 90% FBRs. The simulations include temperature fields at the moment of detonation re-initiation and numerical sootfoil records shown in Figs. 3b, 3d and 4b. Figure 4c illustrates the numerically measured run-up distances, L_{DDT}, derived from sootfoil records for different blend ratios and numerical resolutions. The inviscid Euler method demonstrates a lack of convergence with resolution, consistent with prior studies that attribute diffusion and mixing rates in such methods to resolution-induced numerical errors. While numerical simulations capture key features observed experimentally—such as incident shocks, Mach shocks, transverse shock waves, transverse detonations, and unburned gas pockets—they fail to accurately replicate the run-up distances (see Fig. 4c). For methane-dominant mixtures (0% and 33% FBR), experimental run-up distances are approximately 700 mm and 758 mm, whereas simulations predict a mean value of 102 mm and 755 mm, respectively with standard deviation shown in the error bars. For hydrogen-dominant blends (e.g., Fig. 4a), simulations reveal a distinct go/no-go regime, where quenched detonations either remain quenched or re-initiate almost immediately. Re-initiation in this regime typically occurs within the distance required for 2–3 transverse shock reflections to reach the channel walls. These discrepancies highlight the limitations of the current modeling framework and emphasize the need for further refinement to improve predictive accuracy.

Enhanced mixing in mixtures with lower γ [15] necessitates the incorporation of turbulence models to accurately capture the localized increase in reactivity. To achieve closure on the turbulent combustion interactions and the interplay between chemical and mixing timescales, numerical simulations utilizing



(a)

(c)

(b)

(d)

Figure 3: Temperature field comparison with experiments for FBR of a) 0 and c) 33 at 78 μm, and b) and d) represents corresponding numerical sootfoil

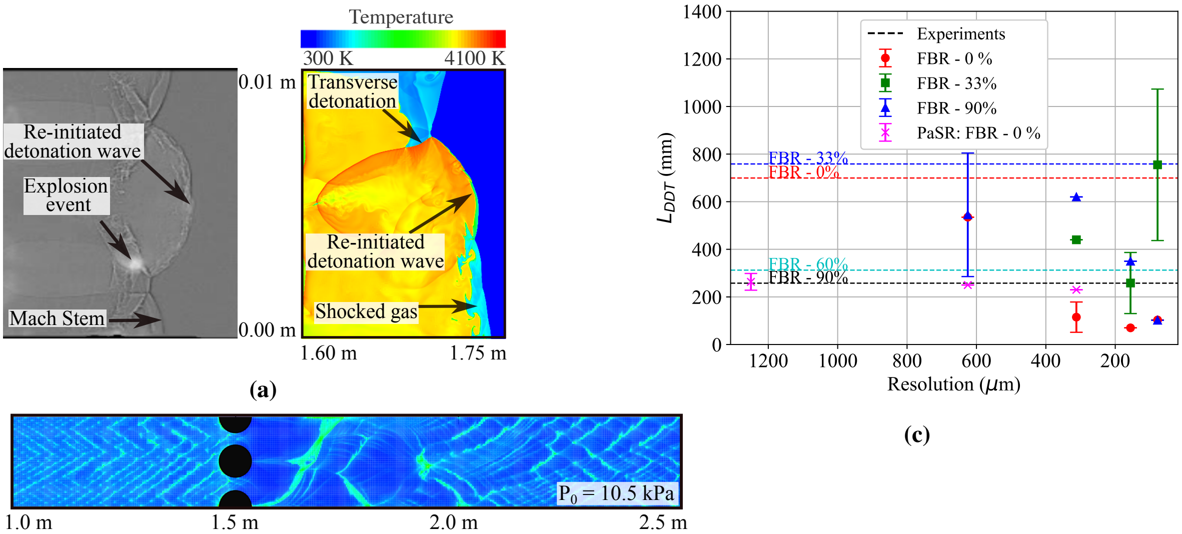
the PaSR model were conducted for pure methane-oxygen mixtures, and the corresponding results are presented in Fig. 4c. Although the PaSR model successfully reproduced key features of the turbulent flow field, it did not accurately capture the run-up distances observed in experiments. Specifically, the predicted run-up distances were consistently underestimated. One potential explanation for this discrepancy is the smoothing of viscosity inherent in the PaSR approach, which may dampen the small-scale turbulent structures and reaction rates that are critical for promoting the localized explosions necessary for detonation re-initiation. We note, this turbulence closure approach is fundamentally different from the previous application of the linear eddy model, where reaction rates due to turbulence were artificially increased to capture the experimental observations [5]. Therefore, this raises the question of what physical phenomenon is missing that leads to increased local reaction rates to permit flame acceleration in the lower-γ mixtures.

In fact, the discrepancies in the numerical results can very likely be strongly attributed to the three-dimensional boundary layer effects present in experiments, as discussed by Kuznetsov et al. [16]. These effects are known to play a critical role in introducing perturbations that significantly enhance flame acceleration through the increased flame surface area in the boundary layer. However, such intricate phenomena that lead to increased reaction rates are inherently absent in two-dimensional numerical simulations, underscoring a fundamental limitation in their ability to replicate experimental observations accurately.

We propose that the observed DDT-type detonation re-initiation cannot be attributed solely to a low-γ value. Instead, it likely results from the interplay between three-dimensional flame-boundary layer interactions and the low-γ sensitivity, which together enable the amplification of small-scale perturbations through enhanced turbulence and gas reactivity. This mechanism merits further investigation.

4 Conclusion

This study investigates the final stage of DDT in methane-hydrogen-oxygen mixtures, comparing experimental and numerical results. From our experiments, we found that two distinct re-initiation behaviours exist. Namely, we found that for $\mathrm{FBR} < 50\%$, quenched detonations were able to accelerate and transition to detonation through a distinct DDT phase, whereas for $\mathrm{FBR} > 50\%$, a go/no-go behavior was characterized for the detonation reinitiation. In this sense, we found that hydrogen-dominated detonations quenched by the obstacle either fail to re-initiate or re-establish immediately. In this regime, we believe the chain-branching crossover regime is likely a pivotal factor in detonation transition, as recently shown by Yang et al. [14]. We also found that the presence of the chain-branching crossover



(a)

(b)

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Figure 4: Temperature field comparison with experiments: a) FBR of 90 at 78 μm, b) corresponding numerical soot foil, c) experimental and numerical L_{DDT} vs. Resolution for various blend ratios.

effects also correlated with a post-shock $\gamma > 1.25$. However, regarding the interplay between the chain-branching mechanism and the specific heat ratio (γ), it is not clear which one of these properties is the dominant controlling factor that governs detonation re-initiation in the go/no-go type of re-initiation in hydrogen-dominant mixtures. We aim to isolate these two effects in future work.

While the CFD simulations using Euler and PaSR models capture several key features of shock-flame dynamics, significant discrepancies persist regarding run-up distances and detonation re-initiation. These discrepancies are likely due to the smoothing of viscosity inherent in the PaSR model, which dampens the small-scale turbulent structures critical for localized explosions and detonation re-initiation. The findings also highlight the crucial role of three-dimensional boundary layer effects, which perturb the flame front, increasing the flame surface area, burning rates, and the global acceleration of the flame front. This, coupled to the tendency of low-γ gases to exhibit fluid motion under pressure, facilitate the transition from deflagration to detonation. These boundary layer effects, absent in 2D simulations, are further explored in a companion study [17] through introduction of controlled perturbations. In this supplemental work, we aim to better understand how perturbations to the flow field influence the flame acceleration process. By controlling the perturbation, we also aim to gain convergence on future two-dimensional simulation approaches with experimental observations.

These insights have significant safety implications, particularly for hydrogen-natural gas pipeline designs. Hydrogen's hypersensitivity in hydrogen-dominated mixtures promotes a go/no-go type detonation re-initiation after interacting with obstacles, while methane-dominated mixtures require stronger disturbances to reinitiate detonation in quenched states. Continued refinement of numerical models and further experimental investigation are essential to bridge the gap between simulations and experiments, enhancing our understanding of DDT mechanisms and their practical implications.

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