Lean detonability of hydrogen-oxygen mixtures in narrow channels

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1 Introduction

As detonation approaches its propagation limits, it exhibits distinct modalities. In mixtures with regular cellular structures, detonation propagates steadily at near-CJ velocity when sufficiently far from the limit, with detonation cell sizes significantly smaller than the confinement length scale. As the limit is approached, velocity deficits increase and cells become bigger, eventually leading to single-headed spinning or zig-zag detonations. The onset of single-headed detonation is often regarded as the critical limit condition [1]. Since this mode corresponds to a cell size comparable to the confinement length, cell size is commonly used to size confining geometries in practical applications, such as the annulus width in rotating detonation engines (RDEs). The annulus width is recommended to be at least 2.4 times larger than the cell width of the fuel/oxidizer mixture [2].

However, it remains unclear whether RDE limits—particularly under lean conditions—follow this behavior. Lean operation is preferred for its higher thermodynamic efficiency and lower NOx emissions [3–5]. As the equivalence ratio (ϕ) decreases, while cell size often increases, cellular structures may also become irregular. While propagation in irregular mixtures away from the limit remains steady near the CJ velocity, approaching the limit leads to significant velocity fluctuations [6–8]. These so-called "galloping" detonations [6] have been observed across various mixtures and chamber geometries [7–16]. Unlike single-headed detonations, galloping modes occur over a broad range of conditions, making precise limit identification difficult [13]. The absence of a dominant cellular length scale in galloping detonations challenges the conventional RDE design strategies based on cell size. Overall, the differing limit behaviors between mixtures with regular and irregular cellular structures suggest that both cell size and stability affect detonation limits. For conditions where both cell size and stability may vary simultaneously, e.g., as mixtures become leaner, how confinement and stability characteristics interact and collectively determine the limit modalities remains unclear.

This study quantitatively assesses detonation limit behaviors in lean mixtures within narrow channels. The effects of confinement and stability are evaluated through experiments and detonation parameter calculations, specifically induction length, Δ_i, and effective activation energy, ε_I. By selecting mixtures with targeted ε_I and Δ_i values, we assess their ability to predict propagation limit behavior. Findings are compared with existing literature to identify quantitative trends, if any.

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2 Preliminary Results

Detonation limit behaviors of lean hydrogen-oxygen mixtures were investigated in a linear narrow channel. The channel has an inner cross-section of 190.5 mm by 19.05 mm, and is divided into a 1.86 m long driver section and a 3.37 m test section. Optical measurements via Schlieren imaging were facilitated by a 152.4 mm diameter quartz window in the test section. Pressure transducers along the top of the chamber provided time-of-arrival measurements for detonation wave front velocity calculations. For further assessment of some mixtures, aluminum plate soot foils were inserted into the chamber. Experiments were conducted at initial pressures (P_0) of 15 kPa and 6 kPa across a range of equivalence ratios (around 0.1–3.5), with rich mixtures included for comparison.

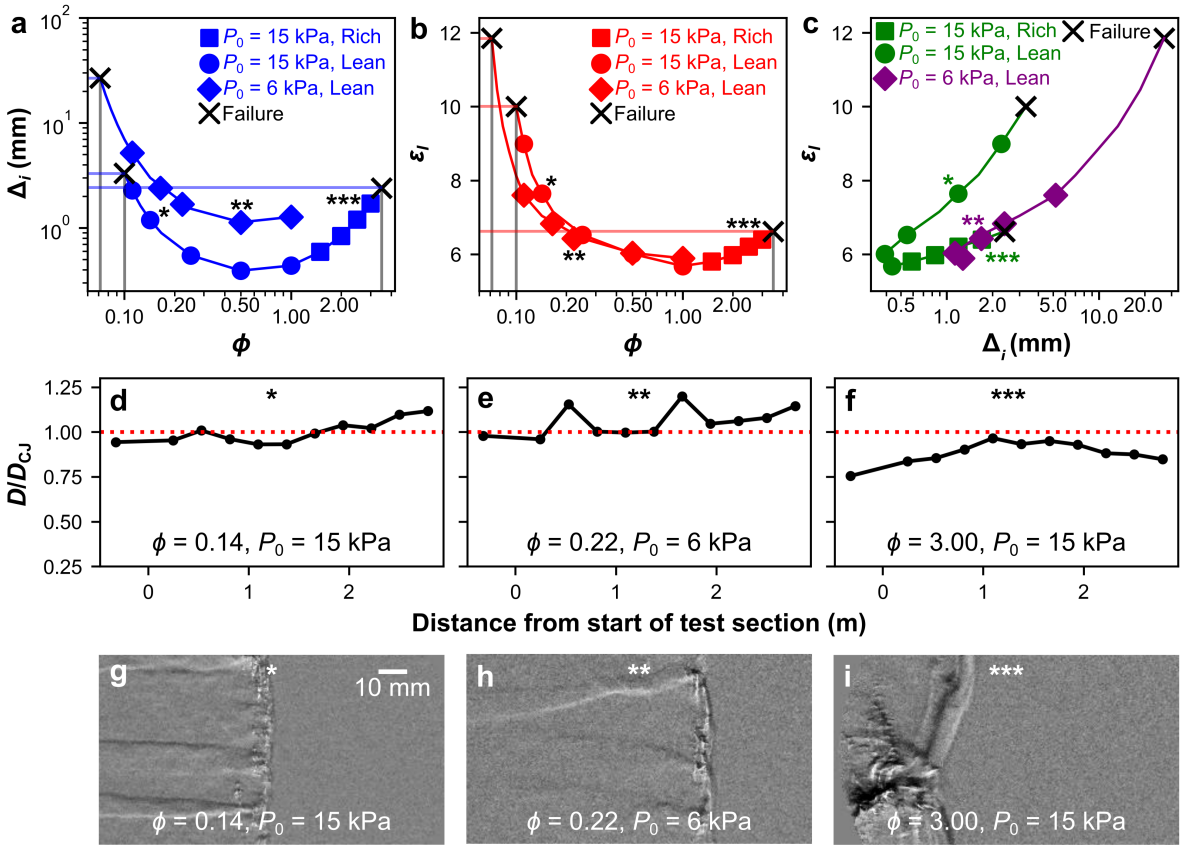

Figure 1: Summary of completed tests: **a** Δ_i vs ϕ; **b** ε_I vs ϕ; **c** Δ_i vs ε_I; **d-f** Propagation velocities of selected cases; **g-i** Schlieren snapshots of selected cases.

The preliminary results are summarized in Fig. 1. Figures 1a-c present the values of Δ_i and ε_I for the tested mixtures, including conditions at which failure occurs. The lean mixtures at 6 kPa were selected such that the values of Δ_i and ε_I in the 6 kPa lean tests overlap with those from the 15 kPa rich tests, as illustrated in Fig. 1c. As shown in Figs. 1a and b, Δ_i and ε_I reach their respective minimum values around stoichiometric conditions and increase as the mixture becomes either leaner or richer. The failure limits for both lean and rich tests at 15 kPa occur at similar values of Δ_i (around 3 mm), but the lean limit corresponds to a significantly higher ε_I (around 10 for the lean limit and around 6.5 for the rich limit). This indicates that in lean mixtures, ε_I increases more rapidly relative to Δ_i compared to rich mixtures. The experimental results support this, where the rich tests appear to fail due to geometric confinement effects characterized by propagation with large cells and steady velocity deficit (e.g., Figs. 1f and i), i.e., the failure mode observed in mixtures with regular structures. In contrast, the lean mixtures, for

both 15 kPa and 6 kPa, exhibited unsteady propagation with highly wrinkled, multi-cellular wave fronts (e.g., Figs. 1g and h). Detonation velocities are characterized by a profile that increases along the length of the chamber (e.g., Figs. 1d and e). This increasing velocity is thought to be indicative of a long-wavelength galloping detonation. These findings are also consistent with the results of Ishii et al. [12], who reported that lean mixtures exhibit a greater ability to propagate in narrow gaps and tend to display unsteady behavior. Furthermore, the results suggest that conventional cell-size-based design strategies for determining confinement dimensions, such as the gap width in RDEs, may not be suitable for lean conditions.

In addition to identifying failure conditions, this study also evaluates the effectiveness of Δ_i and ε_I in predicting detonation limit behavior and structures. Experimental results indicate that these two parameters alone are insufficient for such predictions. This is demonstrated by comparing two mixtures with nearly identical Δ_i and ε_I values: A rich case at 15 kPa (Figs. 1f and i) and a lean case at 6 kPa (Figs. 1e and h). Despite similar Δ_i and ε_I, their propagation behaviors and detonation cell structures are markedly different. As previously stated, the rich case at 15 kPa exhibited a near-limit behavior typical of regular mixtures, with very large cells and a relatively steady velocity profile with notable deficit. In contrast, the lean case at 6 kPa had an unsteady velocity profile with a highly wrinkled front indicative of cells smaller than the rich case. Another quantity often used to characterize mixture regularity, the stability parameter, χ, was also calculated for these two cases. The P_0 = 15 kPa, ϕ = 3.00 case had a value of χ = 2.78, while the P_0 = 6 kPa, ϕ = 0.22 case had a value of 2.54. As with ε_I, these two cases have very similar values of χ, so the selection of effective activation energy over the stability parameter does not affect the results. A third case, a lean mixture at 15 kPa (Figs. 1d and g), also exhibited a wrinkled front structure but with detonation cells smaller than either the 15 kPa rich or the 6 kPa lean case, despite having a similar Δ_i. The structure and behavior of these tests were in parallel validated via soot foils.

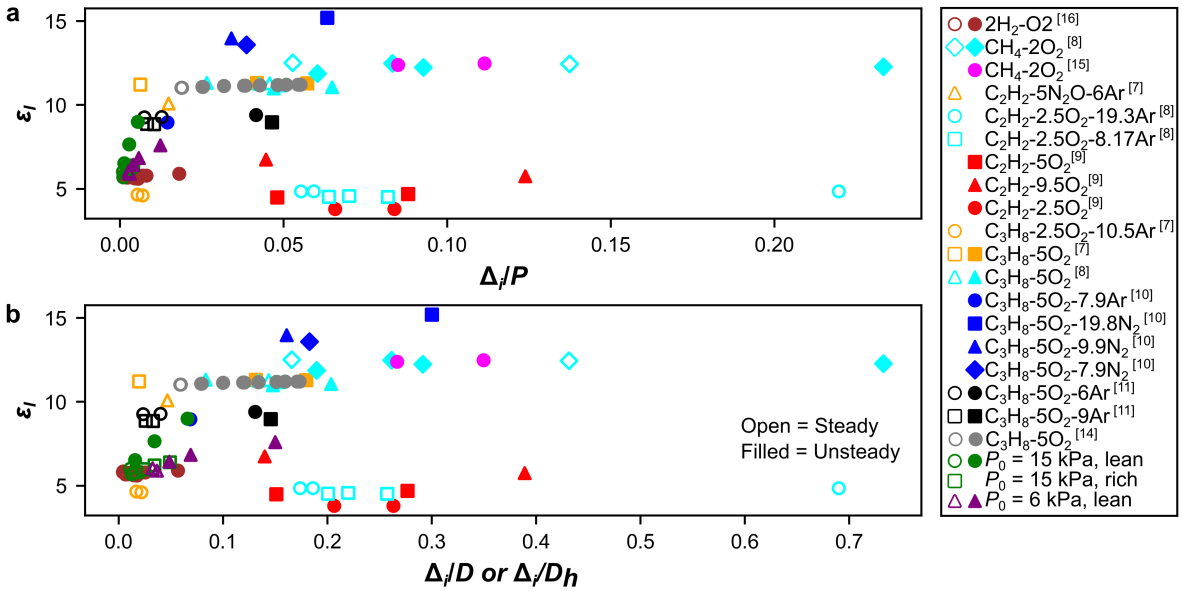

Figure 2: Effective activation energy and induction length data for various mixtures with steady or unsteady propagation behaviors: **a** induction length scaled with channel perimeter; **b** induction length scaled with channel diameter or hydraulic diameter.

The tested mixtures were also analyzed in comparison with tests from several previous studies on unsteady detonation propagation [7–11, 14–16]. The results, shown in Fig. 2, include a broad range of

mixtures and conditions. Open symbols represent steady detonation behaviors, while filled symbols indicate unsteady propagation. The dataset is presented as effective activation energy ε_I versus dimensionless length scales based on Δ_i. To account for variations in chamber geometries across these studies, two scalings for Δ_i were applied. Figure 2a scales the induction length by the channel perimeter, which reflects the geometric accommodation of the detonation structure within the chamber. Alternatively, Fig. 2b shows the induction length scaled by either the diameter or the hydraulic diameter, relevant to the degree of losses to walls. As evident in both figures, regardless of the scaling method, no clear correlation emerges in either ε_I or Δ_i with respect to the exhibited detonation behaviors. Some mixtures with high activation energies exhibit steady behavior [7, 8, 14], while some with relatively low activation energies showed unsteady behavior [9]. A similar analysis was performed replacing ε_I with χ, producing similar results with no trends. This analysis corroborates the experimental findings of this study, further demonstrating that effective activation energy and induction length are insufficient to predict detonation limit behaviors.

3 Work in Progress

Despite these findings, the possibility of using ε_I and Δ_i to characterize detonation limit behavior cannot be entirely dismissed yet, as several factors may influence the actual values of these parameters. One possibility is that various boundary effects can alter both the induction length and effective activation energy [17]. Since the lean and rich mixtures are essentially diluted, with either oxygen or hydrogen as the diluent, their thermodynamic and transport properties differ significantly. Near propagation limits, certain mixtures and their detonation characteristics may be highly sensitive to these boundary effects. Detonation property calculations that account for boundary effects will be performed to assess the corresponding impact.

Additional experiments are planned to investigate the observed transition to unstable propagation as ϕ decreases in hydrogen-oxygen mixtures. A more comprehensive experimental campaign will be conducted by performing equivalence ratio sweeps over a broad range of initial pressures to map out the onset of instability in greater detail. Additionally, to extend the findings beyond hydrogen-oxygen mixtures, ethylene-air and methane-oxygen mixtures will also be tested under similar conditions. Since these hydrocarbon-based mixtures have inherently higher activation energies, they will be diluted with argon to lower their effective activation energy to levels comparable with the hydrogen-oxygen cases, ensuring a meaningful comparison of stability effects across different fuel-oxidizer systems. The goal of these hydrocarbon tests is to determine whether strong nonequilibrium effects exist in hydrogen-oxygen mixtures and to identify additional detonation properties that may help reconcile the similarities and differences observed in this study.

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