DETONATION DYNAMICS IN A CURVED CHAMBER FOR AN ARGON DILUTED HYDROGEN-OXYGEN MIXTURE

C. Jourdain, J. Melguizo-Gavilanes, V. Rodriguez, P. Vidal and R. Zitoun

Institut Pprime, UPR 3346 CNRS, ISAE-ENSMA, BP 40109
86961 Futuroscope-Chasseneuil, France
josue.melguizo-gavilanes@cnrs.pprime.fr

Abstract

The dynamics of detonation transmission from a straight channel into a curved chamber was investigated as a function of initial pressure using a combined experimental and numerical study. Hi-speed Schlieren and *OH chemiluminescence were used for flow visualization; numerical simulations considered the two-dimensional reactive Euler equations with detailed chemistry. Results show the highly transient sequence of events (i.e. detonation diffraction, re-initiation attempts and wave reflections) that precede the formation of a steadily rotating Mach detonation along the outer wall of the chamber. An increase in pressure, from 15 kPa to 26 kPa, expectedly resulted in detonations that are less sensitive to diffraction. Local quenching of the initial detonation occurred for all pressures considered. The location where this decoupling occurred along the inner wall determined the location where transition from regular reflection to a rather complex wave structure occurred along the outer wall. This complex wave structure includes a steadily rotating Mach detonation (stem), an incident decoupled shock-reaction zone region, and a transverse detonation that propagates in pre-shocked mixture.

1. INTRODUCTION

Increasing the use of hydrogen is an attractive strategy to meet current and future CO₂ emission targets, and will support the effort of achieving a sustainable decarbonization of the economy in the not too distant future. While using hydrogen opens interesting possibilities in mobile and stationary applications in the industrial, residential and commercial sectors (i.e. propulsion devices, fuel cells, electrolyzers, etc.), the materialization of a hydrogen economy calls for a thorough understanding of the risks associated with its storage and use [1].

This work is part of an effort on novel propulsion technologies, and focuses on the fundamental understanding of Rotating Detonation Engines (RDE). RDE harness the power of detonation waves to create thrust without moving parts. The simplest RDE chamber is the annular space between two coaxial cylinders in which one or several detonation waves propagate azimuthally consuming the reactive mixture. Literature includes experimental, numerical and theoretical studies investigating detonation propagation inside full RDE [2, 3, 4], curved channels/chambers of constant and varying widths [5, 6, 7, 8, 9], wedges and bends [10], and U-bend tubes [11] (for the most recent reviews on the topic, readers are referred to [12, 13, 14]). Another promising geometry of RDE chamber is the hollow configuration in which the internal wall of the combustor is fully or partially removed resulting in improved specific impulse, and larger pressure and rotation frequencies e.g., [15].
Here, we focus on a simplified hollow geometry amenable to fundamental studies, namely a straight channel connected to a curved chamber with a small center body. The wave dynamics in this configuration is presumably representative of the early stages of detonation propagation inside hollow RDE.

This geometry was experimentally studied in our group recently using a stoichiometric propane-oxygen mixture [5, 6]. A steadily rotating overdriven detonation wave along the outer wall (called a Mach detonation) was observed, and modeling by means of Geometrical Shock Dynamics (GSD) [16] was capable of reproducing, qualitatively, the main global features in the chamber (i.e. wave diffraction, reflections and a steadily rotating Mach wave). However, properly capturing the details of the complex transients observed experimentally requires unsteady, time accurate simulations.

The main objective of the present work is thus the characterization of the flow dynamics inside a curved chamber (i.e. detonation transmission, diffraction, re-initiations, wave transitions, etc.) as a function of initial pressure for an argon diluted hydrogen-oxygen mixture.

2. EXPERIMENTAL METHODOLOGY

2.1. Apparatus and procedure

The experimental apparatus is composed of a detonation tube and a curved chamber. After vaccumming, the entire system is filled with a hydrogen-oxygen-argon mixture at the desired initial pressure (absolute). A deflagration is ignited at one end of the tube, accelerates to detonation by means of a Shchelkin spiral, and reaches the steady Chapman-Jouguet (CJ) regime before entering the curved chamber. Several dynamic pressure transducers are used to record the pressure evolution behind the wave front and obtain an average propagation velocity of the detonation in the tube. The detonation tube is 2 m long and has an inner diameter of 51 mm. The detonation enters the curved chamber and first propagates inside a 200 mm long straight channel with a 30 mm × 20 mm cross section. The detonation then diffracts in a larger volume bounded by a 80 mm radius outer wall and a small 30 mm radius inner wall. The combustion products expand inside a large vessel separated by a 18-µm Mylar foil. More details on the experimental apparatus and procedure are given in [5, 6].

2.2. Flow visualization

The chamber allows for a 217 mm × 275 mm optical access with one UV-silica window on one side and a borosilicate-crown glass window on the other side, both 27 mm thick. Two visualization techniques were used to investigate the dynamics in the chamber: (i) chemiluminescence based on the hydroxyl radical (*OH) to resolve the overall dynamics, and (ii) Schlieren to focus on details of interest. Both were coupled to hi-speed cameras.

*OH visualizations were performed using an intensified Princeton PI-MAX4 camera operated in dual frame imaging mode with an OH filter centered on 311 ± 5 nm. Two pictures were recorded per shot separated by a 10 µs delay. The full-frame resolution was 1024 × 1024 pixels with a 100 ns exposure time. The experimental sequences shown in Figs. 1 and 2 are thus a composite of three shots per initial pressure. This visualization technique has been extensively used as a typical combustion marker [17, 18, 19, 20]. Its most notable limitation is that excited OH molecules have relatively long life times and remain active in burnt gases. This makes the interpretation of the images difficult, especially, in the center of the chamber where different combustion processes interact (i.e. decoupled leading shock-reaction zone, and detonations).
Schlieren visualizations were performed using the classical in-line configuration with a Shimadzu HPV-X2 camera and a set of BK7 lenses, and a 10 cm collimated LED. Cut-off was handled using a razor blade set to block about 70% of the light beam. Videos were recorded at 5 MHz with an exposure time of 200 ns. The image resolution was set to $400 \times 250$ pixels.

3. COMPUTATIONAL METHODOLOGY

3.1. Governing equations and numerical methods

The flow field in the curved chamber was modeled using the reactive Euler equations with detailed chemistry and temperature dependent thermodynamics [21]. The governing equations were solved in a two-dimensional planar geometry using the OpenFOAM Toolbox [22]. The detailed mechanism of Mével for hydrogen oxidation was used to model the chemistry [23]; it includes 9 species and 21 reactions. The spatial discretization of the solution domain is performed using finite volumes (FV); FV methods allow for body-fitted hexagonal meshes avoiding the ubiquitous starcasing present when attempting to integrate numerically curved geometries using finite differences. The numerical fluxes at cell-faces are computed using a central-upwind Kurganov-Tadmor scheme [24, 25]. The flow variables on cell faces are reconstructed through a second order interpolation with a symmetric van Albada flux limiter which results in non-oscillatory bounded transitions across shocks and contact discontinuities. The chemical source terms are computed using a stiff ODE solver (i.e. 4th order Rosenbrock). The PBiCGStab (Preconditioned Biconjugate Gradient Stabilized) method is used for all the linear systems resulting from the discretization of the governing equations, preconditioned through the DILU (Diagonal Incomplete-LU) technique. Finally, the time integration uses a second order Crank-Nicolson method, and the time step is dynamically adapted during the computation with an acoustic Courant number of 0.5. The implementation and validation of this solver follows the methodology presented in [26].

3.2. Domain, initial and boundary conditions

The computational domain is shown in Figs. 1 and 2, and reproduces the curved chamber used in the experiments detailed in [5, 6]. Three initial pressures were considered $p_o = 15, 20$ and 26 kPa to investigate the detonation dynamics in the chamber as a function of pressure. Initial conditions were $T_o = 288$ K, velocity $U_o = (0, 0)$ m/s and mass fractions $Y_{H_2} = 0.034779$, $Y_{O_2} = 0.276021$, $Y_{Ar} = 0.6892$, corresponding to a stoichiometric hydrogen-oxygen mixture with $\%Ar_{vol} = 40$. A slip boundary condition for velocity and zero gradient for temperature, species and pressure were imposed on the curved chamber walls. A hexagonal uniform mesh was used comprising 9,286,953 cells, which resulted in resolutions of 10, 8, 5 points per ZND induction length for $p_o = 15, 20, 26$ kPa, respectively. Simulations were run using 200 processors, and took approximately 10,000 CPU hours per case. The detonations were ignited by imposing three equally spaced hemi-spherical regions ($r = 2.5$ mm) of high pressure ($p_{ign}/p_o \sim 46$) and temperature ($T_{ign}/T_o \sim 14$) at the chamber inlet. This initiation method resulted in steadily propagating cellular detonation fronts before the curved section of the chamber.

4. RESULTS AND DISCUSSION

The numerically predicted and experimentally captured dynamics of the detonation front as it propagated through the curved chamber is presented below. Only results for $p_o = 15$ kPa and 26 kPa are shown because the intermediate pressure case was not found to provide additional insight.
4.1. Overall dynamics in the curved chamber

Figure 1 shows a time sequence of pressure contours superimposed on H atom numerical fields together with experimental *OH chemiluminescence for $p_o = 15$ kPa. H atom is a useful chemical activity marker because it has a short life time; it peaks inside the reaction zone and quickly decays thereafter. The times reported correspond to the time elapsed from the initiation of the detonation at the channel inlet in the numerical simulations, and were selected to match, as closely as possible, the experimental structures observed.

<table>
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<td>$t = 131 \mu s$</td>
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<td>$p$ - contours / H field</td>
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<td>$t = 166 \mu s$</td>
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Figure 1: Overall dynamics for $p_o = 15$ kPa - numerical pressure contours and H atom field vs. experimental *OH chemiluminescence.
Interesting features occur simultaneously along the inner and outer walls. For $131 \mu s \leq t \leq 166 \mu s$, the numerical results show a diffracting detonation front, a subsequent transverse detonation wave that consumes shocked reactive mixture, early stages of decoupling of the leading shock and reaction zone along the inner wall, and the formation of a reactive Mach stem along the outer wall. The experimental images show the regions where chemical reactions are strong. Initially ($131 \mu s \leq t \leq 140 \mu s$), $^*\text{OH}$ is widely spread in the chamber; at later times ($140 \mu s \leq t \leq 166 \mu s$), the highest $^*\text{OH}$ intensity is confined to the outer wall characterized by a white thick line normal to the outer wall representing a Mach detonation front. Inside the chamber, the signal decreases as the combustion front continues to propagate. The last two times of the sequence display the most interesting dynamics with strong chemical activity obliquely attached to the triple point of the Mach stem at $t = 201 \mu s$, and an “S-shape” structure at $t = 236 \mu s$. The numerical fields provide insight into the emergence of these structures. They arise from the interaction of the Mach detonation front with the shocked reactive gas left behind upon the final decoupling of the initial detonation front along the inner wall. A new combustion front propagates in this region consuming the mixture. The bright red regions in the straight section of the numerical domain are remnants of the initiation.

Figure 2 shows the same numerical and experimental fields for $p_o = 26$ kPa. The dynamics of the detonation front are strongly affected by the pressure increase. Notably, the detonation front is less sensitive to the initial area change as it encounters the curved region of the chamber. For $t \geq 143 \mu s$, full decoupling of the leading shock and reaction zone occurs along the inner wall, whereas a regular reflection establishes itself along the outer wall until the last time shown in Fig. 2. Experimental $^*\text{OH}$ fields show a curved transmitted detonation with high intensity regions corresponding to triple-point collisions along the front (see $t = 133 - 143 \mu s$). At later times ($t \geq 161 \mu s$), the only region with strong $^*\text{OH}$ production is located where the regular reflection takes place, and is bounded behind by a tailing wave and the outer wall. Additional details about later stages of propagation are provided in subsection 4.3.

Classical numerical soot foils obtained by tracking the pressure maxima in the computational domain at each time step are presented in Fig. 3. They provide a time history of the triple point trajectories during detonation transmission, and offer insight into local quenching, and re-initiation events. Bright white lines of varying thicknesses represent high pressure regions. The sensitivity to diffusion with increasing pressure is clearly depicted in the figure. For $p_o = 15$ kPa, decoupling occurs immediately upon reaching the curved section of the chamber. For $p_o = 26$ kPa, the cells of increasing length along the inner wall of the chamber are a signature of consecutive decoupling and re-coupling events characterized by combustion fronts that propagate inside these shocked reactive regions. Additionally, numerical soot foils allow to uniquely determine the location where regular-to-Mach detonation transitions take place. Experimental evidence confirms this observation by the presence of fine detonation cells in these regions [5, 6].

4.2. Early stages of propagation

Figure 4 shows a close-up of the early stages of detonation diffraction for $p_o = 15$ kPa. A planar detonation front first enters the curved chamber and, close to the inner wall, it begins to decouple due to the propagation of expansion waves originating from the region where the front first encounters an area change ($96 \mu s \leq t \leq 101 \mu s$). These waves propagate perpendicular to the detonation front towards the outer wall making it curved. An increased detonation front curvature results in a faster local temperature and velocity decrease, so the reaction zone further decouples from the leading shock ($111 \mu s \leq t \leq 131 \mu s$). This decoupling originates from the high sensitivity of chemical reaction rates to temperature resulting in significantly longer induction times behind the leading shock at lower temperature.
Along the outer wall, the detonation appears to be undisturbed initially but quickly transits to a Mach reflection with the leading shock normal to the wall (see $t = 111 \mu s$). Detonation and shock wave reflection types (i.e., regular or Mach) upon interactions with concave wedges/cylinders have been studied extensively. They are known to depend on the wedge angle/cylinder radius, front velocity and mixture characteristics [10, 27, 28]. After the initial Mach stem is established, it grows, reaches a maximum and decreases. The increased pressure and temperature behind the stem results in induction lengths that can be orders of magnitude smaller than the steady ZND length chosen as a reference. Consequently, the cell size significantly decreases, it is thus likely that in these highly compressed regions the numerical

<table>
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<th>$p_o = 26$ kPa</th>
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Figure 2: Overall dynamics for $p_o = 26$ kPa - numerical pressure contours and H atom field vs. experimental $^*$OH chemiluminescence.
Figure 3: Numerical soot-foils for increasing pressure.

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<th>$p_o = 15$ kPa</th>
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Figure 4: Early stages of detonation propagation for $p_0 = 15$ kPa - numerical pressure contours and H atom field.

$t = 96$ µs | $t = 101$ µs | $t = 111$ µs

$\begin{align*}  
  t & = 121 \text{ µs} \\  t & = 131 \text{ µs} \\  t & = 143 \text{ µs} 
\end{align*}$

resolution used in this work may be insufficient to resolve the smaller detonation structure. Nonetheless, we seem to be able to capture the global dynamics. While previous experimental studies suggested that these structures may potentially play an important role in the unsteady flow behavior, the cellular pattern left behind this specific overdriven Mach detonation front is so small that a fair approximation would be to neglect it, which supports the simple GSD modeling in [16]. This is further discussed in the last section.

Figure 4 (111 µs ≤ $t$ ≤ 131 µs) indicates that the first re-initiation mechanism appears to be driven by the competition among reflected expansions from the outer wall, compression waves from downward traveling triple points, and the progress of the decoupled leading shock-reaction zone. A re-initiation center, and the birth of a combustion front that subsequently consumes shocked mixture are visible at $t = 121$ µs. The structure of this combustion front ($t = 131$ µs) is analogous to detonations propagating...
under yielding confinement, namely a curved front, a transmitted shock and a shear layer [29, 30]. A closeup of this structure is shown in Fig. 5. Upon reflection from the inner wall, $t = 143 \mu s$, the early stages of a Mach detonation is shown whose typical features are a Mach stem, an incident curved detonation, and a shear layer.

$$t = 130 \mu s$$  
$$t = 108 \mu s$$

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Figure 5: Close up to detonation diffraction structure close to inner wall for increasing pressure - solid lines are temperature contours.

Figure 6 clearly displays the effect of increasing initial pressure on the early dynamics. As mentioned above, the sensitivity to area changes is significantly decreased for $p_o = 26$ kPa. The detonation front becomes curved in the inner region due to the numerous expansions emanating from the inner wall and propagates intermittently, since the extent of leading shock-reaction zone decoupling is minor along the inner wall (see $t = 108 - 116 \mu s$). These regions will be consumed by transverse waves propagating along the detonation front in the same fashion as for $p_o = 15$ kPa. A closeup to this structure for $p_o = 26$ kPa case is also shown in Fig. 5. Evidence of this intermittent behavior can be seen in the numerical soot foils shown in Fig. 3. Similarly to $p_o = 15$ kPa, the early stages of a Mach reflection along the inner wall appears at $t = 123 \mu s$, while on the outer wall, a stronger and smaller Mach stem forms that decreases rapidly and transitions into the regular reflection described in Fig. 2.

Finally, as the Mach stem along the inner wall continues to propagate into a continuously increasing area, full decoupling occurs regardless of $p_o$. However, for $p_o = 26$ kPa, it takes place earlier but further along the inner wall (see Fig. 7).

### 4.3. Late stages of propagation

Figure 8 shows a close-up of the late stages of detonation propagation in the curved chamber for $p_o = 15$ and 26 kPa.

The global dynamics for both pressures bears similarities with the presence of a regular reflection, a Mach detonation (stem), a decoupled leading shock-reaction zone, a transverse detonation wave, reflected waves, and shear layers. However, differences exist in the reflection transition location (regular-to-Mach) and final wave structure. The critical angle, $\theta_{crit}$ (measured clockwise from the negative $x$-axis), where the decoupled leading shock-reaction zone interacts with the detonation wave propagating along the outer wall, depends on the decoupling of the diffracting detonation along the inner wall (see Fig. 7). When full decoupling occurs, the leading shock velocity decreases significantly allowing for enough time for the detonation propagating along the outer wall to catch up, and for a Mach reflection to redevelop (see Fig. 8). A plot summarizing the transition angles for all pressures considered is shown in Fig. 9; $\theta_{crit}$ increases with increasing pressure and seems to have an asymptote at about 235°. Future experiments and simulations at lower/higher pressures will further explore this trend.

8
\[ p_o = 26 \text{ kPa} \]

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**Figure 6:** Early stages of detonation propagation for \( p_o = 26 \text{ kPa} \) - numerical pressure contours and H atom field.

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<th>( t = 151 \mu s )</th>
<th>( t = 143 \mu s )</th>
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<td><img src="image7.png" alt="Numerical pressure contours" /></td>
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**Figure 7:** Location of full decoupling of leading shock and reaction zone along inner wall for increasing pressure.

The differences in wave structure at the very late stages of propagation, \( t = 236 \) and \( 196 \mu s \) for \( p_o = 15 \) and 26 kPa, respectively, seem to be simply a consequence of the location where transition occurs. In other words, the available arc length for propagation after transition, \( \Delta s = r_e(\theta_{\text{crit}} - \theta_{\text{end}}) \) – where \( r_e \) is the radius of the outer wall and \( \theta_{\text{end}} \) is the angular location at which the outer wall meets the straight section of the chamber – is larger for \( p_o = 15 \text{ kPa} \). This allows for the competition between the transverse detonation that propagates in shocked mixture and the rotating Mach stem propagating along the outer wall to last longer, and an “S–shape” arises as a result. Experimental evidence showing this wave structure is included in Fig. 10.

As a first closing remark, it is worth emphasizing that, as mentioned in [5, 6], the dynamics just described for hydrogen-oxygen-argon mixtures is a universal typical feature of re-initiation of diffracting detonations. Classical experiments on detonation transmission from a straight channel to an open volume...
Figure 8: Late stages of detonation propagation for increasing pressure - numerical pressure contours and H atom field.

Figure 9: Critical angle for transition from regular to Mach detonation along outer wall.

(see [31], for example), have identified a similar behavior (see Fig. 11). In the present work however, the geometry plays an important role as the chamber is effectively an open, diverging volume bounded by a concave wall (which differs from classical diffraction experiments); as a result, the initially diffracting detonation turns into a rotating Mach detonation.
Figure 10: Schlieren images showing “S-shape” wave structure during late stages of propagation in chamber - $p_0 = 15$ kPa.

Figure 11: Experimental evidence of transverse detonation waves in different mixtures and geometries: $0.5\, \text{H}_2 + 0.5\, \text{N}_2\text{O}$ for $p_0 = 47.5$ kPa adapted from [31] (left) and $\text{C}_3\text{H}_8 + 5\, \text{O}_2$ for $p_0 = 12$ kPa adapted from [5, 6] (right).

5. CONCLUSION

Experiments and two-dimensional Euler simulations with detailed kinetics were performed to characterize, as a function of initial pressure, the detonation transmission from a straight channel into a curved chamber using an argon diluted (40%) stoichiometric hydrogen-oxygen mixture. All the computed behavior of a very complex dynamics superimpose almost exactly to those identified in the experiments which provides evidence of the validity/robustness of the implementation of our solver.

Early stages of the evolution included decoupling and re-initiation of the diffracting detonation along the inner wall of the chamber, formation of a Mach stem whose height decreased as it propagated along the outer wall, and transition to regular reflection. At later times, full decoupling of the diffracting detonation occurred along the inner wall, and along the outer wall, an additional transition to a rather complex wave structure took place composed of a Mach detonation, a decoupled leading shock-reaction zone, a transverse detonation, reflected waves and shear layers. A pressure increase from 15 to 26 kPa resulted in differences in the reflection transition location, $\theta_{\text{crit}}$, velocities of the discontinuities and final wave structure. Notably, $\theta_{\text{crit}}$ seems to have an upper limit with increasing pressure. These results suggest that while the transient phenomena occurring along the outer wall at early times seemed to be largely influenced by the dynamics of the leading shock-reaction zone complex propagating along the inner wall, once the final state was engaged, the global dynamics and the rotating Mach detonation in the chamber seemed to be mostly driven by geometry and initial pressure.
The fact that our numerical resolution is unavoidably insufficient to resolve the cellular structure in the highly compressed regions behind the detonation Mach stem and transverse detonation, indicates that a detailed description of the chemistry may not be needed, and that a simpler modeling based on GSD [16] would therefore be sufficient if one is only interested in capturing the most salient features of this dynamics.

Future work will include: (i) a more thorough study of the flow field (i.e. tracking of wave speeds and sonic planes along the outer wall and inside the chamber, as well as their chemical structure - temperature and species profiles) to verify whether the numerically predicted final Mach stem rotates at a normal velocity of about 1.25 $D_{CJ}$ as reported in [5,6]; (ii) increasing the pressure range to lower/higher pressures to investigate further the $\theta_{crit}$ vs. $p_o$ dependence; (iii) Hi-speed Schlieren visualization of the full chamber; (iv) characterization of the transmission dynamics as a function of argon dilution; and (v) to numerically investigate whether a detailed description of the chemistry is required to capture the transient behavior observed inside the chamber by running cases using simplified kinetics (i.e. one-/three-step chemistry).

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