

Hydrogen-Oxygen-Argon Detonation Diffraction in a Narrow Channel

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1 Introduction

At an abrupt area change, a propagating detonation wave undergoes diffraction. Depending on a number of parameters, including on the mixture composition, thermodynamic conditions, detonation velocity at the channel exit, the geometry of the area expansion and channel cross section, the detonation wave can be either quenched (sub-critical regime) or re-initiated (super-critical regime). Detonation diffraction has been studied since the 1950's [1]. Schultz [2] provides a comprehensive review on diffraction studies up to 2000. Gallier et al. [3] summarized the results of more recent studies with emphasis on numerical work. The latest publications on detonation diffraction include the studies of Nagura et al. [4] and of Li et al. [5]. Despite six decades of extensive investigation, the detonation diffraction critical conditions have not yet been predicted from first principles and only semi-empirical models such as that of Schultz [2] are available to estimate the critical tube diameter.

The present study aims at providing a well defined experimental and numerical framework to help establishing a quantitative theoretical model to predict the critical conditions for diffracting detonation failure and re-initiation. Both carefully conducted experiments and Euler numerical simulations with realistic chemistry have been performed for one hydrogen-oxygen-argon mixture for which the chemistry is well established. In addition, simplified models were used to estimate the respective effects of shock front curvature and volumetric expansion on the detonation re-ignition process and the chemical dynamics.

2 Material and method

2.1 Experimental set-up

Figure 1 shows the schematic of the 3.4 m long aluminum rectangular channel with an internal height and width of 203 mm and 19 mm, respectively. It is composed of three sections, a detonation initiation section, a propagation section, and a test section. The mixture was ignited in the first section by a high voltage igniter which can deliver up to 1000 J with the deposition time of 2 μ s. To promote the formation of detonation, mesh wires were inserted in the initiation section. Six PCB piezoelectric pressure sensors (p1-p6), mounted flush to the top wall, were used to measure the detonation propagation velocity in the propagation and test sections. For investigating the diffraction phenomenon, a 165 mm high rectangular polyvinyl-chloride plate was placed in the test section, which was equipped with two glass panels for visualization. The remaining two sensors (p7, p8) were placed for the purpose of recording pressures of the diffracted flow field. The mixture presently studied was 2H₂/O₂/2Ar. It was prepared in a separate tank using the method of partial pressures and was then left to mix for more than 24 hours. Before introducing the test mixture, the channel was evacuated to below 90 Pa. For visualization of the detonation diffraction process, a Z-type schlieren setup with a vertical knife edge

was utilized with a light source of 360 W. The resolution of the high-speed camera is set to 384288 px^2 with the framing rate of 77481 fps. The exposure time was $0.468 \mu\text{s}$. More than 100 diffraction experiments were performed for initial pressures in the range 10.3-23.4 kPa and initial temperature of 298 K.

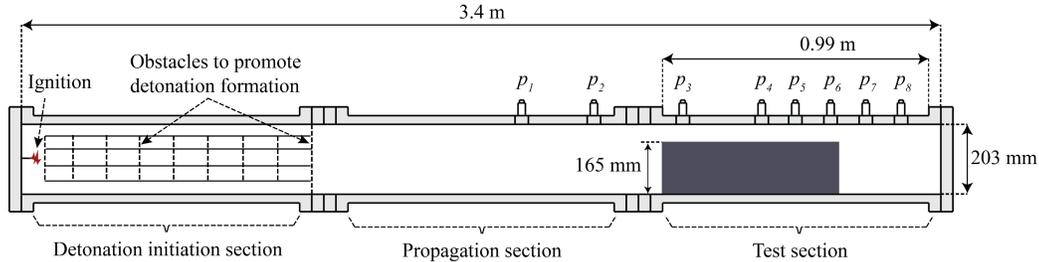


Figure 1: Schematic of the experimental setup used for the diffraction study.

2.2 Numerical simulation and reaction model

Numerical simulations were performed using an in-house code which solves the 2D Euler equations with high-order (5th order WENO) schemes along with AMR (Adaptive Mesh Refinement). Technical details can be found in [3]. The studied conditions are similar to the experiments, i.e. $2\text{H}_2+\text{O}_2+2\text{Ar}$ at different pressures. Detonations are first propagated in 1D until an average steady-state is reached and subsequently in 2D with slight changes of the fresh mixture composition in order to trigger the detonation cellular instability. The channel is 38.1 mm in height and the smallest grid size is $7 \mu\text{m}$. Once the detonation cellular structure is clearly established, the solution is mapped onto the diffraction geometry. It consists of a 38.1 mm high square channel exiting in a larger 203.2 mm high channel.

The reaction model employed was the same as the one used by Gallier et al. [3]. It is composed of 17 reversible reactions and 9 species, including Ar, and corresponds to a slightly reduced version of the mechanism of Mével et al. [6] which was extensively validated against combustion relevant experimental data as summarized in [7].

3 Results and discussion

3.1 Experimental and simulation results

Figure 2 a) presents the evolution of the normalized detonation velocity in the propagation section as a function of initial pressure. Within the range of initial pressure studied, the normalized velocity in the narrow channel increases with initial pressure by 3.5%. At a given initial pressure, the normalized velocity varies by less than 1.5% which demonstrate the repeatability of the experimental procedure. The velocity deficits measured in this experimental facility, 4-8%, are consistent with those measured by Austin [8], 4-5%, for a close mixture: $2\text{H}_2-\text{O}_2-3\text{Ar}$.

Following Loiseau and Higgins' approach [9], the diffraction experiments were analyzed in terms of probability of successful transmission based on 10 experiments performed at the same initial pressure. The evolution of the probability of transmission, referred to as p , as a function of initial pressure is shown in Figure 2 b). The transition between $p=0$ (certain detonation failure) and $p=1$ (certain re-initiation) is smooth rather than abrupt as suggested by the critical tube diameter correlation approach [10]. The range of initial pressure for which $p \in]0, 1[$ extends over 3 kPa. This range of pressure corresponds to approximately 15% of the minimum pressure for which $p=1$.

Numerical simulations were performed for the same mixture and initial temperature as in the experiments. However, only three initial pressures could be tested, 6.9, 10.3, and 13.8 kPa. As the pressure was increase,

sub-critical, critical and super-critical outcomes were observed. The difference in critical initial pressure for successful transmission obtained in the experiments and in the simulations can essentially be attributed to the experimental velocity deficit which was not accounted for in the simulations. For the mixture presently investigated, a velocity deficit on the order of 5% with respect to D_{CJ} induces an increase of the ignition delay-time by more than 50%. Such a difference could be of significant importance for the outcome of the diffraction process at a given initial pressure as was observed for detonation cell size by Mével et al. [11]. Only one reaction model could be tested and different critical pressures for successful transmission might be expected if other chemistry models were used.

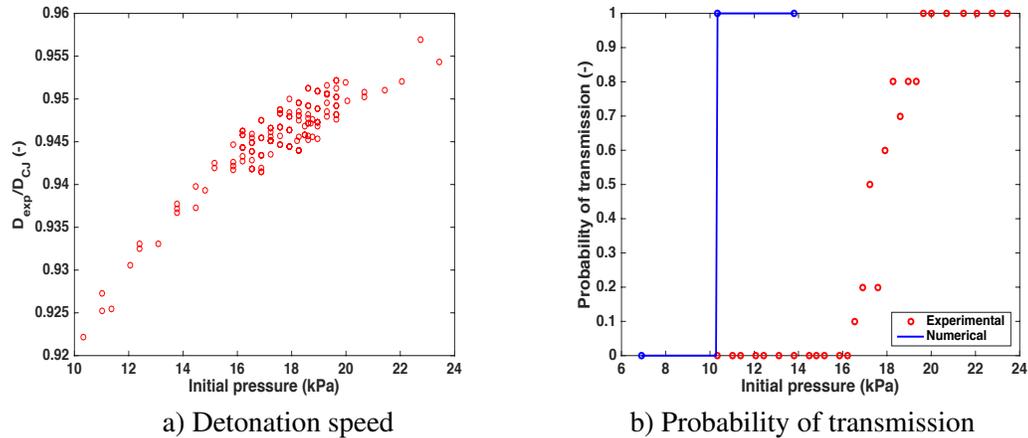


Figure 2: a) Normalized detonation speed in the narrow channel and b) probability of successful transmission as a function of initial pressure for a $2H_2-O_2-2Ar$ mixture at $T_1=295$ K.

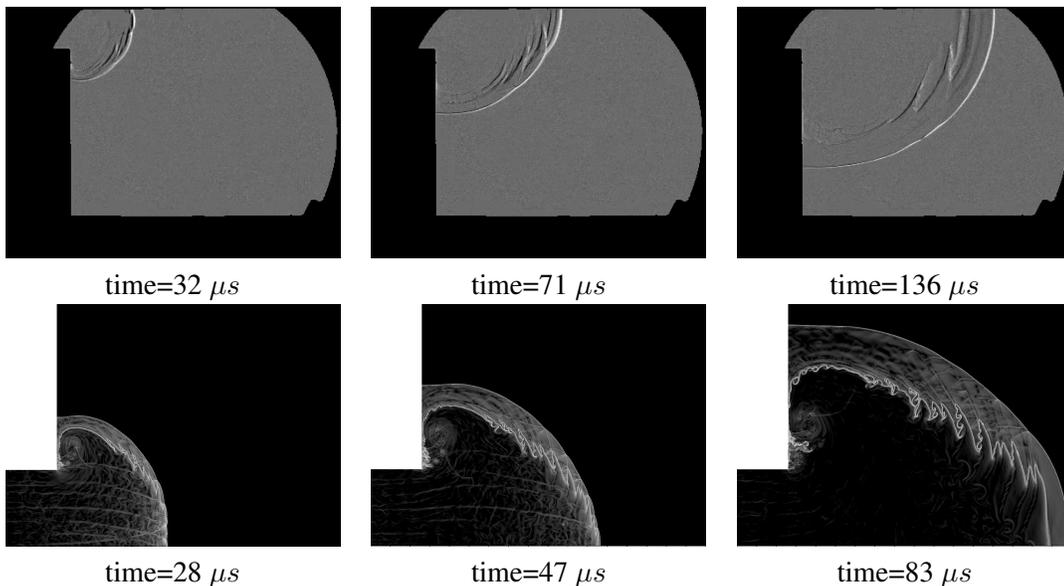


Figure 3: Comparison between experimental (top) and numerical schlieren (bottom) images of a sub-critical diffracting detonation in a $2H_2-O_2-2Ar$ mixture at $T_1=295$ K. Top: $P_1=10.3$ kPa; image height is 250 mm. Bottom: $P_1=6.9$ kPa; image height is 120 mm. The time indicated below the images corresponds to the time after the detonation has exited the channel.

Figure 3 and Figure 4 compares experimental and numerical schlieren image sequences for both outcomes. For

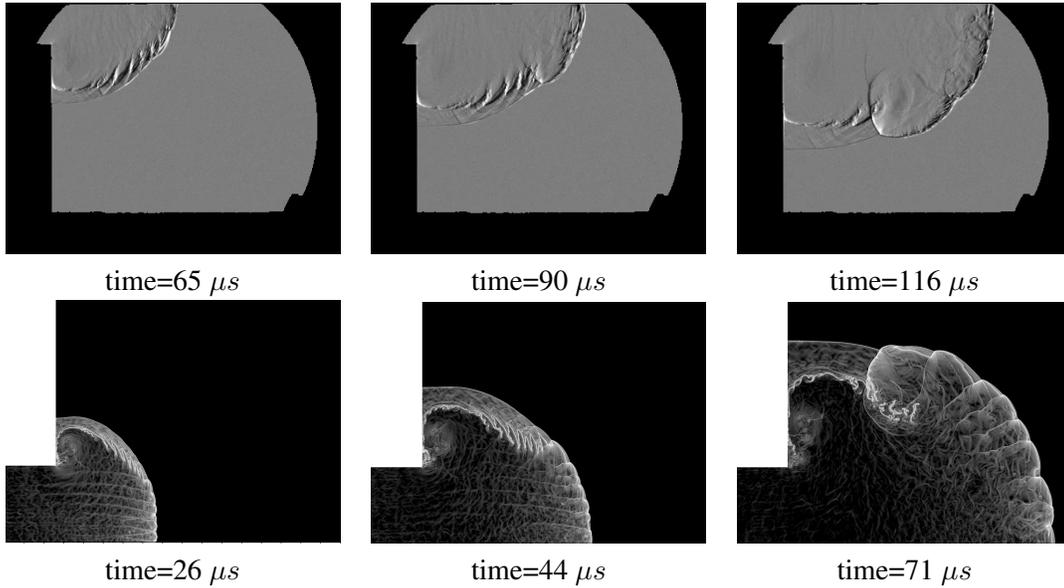


Figure 4: Comparison between experimental (top) and numerical schlieren (bottom) images of a super-critical diffracting detonation in a $2\text{H}_2\text{-O}_2\text{-2Ar}$ mixture at $T_1=295$ K. Top: $P_1=20$ kPa; image height is 250 mm. Bottom: $P_1=13.8$ kPa; image height is 120 mm. The time indicated below the images corresponds to the time after the detonation has exited the channel.

the sub-critical case, the numerical simulation captures some important features including: (i) the progressive decoupling between the shock front and the reaction zone as the expansion wave originating from the corner travels toward the top wall; and (ii) the sawtooth shape of the quenched reaction zone after complete decoupling has occurred. For the super-critical case, the simulation reproduces the local re-initiation event and the amplification process which leads to the formation of a strong transverse detonation within the un-reacted shocked gas.

3.2 Effect of curvature and expansion on ignition

Depending on the studies, detonation transmission failure at area change has been attributed to excess of curvature [5, 12] or to volumetric expansion behind a decaying shock [13]. In order to estimate the respective effect of these two phenomena on diffracting detonation failure, we performed a number of calculations using simplified combustion models.

Locally, the effect of shock front curvature, κ , can be estimated by considering the variation of the thermodynamic state behind an oblique shock as a function of the angle between the shock and the incoming flow in a shock-attached frame of reference. The geometric configuration is depicted in Figure 5 a) based on Hornung's construction [14]. In this configuration, the angle between the flow and the shock wave is given by $\beta = 90^\circ - \arcsin(\kappa|y' - y|)$. The initial thermodynamic state for a 0-D constant pressure reactor behind the curved shock can then be calculated using the jump equations for an oblique shock.

The effect of volumetric expansion behind a decaying shock wave can be estimated by considering a 0-D reactor with a time-dependent specific volume which rate of change depends on the shock deceleration. The situation is depicted in Figure 5 b) as previously described by Radulescu and Maxwell [15].

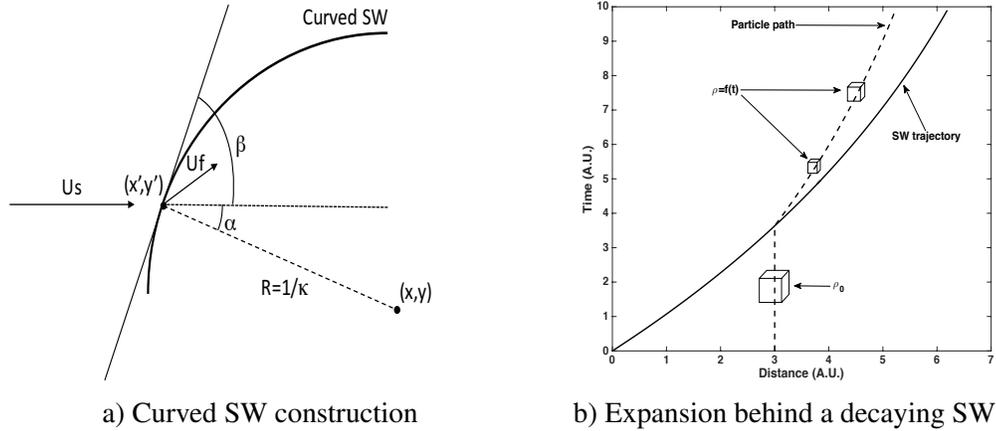


Figure 5: Illustration of a) the geometric configuration for a curved SW in a shock-attached frame of reference and b) of the volumetric expansion resulting from the SW deceleration in a $x-t$ diagram.

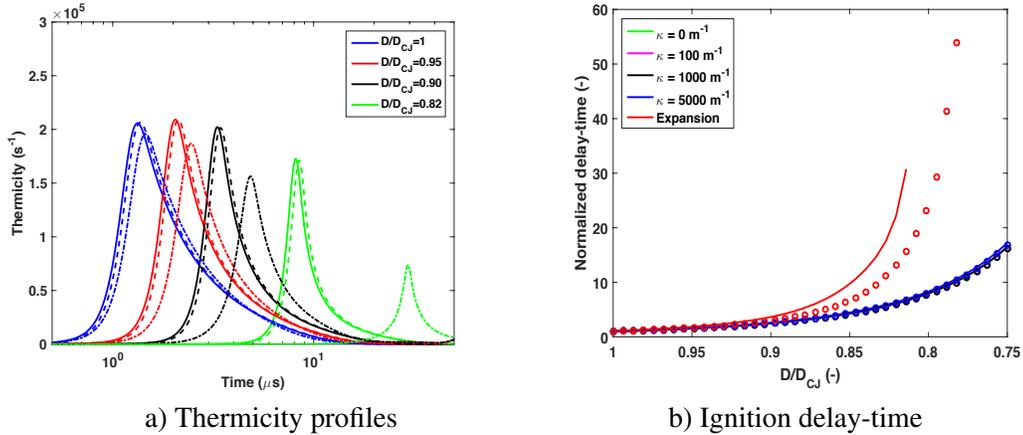


Figure 6: Effect of curvature and volumetric expansion on a) the thermicity profiles and b) the ignition delay-times of a shock heated $2\text{H}_2\text{-O}_2\text{-2Ar}$ mixture at $T_1=295 \text{ K}$. In a), $P_1=6.9 \text{ kPa}$; solid lines: $\kappa=0 \text{ m}^{-1}$; dashed lines: $\kappa=5000 \text{ m}^{-1}$; dashed-dotted lines: expansion. In b), solid lines: $P_1=6.9 \text{ kPa}$; circles: $P_1=10.3 \text{ kPa}$.

In order to consider realistic curvature values, we employed the $D_n-\kappa$ results from Arienti and Shepherd [13]. For a mixture with a reduced activation energy, Θ , equal 4.15, they found a maximum κH of approximately 3.5, where H is the half height of the channel. Applying this relationship to the present mixture with $\Theta=4.8$ and assuming a channel half height of 38 mm, the maximum curvature for our conditions is found to be on the order of 100 m^{-1} . Considering a point on the shock front in the close vicinity of the top wall and assuming that the center of the circle defining the curvature is located at $y=0$, the distance $|y' - y|$ can be assumed to be constant and on the order of 1 mm. The effect of curvature on the ignition delay-time was studied by considering four values of κ : 0, 100, 1000, and 5000 m^{-1} . The effect of volumetric expansion was estimated by considering the decay rate of the normalized shock speed follows a fifth order polynomial in time as extracted from the numerical simulation for an initial pressure of 6.9 kPa. The thermicity profiles obtained at $P_1=6.9 \text{ kPa}$, Figure 6 a), show that even a curvature of 5000 m^{-1} , 50 times higher than expected from Arienti and Shepherd's study, does not influence significantly the dynamics of the energy release rate. On the contrary, the volumetric expansion modifies both the time to thermicity peak and its amplitude. The effects of shock front curvature and volumetric expansion on the ignition delay-time (time to thermicity peak) are shown in Figure 6

a) for two initial pressures of 6.9 and 10.3 kPa. Within the range of values presently considered, the curvature has a very small impact on the ignition delay-time with a maximum increase of less than 5% for $\kappa=5000 \text{ m}^{-1}$ as compared to $\kappa=0 \text{ m}^{-1}$ for a normal shock front. The increase of the specific volume presently considered has a dramatic impact on the ignition delay-time with an increase of 10% at $D/D_{CJ}=1$ and up to about 350% at $D/D_{CJ}=0.814$. At lower initial normalized shock speed, the mixture cannot ignite within 50 μs (final time of the calculation). At higher initial pressure, $P_1=10.3 \text{ kPa}$, ignition is observed at lower initial normalized shock speed, $D/D_{CJ}=0.782$. This is explained by the decrease of sensitivity to expansion of mixtures at higher initial pressure which exhibit shorter ignition delay-time.

4 Conclusion

In the present study, the diffraction of detonation propagating in a $2\text{H}_2\text{-O}_2\text{-2Ar}$ mixture within a high aspect ratio geometry has been investigated both experimentally and numerically. The experimental study has shown that the transition between un-successful and successful detonation transmission extends over a wide range of initial pressure and appears as a statistical process. The numerical study has shown that the main qualitative features of the diffraction process could be captured but that the critical pressure for detonation re-initiation could not be well reproduced. This was attributed to the velocity deficit which was not accounted for in the simulations. Simplified combustion models have been employed to evaluate the respective effects on the ignition dynamics of shock front curvature and volumetric expansion behind a decaying shock. It was found that the expansion was the dominant process responsible for the increase of ignition delay-time and possibly for detonation failure.

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