Numerical Study of Detonation Wave Diffraction in Hydrogen-based Mixtures

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1 Introduction

As a detonation wave propagates from a confined tube to an unconfined space, it undergoes diffraction, which is characterized by a change of geometry from a quasi-planar wave to a cylindrical or spherical wave [1–4]. Depending on the mixture composition, thermodynamic conditions, detonation velocity at the tube exit, the geometry of the area expansion and tube cross section, the detonation wave can be either extinguished (sub-critical regime) or re-initiated (super-critical regime) [2]. Detonation diffraction has been extensively studied both experimentally and through numerical simulations.

Since Zeldovich et al.'s pioneering work [5], numerous studies have been performed on detonation diffraction using a variety of experimental geometry and techniques, as summarized by Schultz [4] in 2000. Since then, a number of investigations have been performed, for example by Khasainov et al. [6], Meredith et al. [7], and Nagura et al. [8]. The most advanced experimental investigation is the study of Pintgen [1, 2] who performed simultaneous imaging of the shock front and reaction zone, using schlieren and Planar Laser Induced Fluorescence (PLIF), as well as multi-exposure and stereoscopic chemiluminescence imaging.

Jones et al. [10–13] and Oran et al. [14, 15] used numerical simulations to study the diffraction of detonation and reignition process at an abrupt tube diameter increase (180° angle). Layered and uniform H_2-O_2(-Ar) mixtures were modeled. The chemical schemes were either 1-step or 2-step models. Arienti et al. [9] and Nagura et al. [8] performed simulations of detonation diffraction from a tube to an unconfined volume (90° angle). Arienti used a 1-step reaction model characterized by different activation energies whereas Nagura employed a 2-step scheme to model a stoichiometric H_2-air mixture. Khasainov et al. [6] studied the diffraction of detonation from a tube to a cone. A stoichiometric C_2H_2-O_2 mixture was considered using a 1-step pressure dependent reaction model. Deiterding [16] studied the failure and reignition of diffracting detonations in a stoichiometric H_2-O_2 mixture diluted with 70% argon. High-resolution numerical simulations with mesh refinement were performed using Euler equations. The reactivity of the mixture was described using a detailed reaction model composed of 34 irreversible reactions and 9 species.

From this literature review, we see that most numerical studies have been performed using an inviscid gas model (Euler equations) and global (1- or 2-step) kinetic schemes. The present study aims at performing numerical simulation of detonation diffraction using a viscous gas model (Navier-Stokes equations) and accurate chemical and thermodynamic models to allow for a more realistic comparison with the experimental data of Pintgen in terms of diffracting detonation behaviour and structure.

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2 Numerical methods

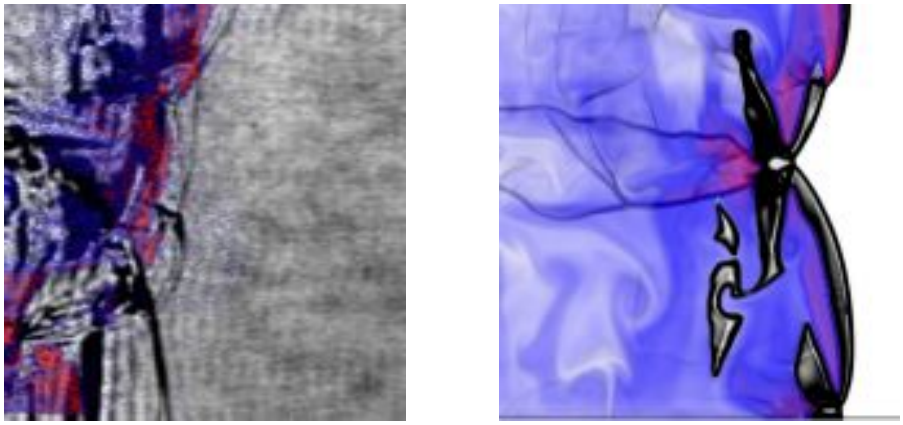
The compressible Navier-Stokes equations are solved for a reacting perfect gas mixture using a proprietary software developed for aerospace applications [17]. This software uses a finite-volume technique on unstructured or structured mesh. Conservative variables are calculated at the center of each computational cell and convective and diffusive fluxes are computed at cell edges using an approximate Riemann solver adapted for multi-species flows (Roe-Toumi scheme [18]). Positivity and monotonicity of species mass fractions are enforced by Larrouturou's method [19]. Computations are second-order accurate in space using a MUSCL approach with Min-Mod flux limiter and second-order accurate in time employing an explicit two-step Runge-Kutta time stepping. Typical CFL numbers used are about 0.5.
An operator splitting is used for chemical source terms. First, conservative variables $\mathbf{W}^n$ are updated without source terms to an intermediate state $\mathbf{W}^*$ for a time step Δt. Then, the ODE $d\mathbf{W}/dt = \mathbf{S}$ is solved from $\mathbf{W}^*$ to the final state $\mathbf{W}^{n+1}$. As the source terms $\mathbf{S}$ are stiff due to the chemistry, especially in the case of detailed kinetics, the ODE is solved using an implicit Runge-Kutta-Rosenbrock method. All computations are performed in 2D axisymmetric formulation, which allows to handle a geometry of revolution while keeping a two-dimensional mesh.
This work considers the Navier-Stokes equations rather than the Euler equations since it has been proposed that diffusion may have a significant role by altering small-scale vortical structures and mixing layers behind unstable detonation fronts [20]. The role of diffusion in the present configuration was not investigated in detail and, in some regions of the flow, numerical diffusion may be larger than physical diffusion. The Sutherland law is used for the temperature dependence of the mixture viscosity; thermal and mass diffusion are modeled using constant Prandtl and Schmidt numbers Pr=Sc=0.6.
Some preliminary simulations of detonations are conducted in a cylindrical tube. The computation is first initialized by mapping a 1D ZND solution on a coarse grid and then run until a steady propagation is achieved. This coarse grid solution is subsequently projected onto a fine grid and the detonation is allowed to propagate. A small disturbance, a square region with slightly modified fresh mixture density, is prescribed in the flow so as to trigger transverse waves and obtain detonation cellular structure. This solution is then mapped onto the final diffraction geometry, which consists of a cylindrical tube exiting into an unbounded half-space. The channel height L is 19 mm, corresponding to the experiment [1] and the numerical "unconfined" space extends up to 80 mm down the tube exit. Walls are modeled assuming free-slip boundary conditions. Since the fluid ahead of the detonation is in its quiescent state, the outflow boundary conditions are irrelevant. The diffraction geometry contains about 65×10^6 elements.
The reaction model used to perform the simulation is a reducted version of the model of Mével et al [21]. It is composed of 17 reversible reactions and 9 species, including Ar. It has been extensivelly validated against shock-tube, flow and jet-stirred reactor, and burning speed experimental data.

3 Results and discussion

3.1 Detonation propagation

An important aspect of the present study was to apply a Laser Induced Fluorescence (LIF) model to the numerical simulation of diffracting detonation so that a realistic comparison with the experiments of Pintgen [1, 2] could be performed. A detailed description of the 3-level LIF model can be found elsewhere [2, 22]. The LIF model has already been applied to 2D numerical simulation of detonation with various levels of instability [22, 23]. However, these simulations have been performed with a different numerical scheme and it was necessary to check the consistency of the results obtained with the two methods. Figure 1 compares experimental and numerical superimposed schlieren-PLIF images [24]. A stoichiometric H_2-O_2 mixture diluted with 60% of N_2 at P_1= 20 kPa, was used for the validation of the LIF model. As in the previous studies [22, 23], there is satisfactory agreement between the experiment and the simulation. The slightly irregular detonation front, typical of moderately unstable detonation, is well reproduced in the simulation. Concerning the OH PLIF field, the sharp onset and subsequent decay

of the fluorescence signal are well predicted. The progressive attenuation of the LIF signal intensity due to the laser sheet absorption is clearly apparent with much less intense portions away from the front.

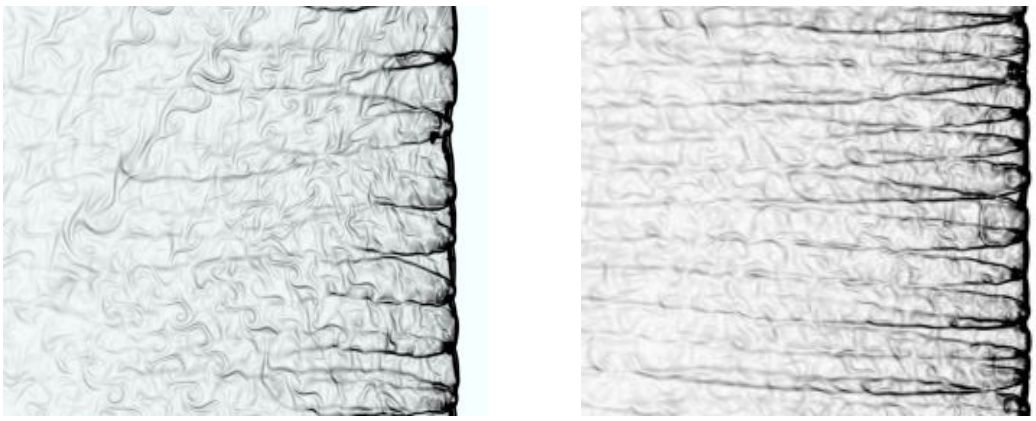


(a) Experimental schlieren-PLIF overlay (b) Numerical schlieren-PLIF overlay

Figure 1: Comparison between experimental [24] and numerical detonation propagating in a H_2-O_2-N_2 mixture. Initial conditions: Φ= 1; X_{N2}= 0.6; T_1= 295 K ; P_1= 20 kPa. Experimental and numerical images are 20 and 12 mm in height, respectively.

3.2 Detonation diffraction

To simulate the experimental results of Pintgen et al [2], two conditions have been numerically investigated, (i) a sub-critical case obtained for a stoichiometric H_2-O_2 mixture diluted with 70% of Ar at P_1= 100 kPa (mixture 1); and (ii) a super-critical case obtained for a stoichiometric H_2-O_2 mixture diluted with 50% of Ar at P_1= 57.5 kPa (mixture 2). In both cases, the initial temperature is 295 K.

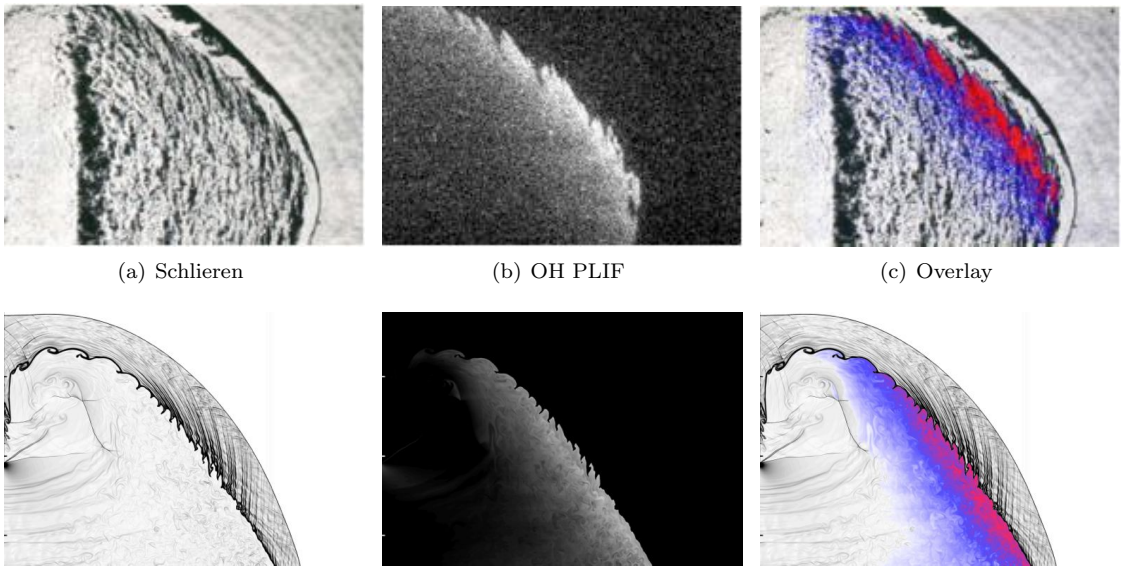


(a) Propagation for mixture 1 (b) Propagation for mixture 2

Figure 2: Numerical schlieren images of detonation propagation in H_2-O_2-Ar mixtures in a tube prior to diffraction. Initial conditions: a): Φ= 1; X_{Ar}= 0.7; T_1= 295 K ; P_1= 100 kPa. b): Φ=1; X_{Ar}= 0.5; T_1= 295 K; P_1= 57.5 kPa. Both images are 5 mm in height.

As demonstrated by Jones et al [12], high spatial resolution is required to simulate a diffracting detonation because the cellular structure plays a fundamental role in the qualitative nature, reignition or failure, of the diffraction process outcome. In the present simulation, a structured uniform numerical grid with cells of 8 μm has been used, this represents approximately 10 grid points per induction length.

Figure 2 shows instantaneous schlieren-like images of the detonation propagation prior to diffraction. In both cases, the cellular structure is satisfactorily resolved. For mixture 1, the cell size, λ, is estimated to be around 1 mm whereas, for mixture 2, the cell size is around 0.8 mm. These cell widths are two to three times smaller than the experimental values [25].
Figure 3 and Figure 4 present the numerical results along with the corresponding experimental data obtained for mixtures 1 and 2, respectively. The two different diffraction regimes observed experimentally, that is sub-critical for mixture 1 and super-critical for mixture 2, are well captured in the simulations. The ratio of the channel height to the cell width is approximately 38 and 48 for mixture 1 and mixture 2, respectively. Jones et al. [12] report a critical length scale in the range L_c=3-7λ, consistent with experimental data for high aspect ratio rectangular channels [26]. Deiterding [16] observed a critical length scale of approximately L_c=10λ, which is in agreement with the value reported for square channels [26]. Although the critical length scale is known to increase as the instability level of a detonation decreases [27], the ratio of mixture 1 appears higher than the expected range of ratio values. The differences observed between the studies could be related to the chemical reaction model, grid resolution and the accuracy of the numerical scheme.



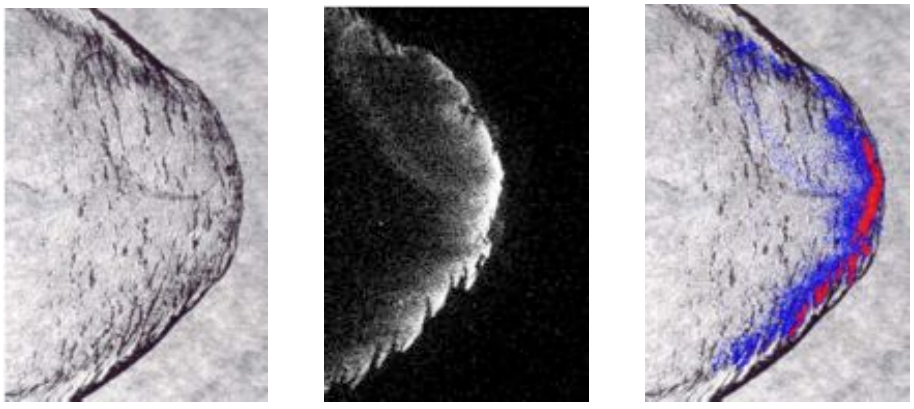
(a) Schlieren (b) OH PLIF (c) Overlay

(d) Schlieren (e) OH PLIF (f) Overlay

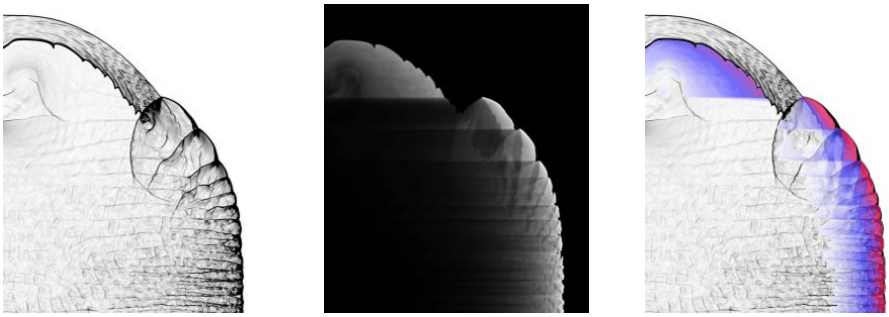
Figure 3: Comparison of experimental [2] (top) and numerical (bottom) images of a sub-critical detonation wave diffraction in a $2H_2$-O_2-7Ar mixture. Initial conditions: T_1=295 K and P_1=100 kPa. Experimental and numerical images are 60 and 32 mm in height, respectively. Detonation propagation is from left to right.

In both the failure and reignition cases, the evolution of the diffracting detonation wave observed in the simulation is consistent with previous experimental and numerical results. As the detonation exits into the unconfined volume, the top part undergoes diffraction and, in the vinicity of the corner, the reaction zone decouples almost intantaneously from the diffracting leading shock. Most of the detonation front remains quasi-planar but the area of the undisturbed front decreases as the expansion waves travel toward the tube axis. For mixture 1, the transverse waves fail in reigniting the unreacted gas volume which was shocked by the diffracting shock. The geometry of the detonation progressively switches from planar to spherical and eventually, the reaction zone completely decouples from the leading shock. For mixture 2, the central part of the detonation front remains undisturbed and quasi-planar. In the unreacted shocked volume, a reactive fan-like structure readily establishes due to the compression by

the transverse waves. Eventually, a transverse detonation is formed between the leading shock and burnt gas and propagates toward the wall. It is to note that the transverse detonation reflects at the wall at a distance of about 13 mm from the wall corner, which corresponds to 16 λ. This result is consistent with the experimental measurements of Nagura et al [8] who reported wall reflection distances in the range 10-15 λ for a wide variety of mixtures including both weakly and highly unstable cases.
Figure 3 and Figure 4 demonstrate qualitative agreement between the experimental and numerical schlieren and PLIF images. In both mixture 1 and 2, the LIF field appears as a very thin layer with a maximum intensity at the reaction zone front. The intensity of the signal decreases very sharply due to the strong absorption of the laser light. For mixture 1, the uncoupled reaction zone exhibits a pronounced sawtooth shape as observed experimentally. For mixture 2, the maximum LIF signal is observed at the undisturbed detonation front and at the front of the fan-like structure which exhibits a keystone shape as observed in propagating detonations. Interestingly, the front of the transverse detonation appears as a zone of low LIF intensity due to the strong absorption of the laser light by the fan-like structure. The uncoupled reaction zone located behind the diffracting shock wave appears as a zone of low LIF intensity with a slight sawtooth shape.



(a) Schlieren (b) OH PLIF (c) Overlay



(d) Schlieren (e) OH PLIF (f) Overlay

Figure 4: Comparison of experimental [2] (top) and numerical (bottom) images of a super-critical detonation wave diffraction in a $2H_2$-O_2-3Ar mixture. Initial conditions: T_1=295 K and (a-c): P_1=60 kPa (d-f): P_1=57.5 kPa. Experimental and numerical images are 70 and 18 mm in height, respectively. Detonation propagation is from left to right.

4 Conclusion

In the present study, the diffraction of detonation waves in hydrogen-oxygen-argon mixtures has been investigated using 2D numerical simulations performed with a Navier-Stokes solver and a realistic ther-

mochemical scheme. The numerical results demonstrate a reasonable agreement with previously obtained experimental and numerical data in terms of diffracting detonation behaviour and structure. Key features observed in the experimental LIF images were reproduced by the synthetic LIF visualization. Future work will focus on the simulation of detonation diffraction in mixtures with high activation energy such as hydrogen-nitrous oxide mixtures.

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