Numerical investigation of detonation failure in non-uniform compositions and comparison to experiments

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1 Introduction

In many engineering problems, detonations propagate in non-uniform compositions. Accidental leaks of fuel from tank or ducts form explosive clouds with atmospheric air which involve a spatial distribution of the mixture components. In detonation-based propulsion systems, such as Pulse Detonation Engines (PDE) and Rotating Detonation Engines (RDE), fuel and oxidizer are injected separately in the combustion chamber and, especially in RDE, some burnt gases remain in the chamber during the injection. Thus, for industrial safety and specific applications of detonation, the behaviors of detonation in mixtures with composition gradients should be investigated.

Several experimental and numerical works have been conducted with, for simplicity, gradients either normal or parallel to the direction of the detonation propagation. A review can be found in Boulal et al. [1, 2]. For the normal-gradient case, experiments, e.g. Ishii and Kojima [3], Boeck et al. [4], have shown that the global curvature and the mean cell width and shape of the detonation wave front are dependent on the local composition concentration. Liebermann and Shepherd [5] also observed local shock-flame decoupling when front curvature was too large. These observations are confirmed by numerical analyses, e.g. Kessler et al. [6]. For the parallel-gradient case, Boulal et al. [1, 2] have conducted experiments with two sets of initial distributions, a first one with monotonic decrease of Equivalence Ratio (ER), from rich or lean to leaner compositions, and a second one with non-monotonic ER distributions, from lean to leaner then to richer compositions. For the first distribution set, they observed two types of failure of an initially self-sustained CJ multicellular detonation: a sudden one with shock-flame decoupling, and a more progressive one through marginal modes of propagation, with a decreasing number of transverse waves. They proposed and validated a criterion for shock-flame decoupling based on the variation of chemical scales, such as the ZND characteristic length and time or the cell mean width of the detonation structure. For the second, they observed critical, supercritical and subcritical propagation regimes and found that re-initiation of a failed detonation was mainly governed by the strength of the Mach reflections of residuals transverse waves at walls.

This study is a numerical investigation into the parallel gradient case with monotonic ER distributions. The purpose is to assess the feasibility of numerical simulations to represent the detonation dynamics observed in [1]. Comparisons between numerical and experimental sooted plates are presented. Based on numerical detonation dynamics, the criterion for shock-flame decoupling, and the influence of the channel transverse dimension on the detonation propagation in a given initial distribution are also investigated.

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2 Numerical Setup

The computational domain is a straight tube made of an initial section which contains a uniform composition and a main section which contains a non-uniform one. The object of the simulation is to describe the detonation transmission and behavior in the main section after propagation in the initial section. The value of the ER (φ_{start}) in the initial section is identical to that at the entry of the main section so as to obtain a smooth transmission of the detonation into the main section, as achieved in [1,2]. The initial and main sections have the same width W, and the main-section length is denoted by L. Figure 1 describes the computational domain and the boundary conditions. Figure 2 shows the two considered ER distributions, specifically a Small and a Large Gradient. Table 1 gives the initial pressure and temperature P_0 and T_0, the ERs φ_{start} and φ_{end} at the main section entry and exit-end, and W and L, for the numerical and experimental distributions. For simplicity, linear variations of φ were considered. Table 1 also gives the initial mean width λ_i of the cellular structure that characterizes the local instabilities of the detonation reaction zone. The initial condition considered in the initial section is the multicellular detonation flow obtained from a preliminary simulation in a uniform mixture with ER φ_{start} after a well-developed two-dimensional cellular detonation with a converged mean cell width λ_i was obtained.

The governing equations are the compressible two-dimensional Euler equations and the conservative equations of chemical species. The 5th-order WENO scheme and the 3rd-order TVD Runge-Kutta method are used for the convection terms and the time integration, respectively. The source term is integrated by the Multi-Time Scale method described in [7]. The considered reactive mixtures were compositions of H_2 and Air, and the detailed chemical kinetics mechanism proposed by Hong et al. [8] was implemented. This model contains 9 chemical species and 20 elementary reactions. In the main section, the ratio of the local half-reaction length to the minimum grid width was always kept larger than 16 to ensure that the chemical kinetics process was properly captured.

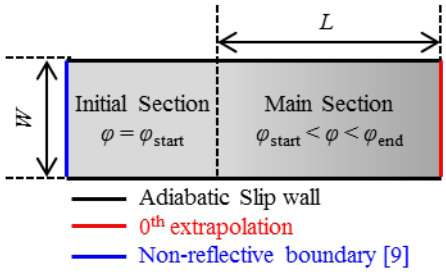

Figure 1. Computational target of this study.

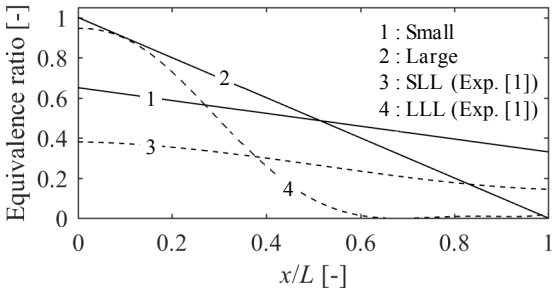

Figure 2. ER distributions in the Main section.

Table 1. Calculation and Experimental conditions of each case.

	λ_i [mm]	W [mm]	L [mm]	T_0 [K]	P_0 [MPa]	φ_{start} [-]	φ_{end} [-]
Small-W9	4.5	9	160	300	0.122	0.65	0.33
Small-W18		18					
Large	1.2	9	45		0.203	1.00	0
SLL (Exp. [1])	15±3	50	665	290	0.203	0.37±0.01	0.18±0.01
LLL (Exp. [1])	5±2					0.93±0.02	0.0±0.01

3 Results and discussion

3.1 Numerical results and qualitative comparison to experiments

Figure 3 is the soot track images from [1] and experimental conditions given in Table 1. The considered mixtures were compositions of C_3H_8/O_2. A self-sustained CJ detonation was smoothly transmitted from a 3570-mm-length ignition tube filled with a uniform mixture to a 665-mm-length chamber filled with a non-uniform one. Both the chamber and the ignition tube had a 50x50 mm^2 square-cross section. In the SLL case (Fig. 2, curve 3), the detonation dynamics resulted in a transverse waves

number adaptation of the front to the chamber confinement. The detonation mean cell width increased and eventually the detonation disappeared in the limiting single-headed regime. This behavior is called the geometric failure. In the LLL case (Fig.2, curve 4), the detonation suddenly quenched through a 1D shock-flame decoupling because of the composition variation being too steep for the front to adjust its structure. This behavior is called the chemical failure. Since, C_3H_8-fuel-based detailed chemical kinetics mechanisms are very heavy in terms of calculation cost, we have considered H_2/Air compositions. From the qualitative point of view the characteristic lengths of this problem are the transverse confinement W and the characteristic mean cell with of the ignition mixture λ_i. To that purpose, the non-dimensional ratio W/λ_i was as best conserved from experiments to numerical simulations. Figure 4 shows the numerical soot tracks obtained. Top and center soot tracks correspond to the Small case (Fig. 2, curve 1), with W = 9 mm (Small-W9) and W = 18 mm (Small-W18), and the bottom one corresponds to the Large Gradient case (Fig. 2, curve 2). We observe that the cells' increase, due to the propagation into leaner compositions, is less significant in the numerical simulations than in the experiments. The reason is that, in the range $0.5 < \varphi < 1$, cell width of H_2/air detonations presents limited variations compared to those of C_3H_8/O_2 detonations [10]. As regards the Small Gradient cases, we observe the same geometric failure through marginal propagation, as in the experiments (Fig. 3). The influence of the transverse confinement can clearly be observed by comparing top and center soot tracks obtained for 9 and 18 mm transverse widths. In the Small-W18 case, triple points are observed at further positions than in the Small-W9 case. As regards the Large Gradient case, sudden failure without transition to marginal modes is also remarkably well reproduced by numerical simulations.

3.2 Simulation of failure processes

Figures 5 and 6 show density field of the Small and Large Gradient cases, respectively, at different mean shock positions x_s. Details of the geometric failure are provided in Figure 5. At start, we observe several shock-induced reactions in both transverse and longitudinal directions. These coupled shock-flame systems are progressively reduced as the number of triple points is decreasing. Transverse shock waves reflections at walls generate local explosions that maintain this marginal propagation in the form of local and periodical process of shock-flame decoupling and recoupling. On the contrary, the chemical failure displayed in Fig. 6 occurs as a whole 1D process with the sudden disappearance of transverse shock-induced reactions. Localization of the shock-flame decoupling can be assessed from maximum pressure history, such as shown in Figure 7. Considering the center line, we observe the disappearance of the large pressure peaks at about the position $x/L \sim 0.5$, in compliance with the disappearance of the cellular structure in Fig. 4 (bottom).

3.3 Simulation of failure criterion

The shock-flame decoupling criterion [1,2] of an initially multicellular detonation in domains of decreasing reactivity is based on the comparison of the non-dimensional number $D\nabla t_c$ with 1, where D is the detonation wave velocity and $\nabla t_c = \partial t_c/\partial x$ is the spatial derivative in the direction of the detonation propagation of the ZND model characteristic time t_c. Values of $D\nabla t_c$ smaller than 1 are necessary conditions for the stable propagation of a multicellular detonation wave. If, subjected to decreasing reactivity compositional variation, $D\nabla t_c$ becomes larger than 1, failure through shock-flame decoupling is likely to appear. We have calculated the shock-flame decoupling criterion number for the Large Gradient case (Figure 8). From the initial ER distribution, t_c and D were obtained by the detonation characteristic analysis code AISTJAN [11]. We observe that $1 \lesssim D\nabla t_c \lesssim 10$ in the range of positions $0.4 \lesssim x/L \lesssim 0.5$, which approximatively well predicts the position of detonation failure from Fig. 4 (bottom). Figure 8 shows OH mass production rate (Ω). When detonation failure occurs, chain-branching reactions drop. Therefore, the detonation failure can reasonably be assumed to occur when $\Omega < 0$. As a matter of fact, the point of $\Omega = 0$ agrees well with that of $D\nabla t_c = 1$. This shock-flame decoupling criterion calculated by a ZND model provide a good validation tool for 2D simulation of detonation in non-uniform compositions.

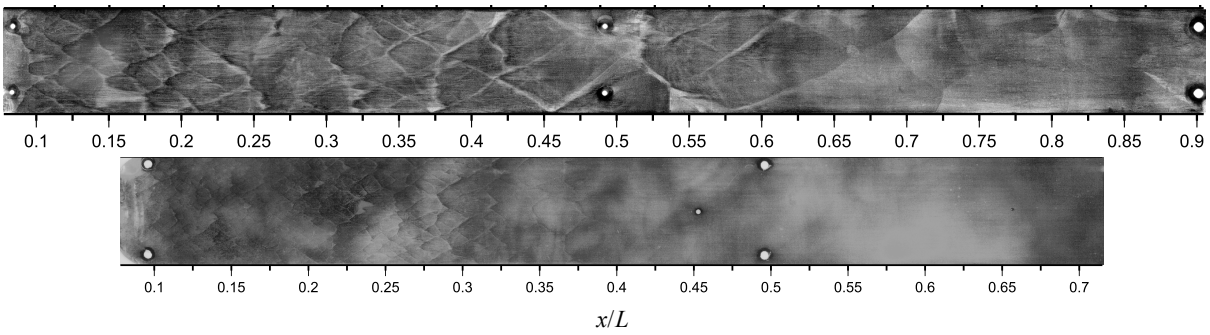

Figure 3. Experimental sooted plate recordings [1].
Top: Small Lean to Leaner Gradient (Geometric failure).
Bottom: Large Lean to Leaner Gradient (Chemical failure).

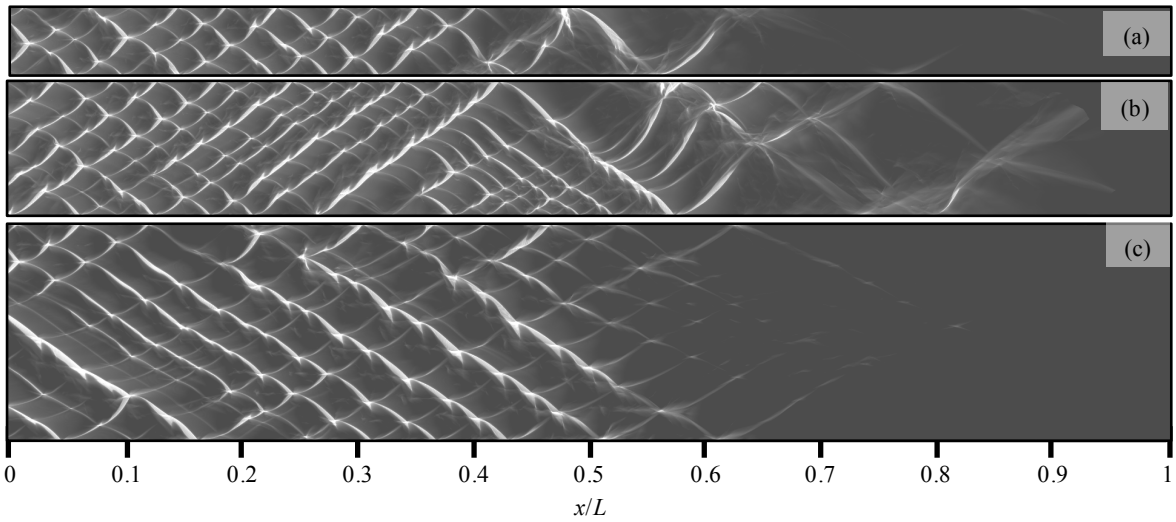

Figure 4. Numerical sooted plates. (2D maximum pressure history):
(a) Small-W9 Gradient, (b) Small-W18 Gradient, (c) Large Gradient.

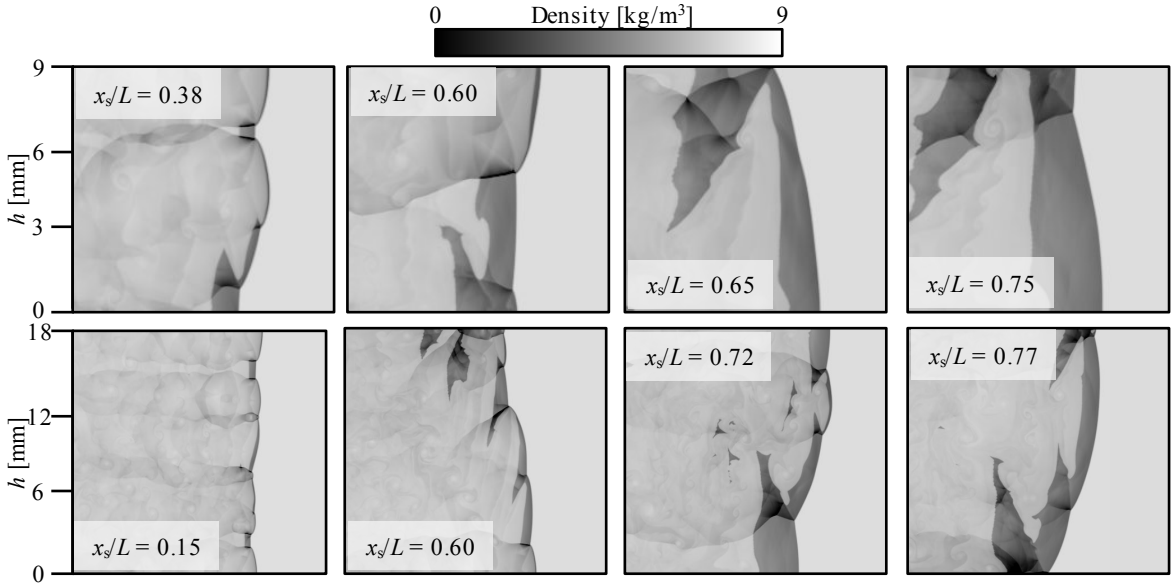

Figure 5. Density distributions in the Small Gradient cases.
(top: Small-W9 Gradient, bottom: Small-W18 Gradient).

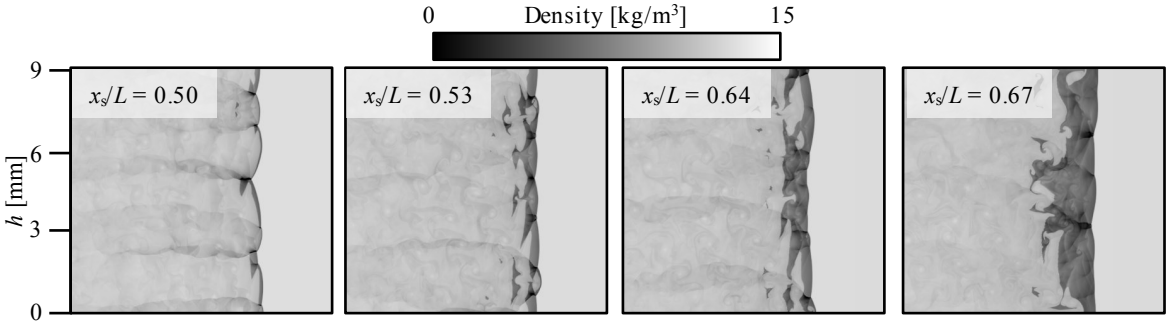

Figure 6. Density distributions in the Large Gradient case.

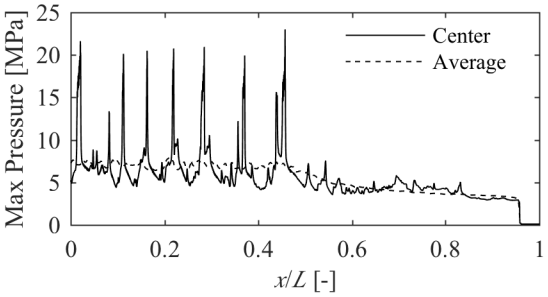

Figure 7. 1D Maximum pressure history in the Large Gradient case.

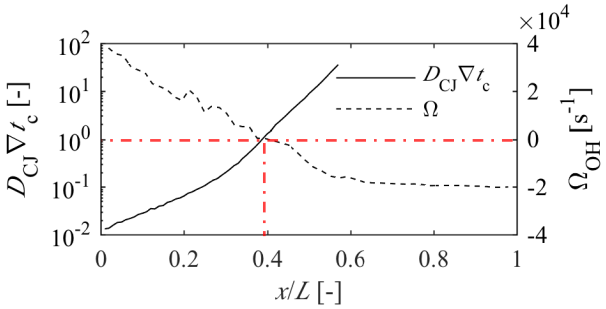

Figure 8. Variation of $D\nabla t_c$ and Ω in the Large Gradient case.

4 Conclusion

Two-dimensional dynamics of detonation waves in mixtures with composition gradients parallel to the direction of propagation were numerically investigated by solving the two-dimensional Euler equations with detailed scheme of chemical kinetics. The ER distributions were monotonically decreasing from stoichiometric or lean compositions to leaner ones. The geometric and chemical dynamics of failure observed by Boulal et al. [1] were successfully reproduced. The influence of the channel transverse dimension was also investigated. For the same initial composition distribution, the larger the transverse width, the farther the propagation of detonation, i.e., towards leaner compositions. The shock-flame decoupling criterion proposed in [1,2] was numerically implemented and found to provide a good prediction of sudden failure and therefore a good validation tool for numerical simulation of detonation propagation in composition gradient. The present work thus demonstrates the ability of numerical simulations to reproduce the complex dynamics of detonation in non-uniform compositions. Future works will address another case of monotonically varying non-uniform compositions, with ER decreasing from rich to lean, and the cases of non-monotonically varying non-uniform compositions, with ERs first decreasing and then increasing.

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