# Numerical Study of Gaseous Detonation Propagation Across a Density Interface

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## 1 Introduction

The transient, multi-dimensional cellular structure of the detonation has been well observed both experimentally and numerically [1]. However, due to various instability features and interaction between compressible turbulence and chemical reactions giving rise to a highly unstable flow field, no detailed theory exists yet to describe the unstable detonation structure. Experimentally, the conventional technique often used to shed light on the dynamics of the detonation structure is to analyze a response to a certain perturbation [2, 3]. The idea is to perturb the detonation and then observe the subsequent relaxation as the detonation re-establishes its asymptotic structure. It is hoped that the relaxation length (or equivalently, the time), will provide a measure of the hydrodynamic thickness of the detonation front in its direction of propagation [4], that is a length scale to characterize the overall thickness of the unstable cellular front and develop empirical correlations or analytical models for the dynamic detonation parameters (e.g., initiation energy, critical tube diameter, limit, etc.).

In this study, numerical experiments are carried out to investigate how the detonation adjusts to a sudden change in mixture conditions. To disturb the detonation front, a step decrease as well as increase in density of the reactants are used. Experiments of similar problems has been previously conducted [5, 6] investigating the interaction of a detonation with a varying concentration gradient. Analytical, as well as experimental and numerical studies were also conducted more recently on the phenomenon and possibility of detonation transmission from one gaseous mixture to another of lower reaction sensitivity [7, 8]. Experimentally, it is challenging to create well-defined concentration gradients or a stable free interface, to observe the interaction at the interface itself and the strong influence of the experimental setup complicates interpretation of the results. Here, numerical simulations are performed to understand the flow field of a simpler well-defined interaction of a detonation with an abrupt density interface. The numerical results provide observation of the detonation wave behavior both upstream and downstream as well as during the transmission.

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For a non-reacting shock wave, the wave patterns resulting from its interaction with a contact discontinuity will depend on the entire gasdynamic flow field in its wake. For a detonation, however, it will depend on the chemical energy release and not on the flow behind the reaction zone. Only the flow in the reaction zone itself can influence the detonation. In the presence of an unsteady heat release in the flow, the detonation will regain its original structure as the perturbation at the front structure relaxes. The study of the relaxation length resulted from the imposed perturbation will thus provide a measure of the effective thickness of the detonation front. For a significant density difference between the donor and acceptor mixtures, the problem can lead to a better understanding of the detonation re-initiation mechanism behind the interface through transmission of detonations or failure caused by the interaction.

## 2 Computational Details

Numerical simulations of gaseous detonations are performed using the reactive Euler equations with the one-step Arrhenius kinetic model. The equations are non-dimensionalized using the unburned gas properties and the half reaction length $L_{1/2}$ (where half of the reactant is consumed) as the reference length scale, see [9]. The governing equations are discretized on a uniform, Cartesian computational grid. For the onedimensional simulation, the governing equations are solved numerically using a second-order SLIC (Slope Limiter Centered) scheme which has been validated and used in previous studies [10]. The one-dimensional computations were performed in the lab-fixed reference frame and initialized with a ZND profile. The computational domain was reinitialized at finite intervals to always contain the leading shock front and allow sufficient length to avoid any disturbance from the back boundary. For the two-dimensional simulation, the MUSCL-Hancock scheme using the HLLC Riemann solver with Strang's splitting is used [11]. A moving control volume with a sufficiently long domain length of $x = 100\ L_{1/2}$ is used with a constant inflow defined at the right boundary. The width of the computational domain is 40 $L_{1/2}$. A region of overpressure $2P_{CJ}$, to facilitate detonation formation, covers three quarters of the domain length from the left edge. The top and bottom boundaries are reflective. The left boundary is relaxed toward the inflow conditions following [12]. The established detonation wave thus remains at approximately the same location in the domain. Unless otherwise specified, a grid resolution of 100 points and 32 points per ZND half reaction zone length $L_{1/2}$ is used for the one and two-dimensional simulations, respectively. The computational setup fixes the dimensionless parameters with the values $Q = 50$ and $\gamma = 1.2$ while varying the activation energy $E_a$ as a control parameter [9]. In both cases, sufficient computational time was used to allow the propagating detonation to fully develop before imposing the density perturbation.

## 3 Results and Discussion

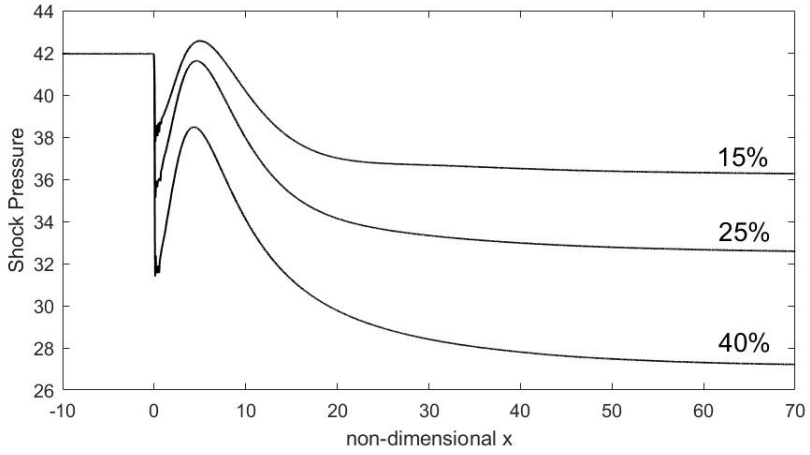


Figure 1. Leading shock pressure history of a ZND detonation interacting with a step density decrease in the reactant

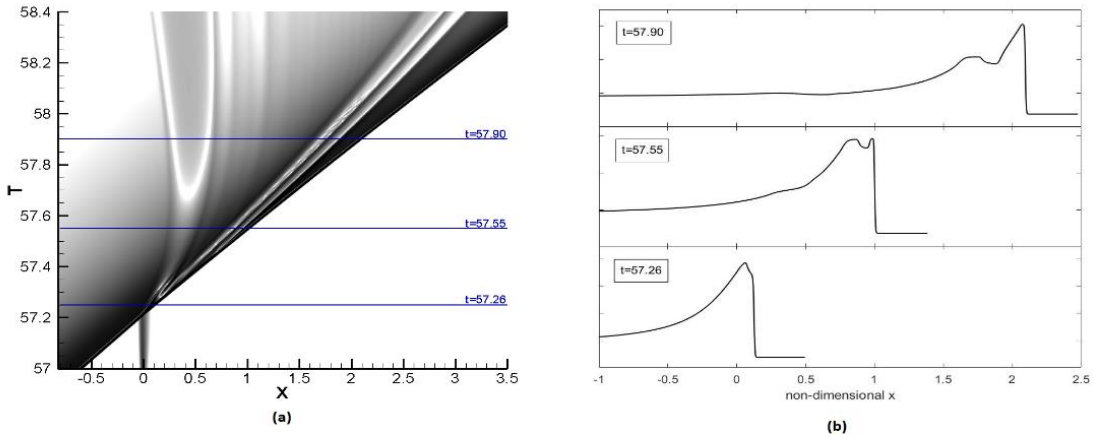


Figure 2 a) Schlieren flow field and b) density profiles within the relaxation region for the case with $\Delta\rho$ = -25%

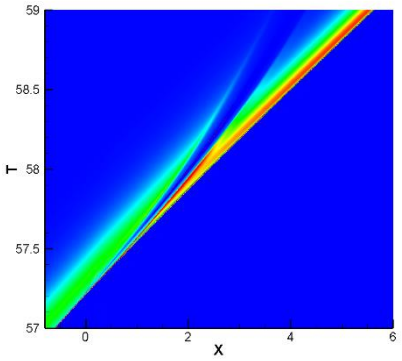


Figure 3. Reaction rate within the relaxation region

Figure 1 shows the leading shock pressure evolution of a stable ZND detonation with $E_a$ = 20 interacting with a negative density discontinuity in the reactant. Results for three magnitudes of density change are plotted. The distance x is non-dimensionalized with respect to the reaction zone length defined by 90% of energy released of the initial ZND wave. Upon interaction, the leading shock pressure drops to a lower level. However, the wave immediately re-accelerates and subsequently relaxes and re-establishes to the structure corresponding to the new mixture condition with a lower reactant density. A transient relaxation region can be clearly observed in the figure. In all three cases, the dynamics and the length for the detonation wave to relax back to the new structure are qualitatively similar. To look at the wave interaction in the early relaxation period, Fig. 2 shows a Schlieren plot and the density profiles at different instants of time as indicated. Fig. 3 shows the change in reaction rate during this period.

When the detonation encounters a step decrease in reactant density, the immediate interaction between the leading shock front and a stationary contact surface is consistent with the non-reacting shock-contact surface interaction [13]. It produces a transmitted shock with lower pressure ratio equivalent to that of the non-reacting shock interaction, a contact discontinuity and a reflected rarefaction wave, as shown in Fig. 2. The reflected expansion wave is deflected as it moves through the reaction zone and the contact surface is convected with the flow behind the detonation wave. Apart from the immediate period after the head-on collision with the density discontinuity, the reaction front stays closely behind and coupled with the leading transmitted shock. Although the transmitted shock strength decreases, a decrease in density gives a higher temperature in the reactant. This causes immediate re-acceleration of the wave via an increase in reaction rate behind the leading shock until x~5 as shown in Fig. 3. There is a subsequent relaxation to the final structure.

By increasing the activation energy of the reactive mixture to $E_a$ = 27, the ZND detonation becomes unstable. The leading shock pressure pulsates with a single mode limit-cycle oscillation as shown in Fig. 4. When the pulsating detonation hits the step change in density, similar wave dynamics as compared to Fig. 1 is observed. Clearly shown in Fig. 4, the detonation undergoes a relaxation process after its interaction with the density perturbation. For a larger density change in the reactant mixture, it is also shown that the detonation propagation is made more stable. This is due to the resulting temperature increase in the reactant which leads to a lower reduced activation energy of the mixture, below the neutral stability limit.

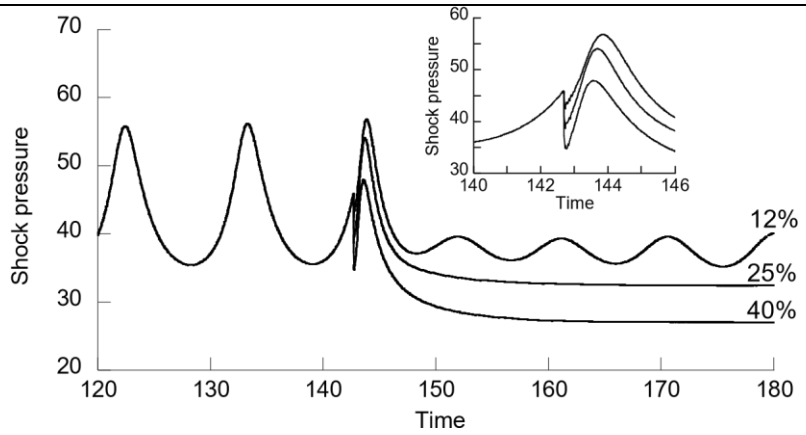


Figure 4. Leading shock pressure history of an unstable one-dimensional pulsating detonation interacting with a density step decrease in the reactant

A two-dimensional simulation is performed to look at the interaction of a cellular detonation with a density discontinuity. Figure 5 first shows the Schlieren flow field for $E_a = 20$ which gives a weakly unstable cellular structure. Both grid resolutions of 32 and 50 per $L_{1/2}$ gives about two and a half cells for the mixture properties and channel size used in the computation, consistent with the work by Sharpe & Quirk [14].

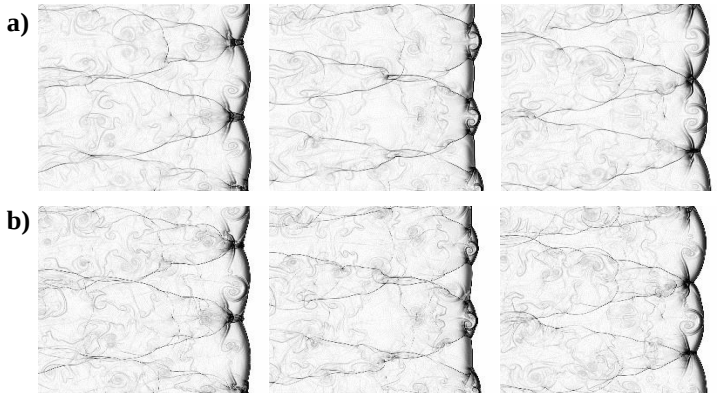


Figure 5. Two -dimensional unstable cellular detonations simulated with a) 32 pts; and b) 50 pts per $L_{1/2}$

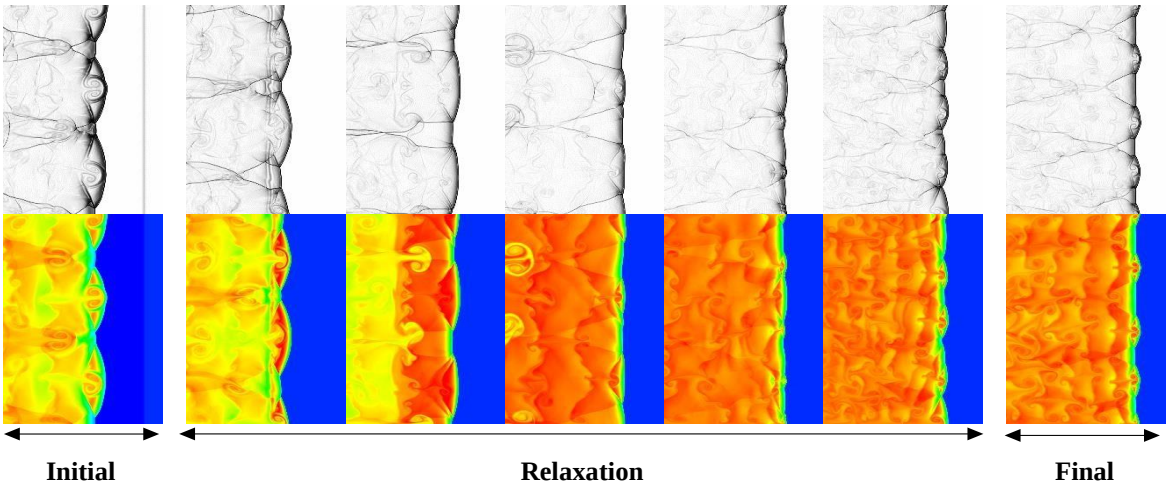


Figure 6. Two-dimensional simulation of a weakly unstable cellular detonation interacting with a negative density discontinuity using $E_a = 20$ and a grid resolution of 32 pts per $L_{1/2}$

Figure 6 shows both the density Schlieren and temperature contours for a weakly unstable detonation interacting with a density step decrease of 40% (i.e., $\rho_{new} = 0.6\rho_o$). After the interaction, it is shown that there is an increase of the number of detonation cells to about four after converging to the final structure. When the detonation front first hits the density discontinuity, there is a sudden increase in the temperature behind the detonation front. The flow field appears to be homogenized. During the relaxation period, new triple points are developed at the leading front and vortices are subsequently regenerated and well selforganized behind the re-established weakly unstable detonation structure.

1-D simulations are also performed to look at the interaction of the ZND detonation with a positive density step in the reactant. Figure 7 shows the results with $E_a = 20$ for three different density step sizes. The head-on collision of the ZND detonation with the density jump first causes an increase in the transmitted shock pressure with a reflected shock into the product, similar to the non-reacting shock interaction with a positive density contact surface. It is followed immediately by a wave decay to a sub-CJ level. After a quasisteady period, the wave re-accelerates and subsequently relaxes to the final detonation structure based on the new reactant density. The observed evolution is very similar to our previous study on the head-on collision with a normal shock wave [2, 3]. Figure 8 also plots out the pressure profiles during the relaxation period. The re-acceleration process is similar to the direct initiation of 1-D detonation [1], whereby it is originated from onset of a pressure pulse within the reaction zone, which is amplified continuously and eventually catches up with the leading front to produce an overdriven detonation.

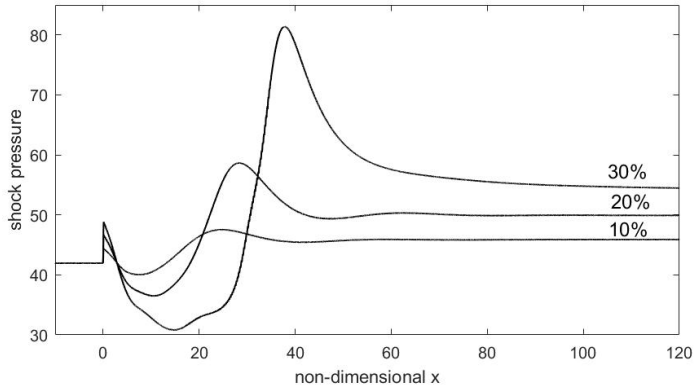


Figure 7. Leading shock pressure of a ZND detonation interacting with a positive density change in the reactant

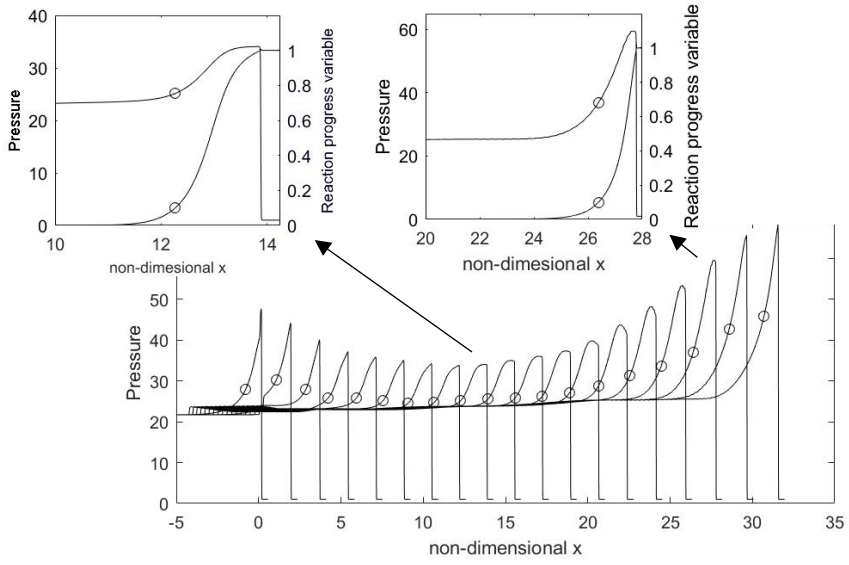


Figure 8. Pressure profiles within the relaxation with $\Delta\rho = +25\%$. The circle indicates the location of $\lambda = 0.10$.

## 4 Concluding Remarks

In this study, the interaction between a propagating detonation with a density discontinuity is analyzed numerically through one- and two-dimensional simulations. The focus of this study is on the detailed relaxation process produced by the imposed perturbation to shed light on the dynamics of the detonation structure and provide a measure of its hydrodynamic thickness. In all simulation cases, the gaseous detonation perturbed by the density step change undergoes a distinct relaxation process toward the final structure. Within the relaxation region, the gas dynamic wave pattern can be more easily revealed from the ZND case. For the negative density change, the increase in the chemical energy release within the reaction zone due to the higher reactant temperature re-accelerates the transmitted shock and re-establishes the final detonation structure very quickly. For the positive density change, the phenomenon is very similar to our previous study on the head-on collision with a normal shock wave [2]. The interaction leads initially to a failure followed by a re-initiation to the final detonation structure corresponding to the new reactant density. The wave amplification process closely resembles the direct detonation initiation phenomenon. Preliminary two-dimensional simulations also show the details of the cellular detonation evolution within this relaxation period for the case of step density decrease in reactant and how new triple points are generated after the interaction to produce the final structure with more cells. Attempt will be made to provide a criterion to describe the relaxation length and to use it to characterize the effective thickness of the detonation front.

## Acknowledgment

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