Transmission of Cellular Detonation Waves across a Density/Temperature Interface

Kelsey C. Tang-Yuk, John H.S. Lee
McGill University
Montreal, QC, Canada

Hoi Dick Ng
Concordia University
Montreal, QC, Canada

XiaoCheng Mi
University of Cambridge
Cambridge, United Kingdom

1 Introduction

The propagation of detonation waves in a non-uniform mixture is of practical interest since in any accidental vapor cloud explosion, the mixture is always non-uniform. Experimental studies of detonation in non-uniform mixtures are difficult to realize in a controlled fashion. Thus numerical studies could be advantageous.

In a previous study [1], the transmission of a planar Zel'dovich-von Neumann-Döring (ZND) detonation across a density interface was investigated numerically. However, real detonation waves posses a three-dimensional, unstable cellular structure [2]. Therefore, in the present study a two-dimensional cellular detonation is considered. Since the pressure has to be uniform across the interface, a density decrease and a density increase are accompanied by a temperature increase and a temperature decrease respectively. Thus the transmission across a density interface is essentially that of a temperature interface as well.

Note that for an infinitely thin detonation front the adjustment to the downstream condition is immediate. Gas dynamics analysis can readily be applied to determine the transmitted and reflected waves by the interface. Thus, in the present study the transient process as the detonation transmits across the interface is dependent on the details of the detonation structure. The adjustment of the initial upstream cellular structure to the final cellular structure corresponding to the downstream state is investigated.

2 Computational Details

The problem is illustrated in figure 1, where the upstream and downstream states of the interface are denoted by subscripts '0' and '1' respectively. The detonation is initiated upstream of the interface by a

Correspondence to: kelsey.tangyuk@mail.mcgill.ca

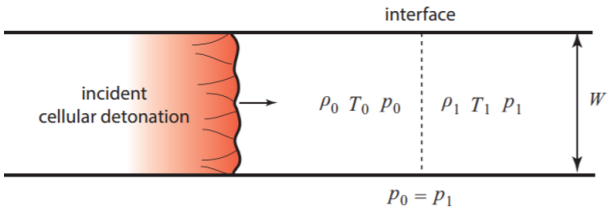

Figure 1: Problem illustration.

high pressure region with a sinusoidal perturbation and initiation is sufficiently far upstream such that a fully developed CJ wave is obtained prior to encountering the interface.

The system is governed by the two-dimensional, reactive Euler equations and the heat release is governed by single step Arrhenius kinetics as follows,

$$\Omega = \frac{\partial Z}{\partial t} = -kZ\exp\left(\frac{-E_\mathrm{a}}{T}\right) \tag{1}$$

The state and flow variables are non-dimensionalized with respect to the initial unburnt state as described by Ng and Zhang [3], and the pre-exponential constant is scaled such that the half reaction zone length, $l_{1/2}$ of the corresponding steady ZND solution is unity. The dimensionless heat release Q and the ratio of specific heats γ are fixed at $Q = 50$ and $\gamma = 1.2$ for all simulations. The domain width, W in figure 1, is defined to be 300 times $l_{1/2}$.

The simulation code is based upon a uniform Cartesian grid with a resolution of 10 grid points per $l_{1/2}$. The MUSCL-Hancock scheme with the van Leer nonsmooth slope limiter and a Harten-Lax-van Leer-contact (HLLC) approximate solver for the Riemann problem are used as described by Toro [4]. A periodic boundary condition is applied to the top and bottom boundaries of the domain. A resolution test at double resolution (20 cells per $l_{1/2}$) was performed to ensure that the salient features discussed in the next section are captured.

3 Results and Discussion

For cellular detonations, the transmission phenomenon across a density interface is best illustrated by soot foils, which show the transient evolution of the structure across the interface. The numerical soot foils of this study were generated by tracking the maximum pressure obtained at each point in the domain.

The change across the interface can be thought of in terms of the change in reduced (or effective) activation energy, $E_\mathrm{a,e}$, due to the temperature change. Since $E_\mathrm{a} = \frac{\tilde{E}_\mathrm{a}}{R\tilde{T}_0}$ is constant in the domain, the downstream effective activation energy is,

$$E_\mathrm{a,e} = \frac{E_\mathrm{a}}{T_1} = E_\mathrm{a}\rho_1 \tag{2}$$

It should be noted that a density decrease always reduces $E_\mathrm{a,e}$ downstream, while for a density increase higher $E_\mathrm{a,e}$ is obtained downstream. Activation energy governs the sensitivity of the mixture to changes in temperature. Therefore, a density decrease renders the wave more stable downstream while a density increase renders the wave less stable downstream.

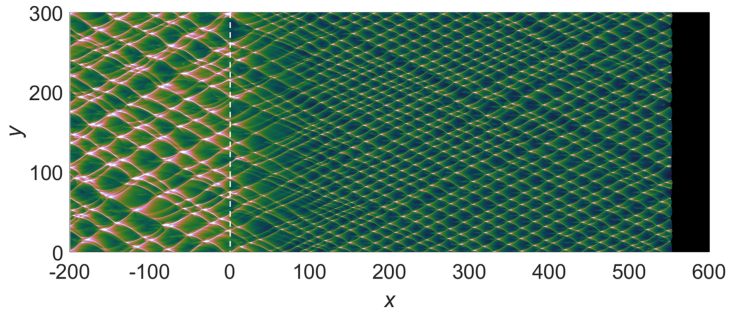

Figure 2: Numerical soot foil for the case with $E_{\mathrm{a}} = 20$ and density decrease $\Delta\rho = -0.3$ across the interface (upstream $E_{\mathrm{a,e}} = 20$ and downstream $E_{\mathrm{a,e}} = 14$).

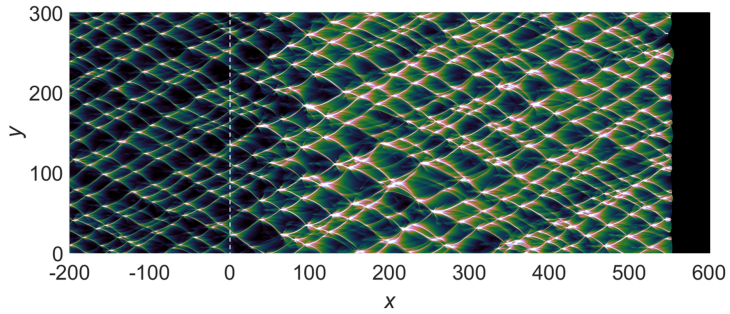

Figure 3: Numerical soot foil for the case with $E_{\mathrm{a}} = 20$ and density increase $\Delta\rho = 0.3$ across the interface (upstream $E_{\mathrm{a,e}} = 20$ and downstream $E_{\mathrm{a,e}} = 26$).

3.1 More stable downstream (density decrease)

First consider a decrease in density (increase in temperature) and thus lower $E_{\mathrm{a,e}}$ (and a more stable mixture) downstream. Figure 2 shows the numerical soot foil. The interface is located at $x = 0$ as indicated by the dashed line. In this case, the upstream $E_{\mathrm{a,e}} = 20$ and a detonation in this mixture has a relatively stable cellular pattern as illustrated in figure 2 for $x < 0$. The downstream $E_{\mathrm{a,e}} = 14$ and thus the mixture is more stable and has a smaller and more regular cellular pattern. This is observed for $x > 0$ far downstream of the interface.

The relaxation region downstream of the interface reveals essentially the development of the finer cellular pattern superimposed on the larger cellular pattern. That is, after crossing the interface the smaller cells can be observed to form within the larger upstream detonation cells. The relaxation process appears to be quite gradual, as new triple points develop on the shock front of the initial larger upstream detonation cells gradually. The relaxation length corresponds to about 150 unit lengths (or 150 times $l_{1/2}$ of the upstream detonation). However, the ZND length scale associated with the downstream mixture is different to the upstream. In terms of downstream mixture, the relaxation length is approximately 380 times $l_{1/2,1}$.

3.2 Less stable downstream (density increase)

Figure 3 shows the case where the detonation transmits across an interface with a density increase (temperature decrease). The upstream detonation, $x < 0$ is the same as before, but in this case the activation

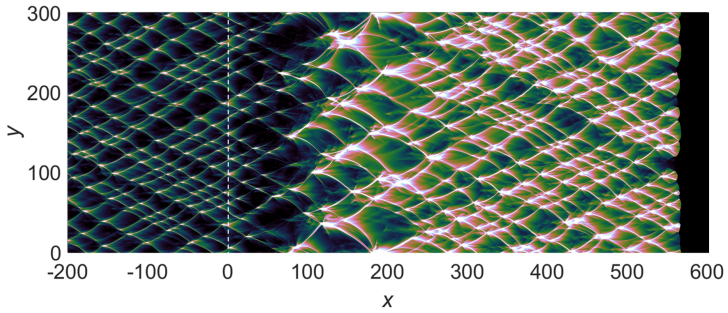

Figure 4: Numerical soot foil for the case with $E_{\mathrm{a}} = 20$ and density increase $\Delta\rho = 0.5$ across the interface (upstream $E_{\mathrm{a,e}} = 20$ and downstream $E_{\mathrm{a,e}} = 30$).

energy is higher downstream of the interface, $E_{\mathrm{a,e}} = 26$. Thus, as is evident in figure 3, in the region far downstream from the interface, the detonation cells are larger and the soot foil is more irregular since the detonation is more unstable.

Immediately downstream of the interface, the cellular pattern corresponds to that of the upstream mixture. However, in the relaxation zone the detonation mach stems strengthen and the larger, more irregular cells develop. As in the previous case, the detonation adjustment to the change appears gradual. Additionally, the relaxation length is about 150 times $l_{1/2}$ as before. Re-scaling this in terms of the downstream mixture, it corresponds to 60 times $l_{1/2,1}$.

As the downstream mixture is made more unstable, either through increased E_{a} or increased $\Delta\rho$, there is a change in the relaxation process dynamics and an accompanying increase in relaxation length. Figure 4 shows the numerical soot foil for a greater density increase $\Delta\rho = 0.5$. The upstream thermodynamic conditions are the same as the previous cases (figure 2 and 3) and hence so is the cellular pattern. However, now the downstream $E_{\mathrm{a,e}} = 30$ and therefore the downstream cells are larger and more irregular.

In the relaxation zone, the detonation wave front weakens and the cells grow larger as transverse waves decay and triple points disappear. Afterward, the wave front abruptly becomes stronger with more intense triple point collisions at the beginning of the cell cycle. Finally, new triple points develop, forming smaller cells within the stronger, larger cells, creating the downstream cellular pattern superimposed on these larger cells. The relaxation process has begun to transition from the gradual process before to a more violent one. Additionally, the relaxation length has approximately doubled and is now about 300 times $l_{1/2}$. Interestingly, if this is re-scaled it corresponds to about 60 times $l_{1/2,1}$ as before.

Finally, in figure 5 the numerical soot foil for a larger activation energy (with the same $\Delta\rho$) is given. Comparing to figure 4, the higher activation energy implies higher temperature sensitivity and thus a more unstable mixture and more irregular cellular pattern. In this case, the downstream $E_{\mathrm{a,e}} = 36$.

Referring to figure 5, after the interface the detonation wave is weakened so dramatically that it is extinguished. It is then re-initiated via localized explosions (for example near the top edge of the domain at around $x = 300$). These form overdriven waves with very fine cellular structure. In this case the relaxation cannot be considered a gradual process. Furthermore, the triple point collisions that are coincident with the interface seem to lead to the re-initiation points downstream. The relaxation length has again increased, however it is not converged and with higher resolution the relaxation process is lengthened. This is likely due to decreased numerical diffusion associated with higher resolution, which would overall hinder the detonation formation [5].

Further increase in activation energy downstream continues to increase the relaxation length. This

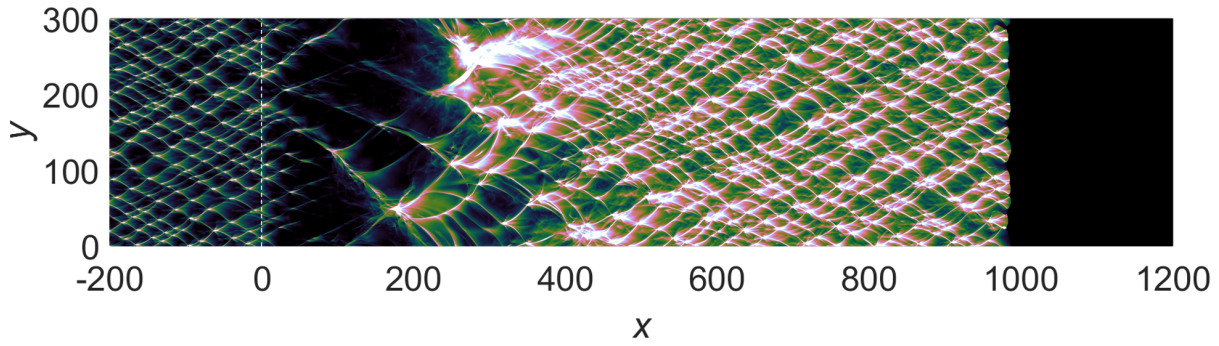

Figure 5: Numerical soot foil for the case with $E_{\mathrm{a}} = 24$ and density increase $\Delta\rho = 0.5$ across the interface (upstream $E_{\mathrm{a,e}} = 24$ and downstream $E_{\mathrm{a,e}} = 36$).

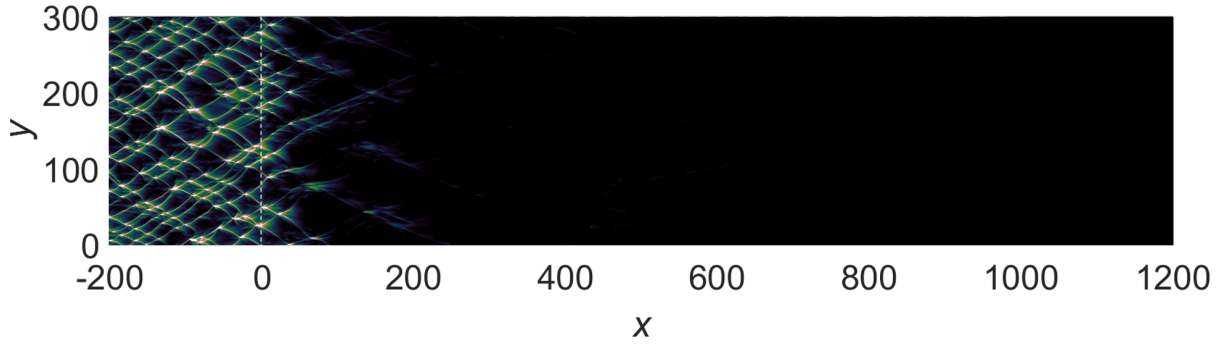

Figure 6: Numerical soot foil for the case with $E_{\mathrm{a}} = 27$ and density increase $\Delta\rho = 0.5$ across the interface (upstream $E_{\mathrm{a,e}} = 27$ and downstream $E_{\mathrm{a,e}} = 40.5$).

reaches a point which is effectively physically impossible, i.e., with a model containing losses and an auto-ignition limit the detonation would not be reformed and a critical limit could be captured. The soot foil for the case where $E_{\mathrm{a}} = 27$ and $\Delta\rho = 0.5$ is given in figure 6. The downstream $E_{\mathrm{a,e}} = 40.5$ and the detonation has not yet re-initiated in the frame length shown.

3.3 Comparison between one and two-dimensional results

The present results were compared with corresponding one-dimensional results previously obtained [1]. For low upstream and downstream activation energy the one-dimensional and two-dimensional results were found to agree well. To illustrate this, the case considered in section 3.1 is presented. The 2D flow field was reduced to an average 1D flow field by by averaging across the vertical y-axis. In figure 7 this average shock pressure is plotted as a function of shock location (blue line). The corresponding one-dimensional shock pressure history is superimposed (black line). The interface is at $x = 0$.

The shock pressure of the 2D simulation approaches a quasi-steady-state downstream that agrees with the shock pressure of the transmitted detonation in 1D. Note that although the downstream detonation has reached an average steady state near to the CJ velocity, it could still be undergoing some transient relaxation. However, comparing to the corresponding soot foil of figure 2, and soot foils later in the

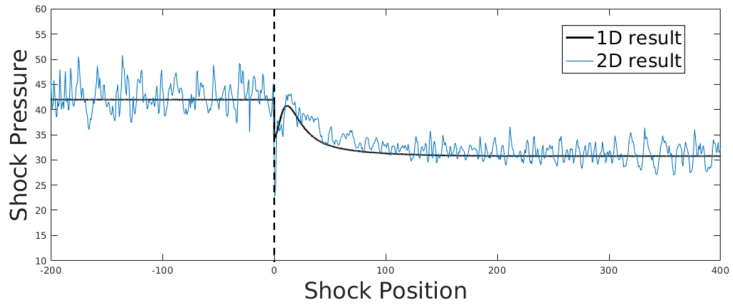

Figure 7: One-dimensional and averaged two-dimensional shock pressure history for $E_{\mathrm{a}} = 20$ and density decrease $\Delta\rho = 0.3$ (upstream $E_{\mathrm{a,e}} = 20$ and downstream $E_{\mathrm{a,e}} = 14$).

process, the detonation cellular structure has also reached a steady state. As was estimated from the soot foil, the relaxation length is approximately 150 unit lengths (or 150 $l_{1/2}$ and 380 $l_{1/2,1}$) for 1D and 2D.

4 Concluding Remarks

The interaction of a two-dimensional cellular detonation wave with a density and temperature discontinuity has been investigated via numerical simulations. The relaxation process is found to depend mostly on the downstream thermodynamic condition, quantified as the downstream effective activation energy, $E_{\mathrm{a,e}}$. For a density decrease, $E_{\mathrm{a,e}}$ is smaller downstream, the cells are smaller and more regular and the detonation is more stable. For a density increase, $E_{\mathrm{a,e}}$ is larger downstream, the cells are larger and more irregular and the detonation is less stable.

For low downstream $E_{\mathrm{a,e}}$, such as a density decrease or small density increase, the relaxation process is smooth and the relaxation length is approximately constant. It agrees with the one-dimensional results, indicating less dependence on the multidimensional cellular structure for such stable cases. However, as $E_{\mathrm{a,e}}$ is increased, changes in the relaxation process become apparent. There is a transition to a case where the detonation fails downstream and localized explosions cause re-initiation. The relaxation length increases dramatically. Dependence on multidimensional cellular effects and resolution is apparent.

References

[1] Tang Yuk KC, Mi XC, Lee JHS, Ng HD. (2018). Shock Waves 28: 967-979.

[2] Radulescu MI, Sharpe GJ, Law CK, Lee JHS. (2007). The hydrodynamic structure of unstable cellular detonations. Journal of Fluid Mechanics 580: 31-81.

[3] Ng HD, Zhang F. (2012) Detonation instability. In: Shock Wave Science and Technology Reference Library (ed. F. Zhang), Volume 6: 107212. Springer.

[4] Toro EF. (1999) Riemann Solvers and Numerical Methods for Fluid Dynamics. Springer-Verlag, Berlin

[5] Radulescu, MI. (2018). A detonation paradox: Why inviscid detonation simulations predict the incorrect trend for the role of instability in gaseous cellular detonations?. Combustion and Flame, 195:151-162.