Influence of the Reaction-to-Induction Length Ratio on the Stability of Cellular Detonations

Bijan Borzou, Brian Maxwell, Matei I. Radulescu
University of Ottawa
Ottawa, Ontario, Canada

1 Introduction

Detonations are self-sustained supersonic reaction waves. The structure of the wave is typically unstable to both longitudinal and transverse perturbations, yielding a characteristic cellular structure [1]. This instability is believed to be due to the sensitivity of the reaction rates to the shock state, manifested by the global activation energy of the induction zone. Indeed, most previous studies used the one-step reaction model to account for the loss of instability of detonations and the non-linear dynamics of the wave.

The one step model is however well known to have severe limitations. By modifying the activation energy, changes in both the induction and the main reaction zone structure occur simultaneously. For very high activation energy cases, an induction zone is present while the reaction zone is thin. On the other hand, for moderate activation energies comparable to those of real mixtures, the reaction zone becomes anomalously long and distributed, while the characteristic thermally neutral induction zone of real mixtures can no longer be reproduced. The behavior of the one-step model thus fails to capture the ZND structure of real detonations.

A number of studies have recently shown that the stability of the ZND structure of detonations is profoundly affected by the size of the main reaction zone length, compared with the induction zone length. Physically, this is expected, as the time scale over which energy is deposited will evidently have a profound influence on the gasdynamic waves generate by the rapid energy deposition, hence expecting more instability with rapid energy release rates in the main reaction layer. Short and Sharpe [2] first demonstrated analytically and numerically the influence of the ratio of induction to reaction zone thickness on the stability of one-dimensional detonations. They used a very simple reaction model of two sequential reactions, one thermally neutral for the induction phase, followed by a state independent exothermic reaction. Using this model, they were able to show that the parameter controlling the instability of one-dimensional pulsating detonations is the product of the activation energy of the induction zone and the ratio of induction to reaction zone length.

$$\chi = \frac{E_a}{RT_s}\frac{\Delta_{ind}}{\Delta_{reac}} \tag{1.1}$$

Further studies by Ng et al. [3] and Leung et al. [4] have further clarified the physical mechanisms by which small reaction zone layers affect one-dimensional detonations, using variations of the same simple two-step model. Experimentally, Radulescu was the first to note that the χ parameter given above correlates very well with the cellular structure regularity of detonations, with irregular detonations typically observed for $\chi > 10$ [5]. The interpretation given to the χ parameter leading to stability in a multi-dimensional detonation is the requirement for coherence of neighbouring power pulses during ignition events, which are promoted for low activation energies and relatively long main reaction zones compared to the induction zone [5]. This was found to be equivalent to the Soloukhin and Oppenheim criterion for strong ignition [5, 6]. Further studies by Liang et al. have also confirmed that the χ parameter correlates well with experimental observations of irregular detonations, in that mixtures with large values of χ yield irregular detonations[7].

The present study extends the previous work on detonation stability using the simple two-step model [2-4] to multiple dimensions. We thus want to verify how χ affects the stability of cellular detonations. The simplicity of the two-step model of Short and Sharpe [2] makes this investigation quite straightforward, as the length, or duration of the main reaction layer can be systematically varied while all other parameters are kept constant, which permits to isolate the effect of the reaction zone on stability.

2 The 2-step model

The two-step chain branching model used by Short and Sharp [2] and Leung et al. [4] has been adapted for this study. It consists of a thermally neutral induction zone whose duration is controlled by an Arrhenius expression. This induction zone is followed by a temperature independent reaction zone. The two-step model offers independent control of the induction and reaction zones. If λ_i denotes a progress variable for the induction zone, with a value of 1 in reactants and 0 at the end of the induction zone, the evolution of this progress variable is given by

$$\frac{D\lambda_i}{Dt} = -K_i H(\lambda_i)\exp\left(-\frac{\tilde{E}_a}{\tilde{R}\tilde{T}_s}\right) \tag{1.2}$$

where K_i is a rate constant and $H(\alpha)$ is a Heaviside function which turns off the progress of λ_i at the end of the induction zone. Immediately following the induction zone is the exothermic reaction zone which proceeds independently of temperature. The evolution of the progress variable is λ_r, which is 0 in the induction zone and 1 in the burned products, is assumed to take the form

$$\frac{D\lambda_r}{Dt} = (1 - H(\lambda_i))\ K_r(1-\lambda_r)^{\nu}$$

where ν denotes the reaction order.

It is straightforward (see Ref. [4]) to show that the χ parameter defined in equation (1.1) yields

$$\chi = \frac{\gamma - 1}{\gamma} t_i K_r E_a Q \tag{1.3}$$

where t_{i} is the non-dimensional induction time, given in our scales [4] by

$$t_{\mathrm{i}} = \sqrt{\frac{2\gamma M_{CJ}^2 - (\gamma - 1)}{\gamma\left((\gamma-1)M_{CJ}^2 + 2\right)}} \tag{1.4}$$

The heat release and activation energy are given by $Q = \tilde{Q} / \tilde{R}\tilde{T}_s$ and $E_a = \tilde{E}_a / \tilde{R}\tilde{T}_s$ where $\tilde{T}_s$ is the shock temperature and the detonation Mach number is given by

$$M_{CJ} = \sqrt{-\frac{-\gamma(\gamma+1)+Q(\gamma-1)(1+(\gamma-6)\gamma)+\sqrt{Q(\gamma-1)(\gamma+1)^3\left(2\gamma+Q(\gamma^2-1)\right)}}{\gamma\left(1-4Q(\gamma-1)^2+\gamma\right)}} \quad (1.5)$$

In the present study, we take $Q = 10.3875$, $E_a = 5$, $\gamma = 1.2$, $\nu = 1/2$ and vary only K_r, which controls the duration and length of the main reaction zone layer. For reference, the value of $K_r = 0.36$, yielding $\chi = 8.7$, corresponds to the neutral stability of one-dimensional pulsating detonations[4]. Figure 1 shows the influence of the reaction rate parameter on the ZND pressure profiles for various values of K_r. As can be seen, since the induction rate parameter is kept constant, the induction zone thickness is the same for all three cases but the reaction zone thickness is larger for small values of the reaction rate parameter K_r.

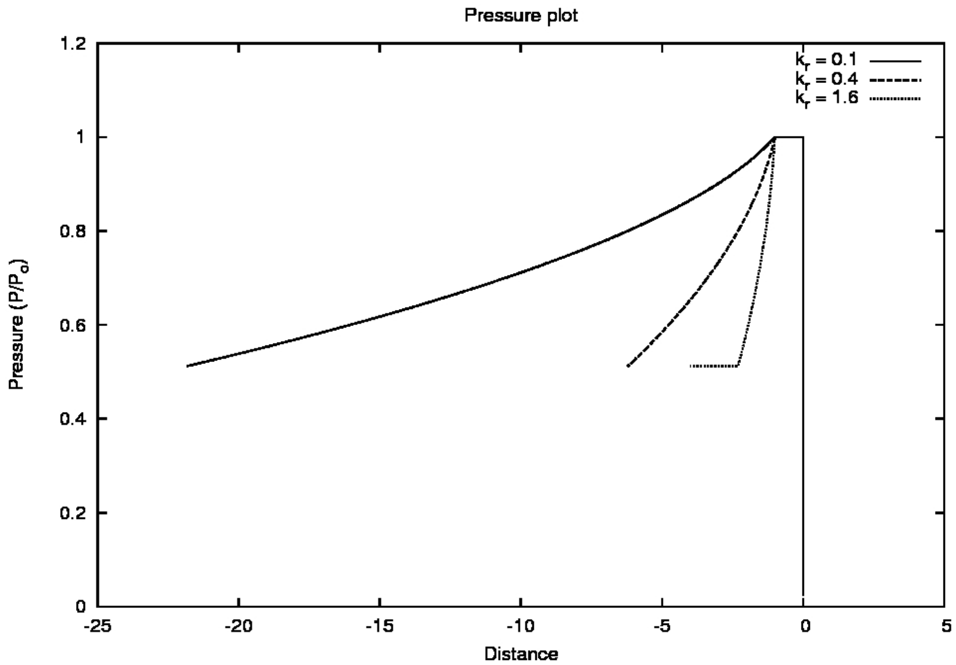

Figure 1. ZND pressure profiles for different reaction rate parameter values.

3 Numerical Implementation

The detonation dynamics were computed numerically by solving the reactive Euler equations coupled with the two step model using the AMRITA computational facility developed by J.J. Quirk[8]. A Roe solver was used to evaluate the fluxes in the Euler equations. To initialize the simulations, the ZND profile was imposed onto the domain. The detonation propagates across the fixed domain, where the non reacted material ahead of the detonation wave is stationary. The rear boundary was prescribed at the CJ condition. The length and width of the computational area have been taken as 1000 and 25 induction lengths respectively. The resolution covering the reaction zone structure was 32 grid points per induction length.

Figure 2 shows the path of the triple shock interactions (triple points) on the detonation front which propagated from left to right for K_r = 0.4. These trajectories were obtained by recording the maximum vorticity, which illustrates the time history of the detonation cellular structure. The evolution of the wave structure illustrates the relation between the multi-scale complex cellular dynamics and the reactive compressible gas dynamics phenomena occurring in the reaction zone at much smaller length scales.

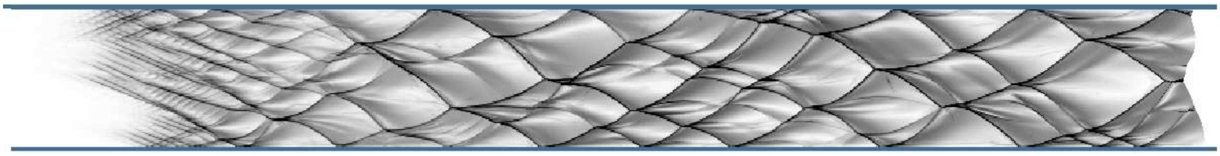

Figure 2. Detonation zone's cellular structure for $K_r = 0.4$.

Triple points, shock waves and slip lines can be clearly identified in the density gradient fields (numerical Schlieren picture) shown in Figure 3 at a specific time for the same value of $K_r = 0.4$.

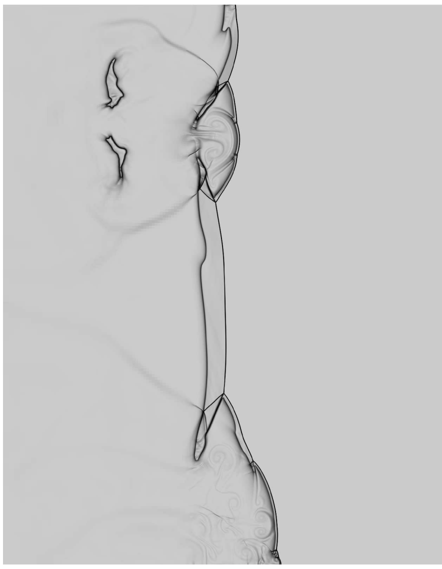

Figure 3. Density gradient field (numerical schlieren image) for a sequence of time for $K_r = 0.4$.

These complex wave dynamics give rise to continuous merging and re-generation of new modes on the surface of the detonation waves. The merging of transverse waves of the same family reinforces their strength and results in larger cells. Following transverse wave collisions, new modes arise from disturbances originating from the shock/jet interactions, producing new smaller cells.

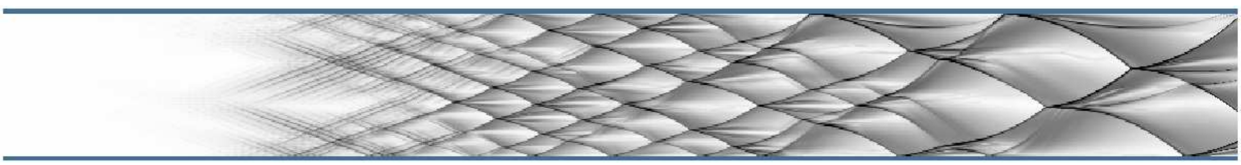

Figure 4. Detonation zone's cellular structure for $K_r = 0.1$.

Figures 4 and 5 respectively show the cellular structure for $K_r = 0.1$ and 1.6, while activation energy, heat release and induction rate parameter have been kept constant compared to above results. As can be seen, for $K_r = 0.1$, cells are very large and quite regular, while for $K_r = 1.6$, they are smaller and less regular. Therefore, decreasing the reaction zone thickness leads to an increase of instability.

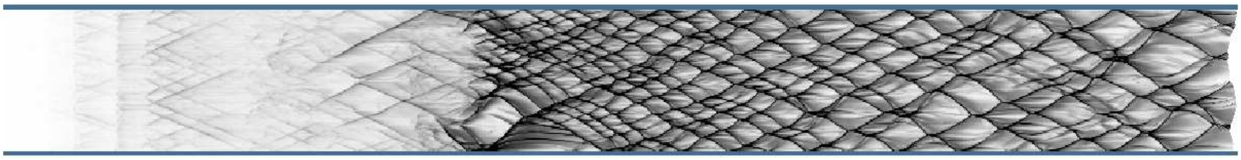

Figure 5. Detonation zone's cellular structure for K_r = 1.6.

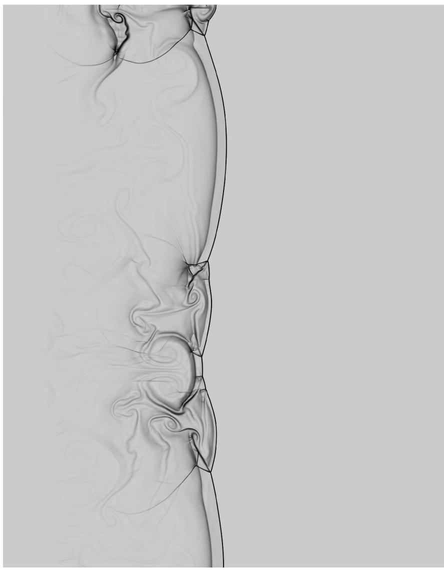

Figure 6. Density gradient field (numerical schlieren image) for a sequence of time for K_r = 0.1.

The same observations can be drawn from the reaction zones shown in Figures 6 and 7. Again, increasing the reaction rate constant and therefore decreasing the reaction zone thickness, the number of triple points is increased and the structure appears to have a more irregular dynamics with the appearance and disappearance of cells.

It is interesting to also compare the values of the stability parameter χ, which takes the values of 2.4, 9.4 and 38 for respectively $K_r = 0.1, 0.4$ and 1.6. The irregularity thus appears at approximately $\chi \approx 10$, in good agreement with previous observations of cellular detonations [5] and the neutral stability boundary of pulsating one-dimensional detonations [4].

3 Concluding Remarks

The effect of the thickness of the main reaction layer, compared with the induction layer non-linear two-dimensional detonation instability, on the cellular structure stability was studied through numerical simulations. This study was facilitated by the simplicity of the two-step model. The results showed that thin reaction zones have a destabilizing effect, yielding smaller, more irregular cells. Therefore, as proposed in previous one-dimensional studies and previous empirical correlations, the degree of stability of two-dimensional detonation structure correlates well with the main reaction zone thickness. The loss of stability also agrees qualitatively with the $\chi > 10$ experimental criterion[5]. This limit also correlates well the stability boundary of one-dimensional pulsating detonations.

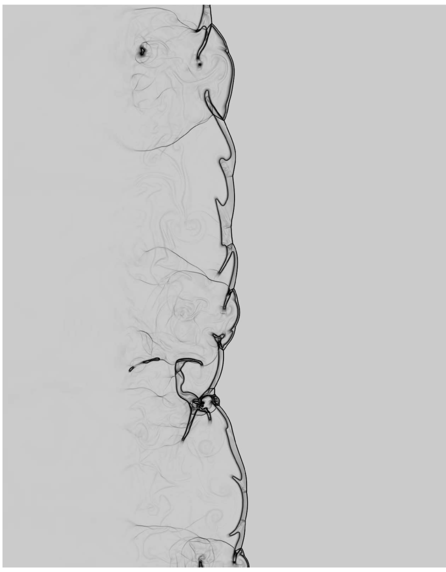

Figure 7. Density gradient field (numerical schlieren image) for a sequence of time for $K_r = 1.6$

Acknowledgements

This work was supported by the H2CAN NSERC Strategic Network.

References

[1] J. H. S. Lee, *The detonation phenomenon*. Cambridge University Press, 2008.

[2] M. Short and G. J. Sharpe, "Pulsating instability of detonations with a two-step chain-branching reactionmadel: theory and numerics," *Combustion Theory and Modelling,* vol. 7, pp. 401-416, Jun 2003.

[3] H. D. Ng, *et al.*, "Numerical investigation of the instability for one-dimensional Chapman-Jouguet detonations with chain-branching kinetics," *Combustion Theory and Modelling,* vol. 9, pp. 385-401, 2005.

[4] C. Leung, *et al.*, "Characteristics analysis of the one-dimensional pulsating dynamics of chain-branching detonations," *Physics of Fluids,* vol. 22, 2010.

[5] M. I. Radulescu, "The propagation and failure mechanism of gaseous detonations: experiments in porous-walled tubes," Ph.D. Thesis, McGill University, Montreal 2003.

[6] J. W. Meyer and A. K. Oppenheim, "On the shock-induced ignition of explosive gases," presented at the 13th Symposium (International) on Combustion, 1971.

[7] Z. Liang, *et al.*, "Detonation front structure and the competition for radicals," *Proceedings of the Combustion Institute,* vol. 31, pp. 2445-2453, 2007.

[8] J. J. Quirk, "Amrita — A computational facility for CFD modelling," in *29th Computational Fluid Dynamics VKI Lecture Series, von Karman Institute.*, H. Deconinck, Ed., 1998.