The Origin of Shock Bifurcations in Cellular Detonations

Matei I. Radulescu[1], Andrea Papi[2], James J. Quirk[3],

Philip Mach[1], Brian M. Maxwell[1]

[1]Department of Mechanical Engineering, University of Ottawa, K1N6N5, Canada

[2]Department of Aerospace Engineering, University of Rome “La Sapienza”, Italy

[3]Los Alamos, NM

1 Introduction

Recent numerical simulations of the structure of cellular detonations have revealed that shock bifurcations may be present on the front of detonations [1-3], accounting for part of the cellular sub-structure [1]. An example of such a wave bifurcation, first identified by Sharpe [2], is shown in Figure 1. The figure illustrates how the triple shock of a cellular detonation reflects on one of the walls and forms a new Mach shock with a distinctive kink (k). Such wave bifurcations have been identified in simulations using generic one-step models with parameters typical of unstable detonations [1-3]. However, recent simulations of hydrogen-oxygen-argon cellular structures did not show such phenomena [3-5]. At present, the origin and effect of such bifurcations on the reaction zone structure is unknown. The present study thus seeks to elucidate the origin of such bifurcations, the conditions for which they are present, and their effect on the structure of detonations.

The short transient involving the reflection of the triple point illustrated in Figure 1 depends primarily on the gasdynamic shock reflection problem driven by the sudden change in flow direction θ (see Figure 1) once the incident shock interacts with the wall (or a triple point of the opposite family). The problem is thus perfectly analogous to the reflection of a shock wave at a compressive corner in a reacting gas with a ramp angle θ. Analysis of the numerical results of Radulescu et al. [1] revealed that the leading shock's strength at the moment of collision is close to the CJ value. From their simulations, it was found that the flow deflection angle at the instant of collision of triple points was

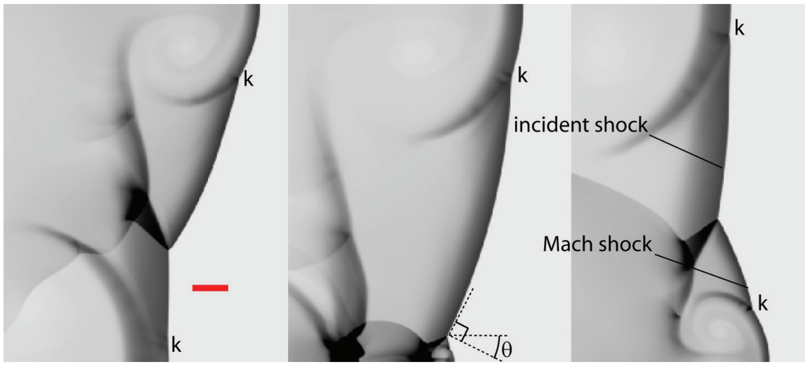

Figure 1. Triple shock reflection in a cellular detonation giving rise to wave bifurcations (*k*), from [1]; red marker marks the unit ZND half-reaction length $\Delta_{1/2}$

Correspondence to: matei@uottawa.ca

approximately θ = 34°±2. The problem that we thus set to solve is the reflection of a ZND wave on a compressive ramp of θ = 34°. The study of this well-defined problem thus permits us to use sufficiently high resolutions to temporally and spatially resolve the reaction zone structure formed immediately after triple point collisions in detonations, using well-defined reproducible initial and boundary conditions.

2 Numerical details

The governing reactive Euler equations are solved using the AMRITA environment developed by J. J. Quirk [6]. An idealized one step reaction and perfect gas behavior are assumed. The hydrodynamic solver uses Roe's method and the *minmod* limiter. The gas parameters studied are (γ=1.2, Q/RT_o=50, E_a/RT_o=27), a generic case investigated in detail in [1], from which Figure 1 was adapted. Adaptive gridding is chosen so that the maximum resolution is on the order 800 grid points per ZND half reaction length $\Delta_{1/2}$. The dynamic mesh refinement is chosen so that the finest grid always covers the entire detonation front (the reaction zones and regions where shocks exists). The solution is initiated by placing the ZND solution on the grid before the start of the ramp. The ramp is treated using the embedded boundary technique developed in Ref. 7 using the level-set method. Simulations of inert shock reflections were also performed using the same method.

3 The origin of shock bifurcations

At an early time after reflection, the reflection of a ZND detonation was found to agree very well with the reflection of an inert shock of the same strength over a ramp of the same angle. The good agreement was obtained when no appreciable reaction has taken place behind the Mach stem. An example of the resulting self-similar density profile obtained is shown in Figure 2 for the inert case and θ = 34°. A bifurcation is observed in all cases where a bifurcation was observed in the cellular detonations. It is thus remarkable that the structure of the shock reflection is not due to the exothermicity in the gas, but rather to the problem of shock reflection at triple point collisions before any reaction has taken place.

Figure 2. The self-similar density profile of an inert shock reflection with (γ =1.2, M = 6.22, θ = 34)

4 The shock bifurcation régime

The questions that arise are thus, "when do these wave bifurcations occur?", and "what role do they play at later times in detonations?", when chemical reactions occur in the gases processed by the different portions of the wave fronts of the bifurcated shocks. Surprisingly, the literature on shock bifurcations in inert shock reflections over a ramp is very limited [8]. Furthermore, to the best of our knowledge, experimental observations of such phenomena are still lacking. It appears that such wave bifurcations only appear in the régime of irregular shock reflections when the angle of the ramp is sufficiently large (but below the RR-IR reflection boundary), the specific heat ratio is sufficiently low, and the shock strength sufficiently high. We are in the course of determining the exact boundary using numerical simulations and the results will be communicated at the conference.

The bifurcations appear to require as a *necessary* (but not sufficient) condition the wall-jetting effect, recently studied in [9]. The transition from a jetting shock reflection to the appearance of the bifurcated shock is shown in Figure 3 for increasing ramp angles. At a deflection angle of θ = 10°, the slip line is diverted towards the Mach shock by a strong pressure gradient, creating a forward jet.

The jet, previously observed in all detonation simulations, rolls up into a vortex where layers of the gas shocked by the incident and reflected shocks alternate with layers of the gas shocked by the Mach shock. With an increase of the wall angle, the resulting jet is found to become stronger, and penetrates further towards the Mach shock, which becomes locally curved. Eventually, for a sufficiently high angle, the jet gives rise to a bifurcated Mach shock. It is found that the bifurcation introduces a new triple point, with its own transverse shock and slip line. After a sufficient time (or for sufficient resolution), the self-similar solutions develop Kelvin-Helmholtz instabilities and eventually become turbulent due to the entrainment of these coherent structures into the vortex.

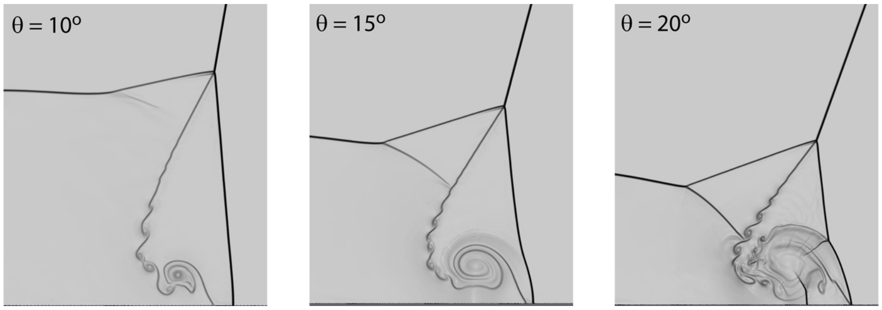

Figure 3. Schlieren profiles of inert shock reflection and the onset of shock bifurcation (γ =1.2, M = 6.22)

5 The effect of shock bifurcations on the structure of cellular detonations

We have further explored how these shock bifurcations affect the reaction zone structure at later times. Figure 4 shows the density and reaction progress variable fields at a time where the Mach shock traveled approximately 10 $\Delta_{1/2}$ along the ramp. Although the flow details obtained in the reflection problem are no longer directly indicative of the reaction zone structure of detonations at these late times, the results nevertheless give very useful information of the coupling of the exothermicity with the bifurcated shock structure. A close inspection of the results of Figure 4 shows clearly how the bifurcated shock structure affects the local reaction rates and the resulting reaction zone structure.

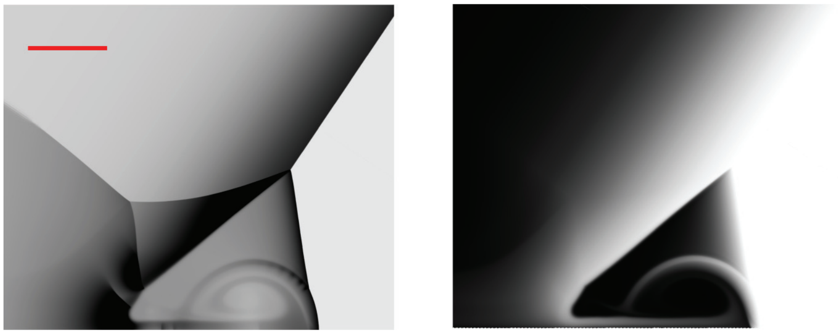

Figure 4 Density and reaction progress variable during the reflection of a ZND wave over a wall with θ = 34° at a time where the Mach shock traveled approximately $10\Delta_{1/2}$

It is seen that the gas ignites first behind the straight non-bifurcated segment of the Mach shock. The gas processed by the curved Mach shock reacts at a lower rate. For the conditions of the simulations, this stream of gas does not ignite behind the new transverse shock of the bifurcation, and extends as a thin curved tongue of unreacted gas. The third stream of gas, shocked by the incident and the two reflected shocks ignites with the longest delay, as determined in [1]. It is thus found that the presence of shock bifurcations gives rise to a supplementary front triple point and the resulting layer of unreacted material. This third entropy layer in the shocked gases has a reactivity intermediate to the other two, which prevail in the absence of shock bifurcations.

A shock polar analysis conducted in this regime, assuming the Mach front as an overdriven detonation and the other shocks as inert, has yielded very good agreement with numerics. The results will be communicated at the conference.

6 Concluding remarks

In conclusion, the present study determined that the shock bifurcations previously observed in some detonation simulations stem from inert shock reflection hydrodynamics occurring after the triple shock collisions. These bifurcations couple with the chemical reaction fields and give rise to finite strength secondary modes on the detonation structure. They are promoted for mixtures with lower specific heat ratios and larger shock strengths. This is compatible with the existing evidence, whereby these bifurcations have not been observed in mixtures with a high-γ and low exothermicity (such as mixtures diluted by a mono-atomic gas). It is important to note, however, that the present mechanism may not be the only responsible for cellular sub-structures. The amplification of acoustic perturbations in reactive flow, through the exponential dependence of the reaction rate on local conditions, cannot be ruled out. Future study should be devoted at determining the growth rates of perturbations in both mechanisms. Furthermore, the present bifurcations, and their own hydrodynamic instabilities illustrated above, could provide the seed of the instability and couple with the exothermicity in the gas in highly unstable cellular detonations.

Acknowledgements

We wish to thank the financial support of NSERC.

References

[1] Radulescu MI et al. (2007). The hydrodynamic structure of unstable detonations. J. Fluid Mech. 580:31

[2] Sharpe GJ (2001). Transverse waves in numerical simulations of cellular detonations. J. Fluid Mech. 447:31.

[3] Deiterding R (2003). Parallel adaptive simulation of multi-dimensional detonation structures. PhD thesis, Brandenburgischen Technischen Universitat Cottbus.

[4] Hu XY et al. (2004). The cellular structure of a two-dimensional H2/O2/Ar detonation wave. Combust. Theory Modelling 8:339.

[5] Liang Z et al. (2007) Detonation front structure and the competition for radicals. Proc. Combust. Inst. 31:3445.

[6] Quirk JJ (1998) AMRITA: A Computational Facility (for CFD Modelling). In ``29th Computational Fluid Dynamics," von Karman Institute Lecture Series, edited by H. Deconinck (ISSN0377-8312).

[7] Xu S et al. (1997) High resolution numerical simulation of ideal and non-ideal compressible reacting flows with embedded internal boundaries. Combust. Theory Modelling 1:113.

[8] Collela P & Glaz HM (1985). Numerical calculation of complex shock reflections in gases. Ninth International Conference on Numerical Methods in Fluid Dynamics, Lecture Notes in Physics, Vol. 218, Springer (ISSN 1616-6361).

[9] Henderson LF et al. (2003) The wall-jetting effect in Mach reflection: theoretical consideration and numerical investigation. J. Fluid Mech. 479:259.