Mach Reflection during the Oblique Interaction of a Condensed-Phase Explosive Detonation Reaction Zone with a Rigid Wedge

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1 Introduction

The equation-of-state (EOS) and reaction-zone (RZ) models used for gas-phase and condensed-phase explosives are substantially different. The EOSs used for condensed-phase explosives are much stiffer and the mass densities are much larger than those of gaseous explosives. Also, the power delivered by condensed-phase explosives is orders of magnitude greater than what a gas-phase explosive can deliver. Additionally, the reaction rates used to model condensed-phase explosives are often taken to be weakly pressure dependent, while those used for gaseous explosives are taken to be highly temperature dependent. All this taken together along with the fact that pressure decreases while temperature increases through the RZ, leads to the reaction rate being greatest near the shock front for condensed-phase explosive while it is greatest near the end of the RZ for gas-phase explosives. These differences lead to the hydrodynamic structures resulting from the RZ models used for these two classes of explosives being different. Because of the high pressures generated by condensed-phase explosives, any material confinement is deformed in multidimensional configurations, and due to the stiffness of their EOSs, the detonation shock is relatively smooth but broadly curved, with shock curvature being measured in distances of many Zeldovich-von Neumann-Doring (ZND) RZ lengths. In similar multidimensional configurations, the detonation shock in gaseous explosives is rough when measured on the RZ length scale, with the lead shock being flat on average.

These observations are consistent with the results of hydrodynamic stability theory for the ZND steady-state RZs for condensed-phase and gas-phase explosives. Using model parameters for gas-phase explosives that are representative of those for real gaseous explosives, the ZND RZ is unstable to longitudinal (galloping) instabilities in 1D and to transverse instabilities for a broad range of transverse wave numbers, even when the Arrhenius reaction rate's state sensitivity is unrealistically low [1]. High-resolution, direct numerical simulations confirm these findings and show the development of a complex pattern of transversely traveling Mach stem structures moving along the lead shock [2]. More recent work detailing the hydrodynamic stability of detonations with condensed-phase explosive RZ models [3] shows longitudinal instability only occurs for unrealistically large, reaction rate pressure exponents, n, with $n > 6$, while detonation is totally stable to transverse disturbances unless $n > 2$ for the simplest and $n > 3$ for a more realistic condensed-phase models. Since typical values for the reaction-rate pressure exponents have $n \le 2$, then theory argues that the

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multidimensional RZ will be stable for condensed-phase explosive models. High-resolution simulations confirm the results obtained with detonation stability theory [4] and show smooth, multidimensional detonation shocks for the problem of detonation diffraction [5].

When linearized stability theory reveals a multidimensional transverse instability, this is realized as a traveling Mach-stem configuration that supports detonation combustion in the RZ. Although this problem has been well studied for gas-phase explosives, the phenomenon of Mach reflection in the detonation RZ has remained largely unexamined for condensed-phase explosives. Multidimensional experiments performed on liquid nitromethane, which is presumed to have a highly temperature-dependent reaction rate, do show a small number of prominent Mach wave features on the lead detonation shock [6]. In this paper we explore the problem of the oblique interaction of the detonation RZ for a condensed-phase explosive with a rigid wedge, as displayed in Fig. 1.

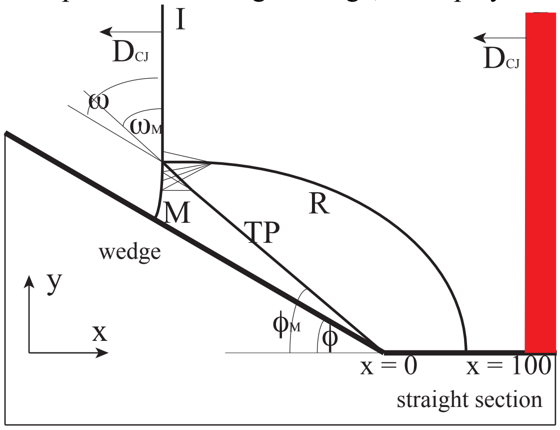

Figure 1. A rigid wedge is used to generate an oblique interaction of detonation with the wall (the case with $\phi = 30^o$ is displayed). The shock/detonation moves to the left. For the inert shock examples, the vN state, corresponding to a CJ detonation, is maintained with a piston at the right boundary. For the resolved RZ examples, the CJ state is maintained at the right boundary.

2 The Shock Polar Theory Description of Mach Reflection

We study two condensed-phase explosive detonation RZ models: 1) the Aslam-Bdzil-Stewart (ABS) model and 2) the Ignition-and-Growth (IG) model. The Mach number of the detonation shock is essentially infinite for the ABS model while it has an $O(1)$ value for the IG model. The ABS model uses the same EOS for reactants and products, for which the scaled specific volume is $V = \rho_0/\rho$ and the specific internal energy is [7]

$$E(Mbar\cdot\frac{cc}{cc}) = \frac{PV}{(\gamma-1)} - q\cdot\lambda\,, \tag{1}$$

and where q is the heat of detonation and λ is the reaction progress variable. The IG model uses separate EOSs for reactants and product phases, with the mixture EOS obtained assuming ideal mixing and pressure and temperature equilibrium between the phases. The specific internal energy for each phase, labeled with the subscript i is given by [8]

$$E_i(Mbar\cdot\frac{cc}{cc}) = E_{0i} + \frac{PV_i}{\Gamma_i} - A_i\left(\frac{V_i}{\Gamma_i} - \frac{1}{R_{1i}}\right)\exp(-R_{1i}V_i) - B_i\left(\frac{V_i}{\Gamma_i} - \frac{1}{R_{2i}}\right)\exp(-R_{2i}V_i)\,. \tag{2}$$

Significant among the differences between these two forms is that as $P \to 0$, Eq. (1) yields a zero sound speed while Eq. (2) yields an $O(1)$ sound speed in the upstream state. These EOS differences lead to differences in the predictions of shock polar theory for the reflected shock coming from the interaction of the incident detonation shock with the wedge. [Shock polar theory predicts the reflected shock pressure, P_2, vs. the streamline turning angle, Θ_2, as a function of the angle of the rigid wedge, ϕ.] Displayed below are the shock polar theory predictions for Mach reflection when the wedge angle is small. These calculations use only the EOS for the unreacted explosive.

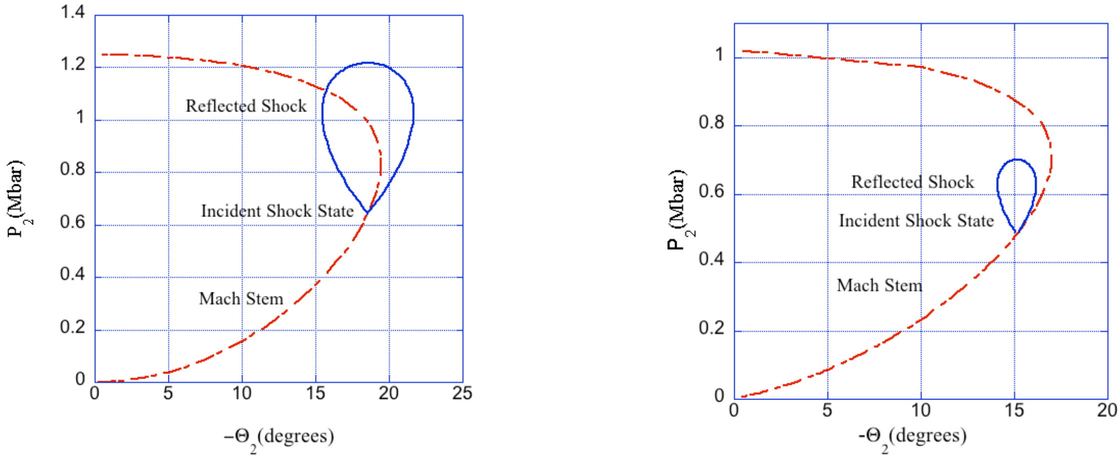

Figure 2. The ABS model, displayed on the left for a wedge angle of $\phi = 30^o$ is consistent with classical Mach reflection existing down to very small wedge angles (to near zero). The IG model, displayed on the right for a wedge angle of $\phi = 30^o$ shows that classical Mach reflection is not possible for wedge angles below $\phi \leq 40^o$.

Direct numerical simulation (DNS) for the two cases displayed in Fig. 2 reveal the differences predicted by shock polar theory. The simulated Mach-stem pressure for the ABS model agrees with the predictions of shock-polar theory displayed in Fig. 2. This comparison of the ABS and IG models reveals the sensitivity of Mach reflection to the shock Mach number.

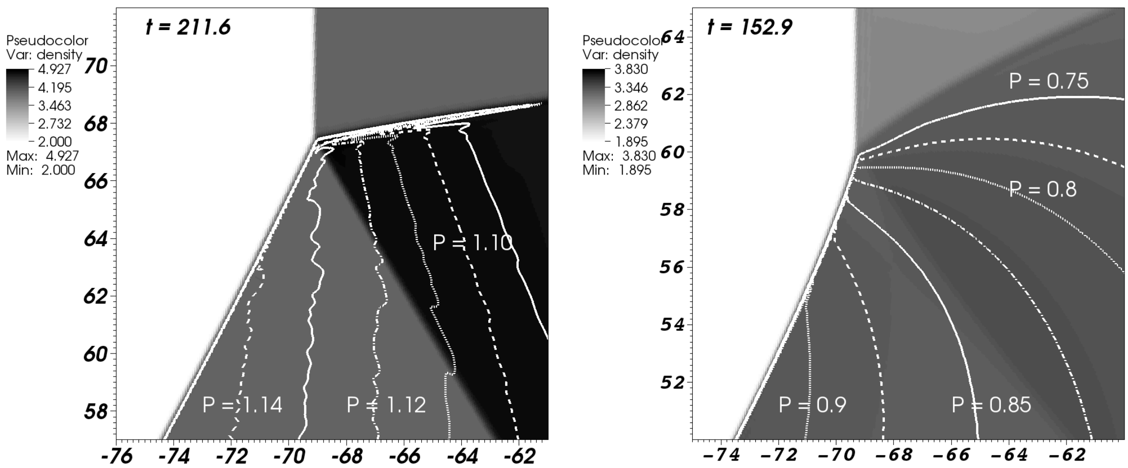

Figure 3. The density palette and pressure contour plots obtained with DNS for the non-reactive models. The DNS for the ABS model, displayed on the left for a wedge angle of $\phi = 30^o$, shows very little variation of pressure and a nearly straight Mach-stem shock (the feature in the lower left of the subfigure). The simulated Mach-stem pressure agrees with the shock polar predictions in Fig. 2. The DNS for the IG model, displayed on the right for a wedge angle of $\phi = 30^o$, shows the pressure varies along what appears as a curved Mach shock. The slip line is a very fuzzy feature near the shock interaction point for the IG model case, suggesting a non-classical von Neumann-like reflection [9].

3 Resolved Reaction Zone Simulations of Mach Reflection

Shock-polar theory combines the scale-free simple waves that can exist in the unreacted explosive into the solution of the problem of streamline turning and shock reflection. An explosives heat-release rate also makes a contribution to streamline turning. No simple theory is available to describe this scale-dependent problem of Mach reflection for a resolved RZ detonation. Here we use DNS to show how the explosives' resolved RZ affects Mach reflection. The resolved RZ simulations use the rate law

$$rate = k \cdot H\left(\rho/\rho_o - 1.25 \right) \cdot \left| \rho/\rho_o - 1.25 \right|^n \cdot (1-\lambda)^\nu , \tag{3}$$

where $H(\ )$ is the Heaviside function and ν, n, k are parameters. Here we specialize to the ABS model and set $\nu = 1$, $n = 1$ and $k = 1.6487/\mu s$, which yields ZND 50% and 90% completion RZ lengths of $x_{\lambda=0.5} = 0.45cm$ and $x_{\lambda=0.9} = 2.05cm$. We explore other models and parameter values more fully in the paper.

The results for the unreacted explosive DNS are displayed in Fig. 4, while the results for the resolved RZ DNS are displayed in Fig. 5. In both Figs. 4 and 5, the result on the left corresponds to a wedge angle of $\phi = 30^o$ while those on the right correspond to $\phi = 15^o$.

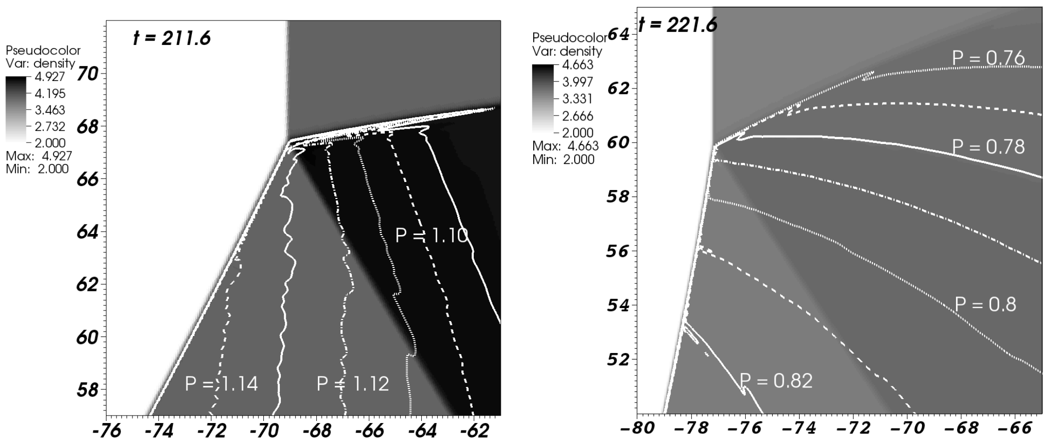

Figure 4. DNS results for the unreacted case. $\phi = 30^o$ is on the left and $\phi = 15^o$ is on the right.

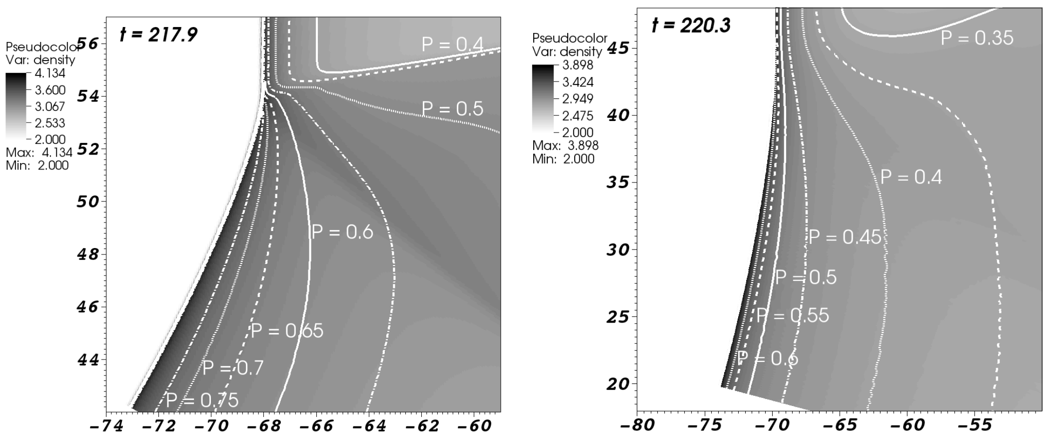

Figure 5. DNS results for the resolved RZ case. $\phi = 30^o$ is on the left and $\phi = 15^o$ is on the right.

Comparing the results from the unreacted DNSs displayed in Fig. 4 with the corresponding resolved RZ DNSs displayed in Fig. 5, we see that the slip line for the $\phi = 30^o$ resolved RZ case has essentially disappeared near the lead shock when compared with the very prominent slip line for the unreacted example. The lead Mach-stem shock is curved and smoothly blends with the lead incident shock. For the $\phi = 15^o$ resolved RZ case, there is neither a reflected shock nor a slip line evident in the RZ. Other than the lead shock, there are no discontinuities of any kind that are visible.

The results for the resolved RZ DNSs for the cases $\phi = 30^o$ and $\phi = 15^o$ show the strong influence the resolved heat-release rate has on streamline turning. Compared with the unreacted cases, where reflected shocks and streamlines are needed to turn the flow, in the resolved RZ cases, neither reflected shocks nor slip lines are needed to turn the flow. As one moves back in the flow and away from the RZ, both the reflected shock and slip line are seen to appear. The takeaway from these results is that for the EOSs and reaction rates used to model condensed-phase explosives, one observes that the RZ has a smoothing effect on the flow near the lead shock. So compared with gas-phase models where the reaction reinforces the reflected shock and slip lines when compared with the non-reactive cases, for condensed-phase explosives the resolved RZ has a strong smoothing effect on Mach reflection.

In the full paper, we describe how changing the parameters in the reaction-rate model affect the flow. Generally, we find that changes that move the heat-release towards the front of the RZ have a smoothing effect on Mach reflection.

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