The Hydrodynamic Origin of the Detonation Cell

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1 Introduction

A characteristic feature of a detonation wave is the cellular structure, i.e., the autonomous generation of locally overdriven detonation fronts, which subsequently decay and vanish with the birth of a new overdriven wave [1–5]. As will be shown, the overdriven regions are born from the localization of energy behind the nascent Mach stem, a necessary condition for detonation propagation. Energy bifurcation is exceedingly rare in nature, but marvelously the detonation wave can produce this structure from essentially homogeneous conditions, e.g., DDT in a tube [6]. Despite significant effort expended in modeling the kinematics of the detonation cell, the origin of the detonation cell (i.e. the mechanism of energy bifurcation) remains speculative [3, 5].

In the present study, we propose that the origin of the detonation cell is hydrodynamic in nature, arising from high-speed fluidic jetting behind the nascent Mach stem. We will show that chemical heat release alone is insufficient to produce the overdriven Mach stem. Instead, a virtual piston is required to provide mechanical work to drive the nascent Mach stem. We will demonstrate this mechanism through a theoretical analysis of overdriven shock waves and reacting flow simulations of cellular detonations. Simulation results reveal that a vortex pair (ring) behind the Mach stem is responsible for the energy bifurcation that produces the cellular structure. The vortex pair draws in burnt fluid from downstream of the Mach stem, and accelerates the fluid toward the Mach stem, producing the high-speed jet. This jet then stagnates behind the Mach stem, providing a virtual piston to drive the Mach stem. In fact, the observation of Mach stem bifurcations in cellular detonations, a consequence of the impingement of a high-speed jet on the Mach stem, alone confirms that hydrodynamic phenomena can alter the evolution of the overdriven Mach stem [7–10].

2 Numerical Methods

To complement the theoretical analysis, direct numerical simulations (DNS) of the compressible Navier-Stokes equations are performed using the massively parallel code `Athena-RFX` [11, 12], a reacting-flow extension of `Athena` [13]. Chemistry is modeled using the mechanism described in Ref. [10],

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consisting of a 13-species H_2 sub-model from FFCM-1 [14] and the Princeton ozone model [15]. For simulations, the detonation propagates into a quiescent mixture of $2H_2$-O_2-CO_2, with 9000 PPM of O_3 added to regulate the detonation. Quiescent pressure and temperature are 40 kPa and 300 K, respectively. Simulations were conducted on a uniform grid, and the detonation structure is resolved with 50 computational cells per induction length Δ_i. The computational domain is $200\Delta_i \times 10\Delta_i$. Both spanwise boundary conditions are symmetric. The upstream boundary is quiescent gas, and the downstream boundary imposes the CJ state. A grid recycling technique is employed to mitigate computational cost. Further details on the computational methods can be found in Ref. [10]. The domain is designed to produce a single-headed detonation that approximately matches the average cell width λ for the mixture [10]. The imposed symmetry allows us to isolate the essential components of the detonation structure. For ease of visualization, simulation results are tiled above and/or below the symmetry planes to show a full detonation cell.

3 The Virtual Piston Model

The subsequent discussion will present results for a stoichiometric mixture of hydrogen and oxygen, diluted with 25% carbon dioxide by mole. Ignition sensitivity is tuned by adding 9000 PPM of ozone. This mixture was selected specifically for its low ignition sensitivity ($\epsilon_i = 4.70$) and propensity for forward jetting ($\gamma = 1.27$). Preliminary results for different mixtures indicate the mechanisms outlined in the following sections can be generalized to all cellular detonations.

Figure 1(a) presents the instantaneous pressure field from simulation along the centerline of the detonation cell. Here, and throughout the study, the spatial coordinates are normalized by the detonation cell length ℓ. Superimposed over the pressure are streamlines computed from the instantaneous gas velocity in a frame traveling at the Mach stem speed D. Noteworthy is the existence of a stagnation streamline, drawn in red. To the Mach stem, the fluid enclosed by this streamline is indistinguishable from a solid body, e.g. a piston. It follows that we can then model the Mach stem as a shock driven by a piston. Figure 1(b) provides a schematic of this model. We treat the Mach stem as a cylindrically expanding shock wave propagating down a diverging duct at a speed $D(t)$, with a piston some discrete distance behind traveling at D_{piston}.

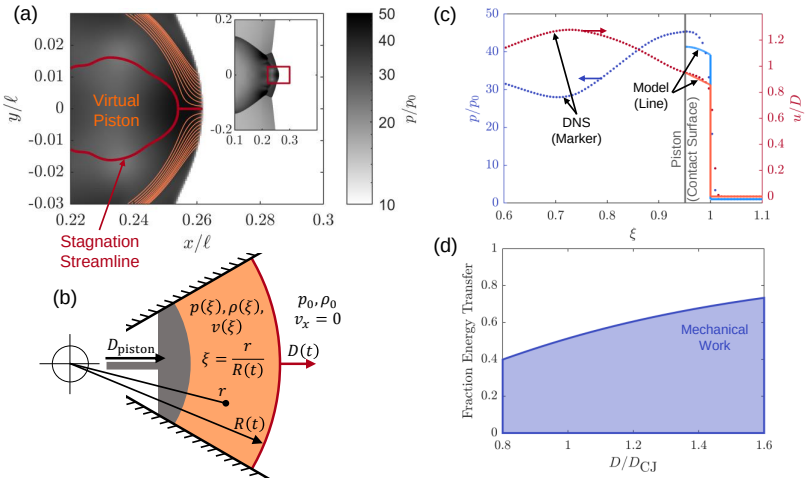

Figure 1: (a) Simulation results illustrating the existence of a stagnation streamline in a frame moving with the Mach stem. (b) Schematic of the simplified model showing the cylindrically expanding shock-wave driven by a piston. (c) Comparison of both pressure and gas velocity from the simplified model and simulation. (d) Fraction of energy tranfer into Mach stem by mechanical work done by piston.

3.1 A Similarity Solution for Diverging Piston Driven Shocks

To resolve the structure of the flow field between the shock and the piston, we derive a similarity solution to the Euler equations,

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial r} + \frac{j \rho u}{r} = 0, \tag{1}$$

$$\rho \frac{Du}{Dt} = -\frac{\partial p}{\partial r}, \tag{2}$$

$$\rho \frac{Dh_{\mathrm{T}}}{Dt} = \frac{\partial p}{\partial t}, \tag{3}$$

where r is the radial position of the shock and j indicates the coordinate system ($j = 0, 1, 2$ for planar, cylindrical, or spherical respectively) [16]. ρ, u, p are the gas density, velocity, and pressure respectively. The stagnation enthalpy is $h_{\mathrm{T}} = (\gamma/(\gamma-1))(p/\rho) - \lambda Q + u^2/2$ where γ is the ratio of specific heats, and Q is the heat of combustion. The progress variable λ is 0 in the quiescent mixture, and 1 in the burnt products.

To solve, we first assume the existence of a similarity variable $\xi = r/R(t)$, where $R(t) = \int_0^t D(\tau) d\tau$ is the location of the shock. We also assume the shock speed is given by some power law in time, such that $D(t) = At^a$. With these simplifications, a general set of governing differential equations is identified,

$$\tilde{\rho}' = \frac{\gamma j \tilde{\rho} \tilde{u} \tilde{p}}{\xi f (\gamma \tilde{p} - f^2 \tilde{\rho})} - \frac{(\gamma-1)\tilde{\rho}^2 \tilde{Q} \Lambda}{\xi f (\gamma \tilde{p} - f^2 \tilde{\rho})} - \frac{j \tilde{\rho} \tilde{u}}{\xi f}, \tag{4}$$

$$\tilde{u}' = -\frac{\gamma j \tilde{u} \tilde{p}}{\xi (\gamma \tilde{p} - f^2 \tilde{\rho})} + \frac{(\gamma-1) f \tilde{\rho} \tilde{Q} \Lambda}{\xi (\gamma \tilde{p} - f^2 \tilde{\rho})} - \frac{\alpha}{\xi} \tilde{u}, \tag{5}$$

$$\tilde{p}' = \frac{\gamma f j \tilde{\rho} \tilde{u} \tilde{p}}{\xi (\gamma \tilde{p} - f^2 \tilde{\rho})} - \frac{(\gamma-1) f^2 \tilde{\rho}^2 \tilde{Q} \Lambda}{\xi (\gamma \tilde{p} - f^2 \tilde{\rho})} - \frac{2\alpha}{\xi} \tilde{p}, \tag{6}$$

where primes indicate $d/d\xi$. Normalized pressure, gas velocity, and density are given by $\tilde{p} = p/\rho_0 D(t)^2$, $\tilde{u} = u/D(t)$, and $\tilde{\rho} = \rho/\rho_0$, respectively. ρ_0 is the quiescent gas density. The normalized heat of combustion is $\tilde{Q} = Q/D(t)^2$. The additional parameters are $\alpha = -a/(a+1)$, $\Lambda = \xi \lambda' + 2\alpha\lambda$, and $f = \tilde{u} - \xi$.

The parameter f is responsible for the existence of the piston. To this point, we have in no way imposed a piston onto the solution field. Instead, the parameter f naturally appears, which serves to indicate the location of the piston face (contact surface). It can be shown that a surface of constant ξ travels with a speed $\xi D(t)$. Clearly, when $f = 0$, the local gas velocity $u(\xi_{\text{piston}})$ matches the speed of the constant ξ_{piston} surface. A parametric study has shown that the solution contains a point where $f = 0$ for detonation relevant conditions, and thus the existence of a piston is a natural and necessary condition for the propagation of the Mach stem.

3.2 Decoupling Chemical Heat Release From Hydrodynamics

For the present study, we will consider the case of cylindrical shock and piston, thus $j = 1$. We will also decouple the effects of chemical heat release from the hydrodynamic structure behind the shock by treating the flow as inert, i.e. $\lambda = 0$ for all ξ. Finally, we will assume the change in shock speed can be neglected, such that $D(t)$ is a constant D. Thusly,

$$\tilde{p}' = \frac{\gamma f \tilde{\rho} \tilde{u} \tilde{p}}{\xi (\gamma \tilde{p} - f^2 \tilde{\rho})}, \tag{7}$$

$$\tilde{u}' = -\frac{\gamma\tilde{u}\tilde{p}}{\xi(\gamma\tilde{p} - f^2\tilde{\rho})}, \tag{8}$$

$$\tilde{\rho}' = \frac{\gamma\tilde{\rho}\tilde{u}\tilde{p}}{\xi f(\gamma\tilde{p} - f^2\tilde{\rho})} - \frac{\tilde{\rho}\tilde{u}}{\xi f}. \tag{9}$$

Figure 1(c) compares the results from the piston model based on Eqs. 7,8, and 9 for pressure and gas velocity, to the DNS results along the center of the Mach stem for an equivalent shock speed D. The model is evaluated from $\xi = 1$ to ξ_{piston}. Exceptionally good agreement in gas velocity is observed, and only a minor under-prediction of pressure is observed, arising from the treatment of the model as inert. Most critically, both the model and the simulation capture $dP/d\xi < 0$ and $du/d\xi < 0$ at the shock ($\xi = 1$). This is in direct contradiction to decaying Sednov blast waves, where the maximum in pressure and gas velocity is coincident with the lead shock. Clearly, the Mach stem is not a decaying blast, and is rather a diverging shock driven by a virtual piston.

3.3 Simple Thermodynamic Analysis of the Mach Stem

Finally, we will employ a simple thermodynamic analysis to demonstrate that the virtual piston, and not chemical reaction, is key to the formation of the nascent Mach stem. Drawing a control volume containing the shock and the compressed gas behind it, there exist four sources of energy transfer into the volume. The first two, internal energy transport from the quiescent gas and pressure work by the expansion of the control volume into the quiescent gas, are negligible for detonation relevant Mach numbers. The remaining two are mechanical work done by the piston on the control volume, and chemical heat release behind the lead shock. Mechanical work done by the pressure at the piston p_{piston} is computed as,

$$\dot{W}_{\text{piston}} = 4\pi D^3 t^2 \xi_{\text{piston}}^3 p_{\text{piston}}. \tag{10}$$

Similarly, the maximum energy transfer via chemical reaction is simply the product of the heat of combustion in mass units Q, and the rate of mass entrainment by the leading shock,

$$\dot{Q}_{\text{chem}} = 4\pi D^3 t^2 \rho_0 Q. \tag{11}$$

Neglecting the minor terms, the fraction of energy transfer by the piston is $\dot{W}_{\text{piston}}/(\dot{W}_{\text{piston}} + \dot{Q}_{\text{chem}})$, and is plotted in Fig. 1(d) for typical detonation overdrives. In the region of interest for the formation and early evolution of the Mach stem ($D/D_{\text{CJ}} \geq 1.4$), mechanical energy is the dominant energy source for the Mach stem. Therefore, this simplified thermodynamic analysis is sufficient to prove that the nascent Mach stem can only be produced by a virtual piston, and that chemical heat release alone cannot provide the energy necessary to generate the overdrives typical of detonations.

4 Origin of the Fluidic Jet

Finally, we will elucidate how the flow structure behind a nascent Mach stem produces the virtual piston, and the mechanism by which the jet provides directional, focused energy into the detonation front. Beginning with Fig. 2(a), the gas vorticity is superimposed with arrows showing the instantaneous velocity field in the frame attached to the lead shock. A vortex pair is apparent behind the Mach stem. In front of and behind this vortex pair, along the centerline of the Mach stem where $y/\ell = 0$, there exist two stagnation points. These flow features are shown schematically in Fig. 2(c), where blue or gray arrows indicate the path of a fluid element, and the red dashed lines indicate regions of high vorticity. The forward stagnation point is the virtual piston which serves to drive the Mach stem, located at the

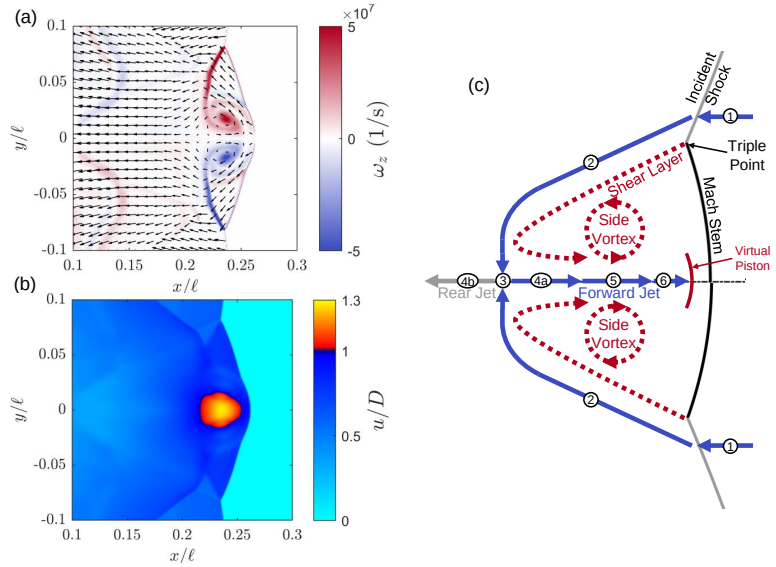

Figure 2: (a) Vorticity ω_z in color, superimposed with velocity vectors in the frame of the Mach stem. (b) False color plot of gas velocity u normalized by the Mach stem speed D. (c) Schematic of the jet/vortex structure which gives rise to the overdriven Mach stem.

front of arrow ⑥, and the rear stagnation point is shown as ③. The vortex pair (side vortex) are fed with vorticity originating at the triple points. The path ③→④a→⑤→⑥ lies between the two side vortices, and here we see the formation of a high speed fluidic jet at ⑤, where the local gas velocity typically exceeds the instantaneous Mach stem speed (see Fig. 2(b)). From ③ to ④a, the vortex pair draws in and compresses burnt fluid from behind the vortex pair. This fluid is accelerated to a maximum velocity at ⑤. This focused stream of high kinetic energy gas then impinges on the nascent Mach stem, producing the virtual piston which drives the lead shock. Clearly, the bifurcation of energy which produces the forward jet and the virtual piston is a consequence of hydrodynamics, particularly the formation of a vortex pair fed by vorticity originating at the triple points.

5 Concluding Remarks

In the present study, we demonstrated a hydrodynamic, high-speed jetting process that is responsible for the origin of the detonation cell. Starting with a simplified model of a piston-driven diverging shock, thermodynamic considerations suggested that chemical energy release alone is insufficient to drive the Mach stem. Instead, mechanical work originating from a virtual piston is essential to produce an overdriven Mach stem. A vortex pair, formed behind the nascent Mach stem and originating from the two triple points, serves to drive this virtual piston in the direction of detonation propagation. The virtual converging-diverging nozzle formed by the vortex pair serves to spatially bifurcate energy, focusing and delivering kinetic energy through high-speed jets into the Mach stem. This jet then impinges on the Mach stem, serving as the virtual piston providing the necessary mechanical energy.

6 Acknowledgements

The work was supported by the Air Force Office of Scientific Research (AFOSR) under Grants FA9550-18-1-0173 (XZ) and FA9550-20-1-0398 (HW) with Dr. Chiping Li as Program Manager, and the Office of Naval Research under Grant N00014-22-1-2606 with Dr. Steven Martens as Program Manager. The

computational resources are provided in part by the DoD High Performance Computing Modernization Program. The authors wish to thank Alexei Y. Poludenenko and Sai Sandeep Dammati for providing access to `Athena-RFX`.

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