Shock dynamics from quenched detonations: diffraction and gallop problems

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1 Introduction

In most reactive gases of practical interest, the rates of chemical reactions behind the lead shock front of detonation waves are exponentially dependent on temperature. When the lead front is exposed to sudden losses, the reaction process is often quenched, and the lead shock evolves as an inert shock. An example is the sudden diffraction of detonation waves at a corner. The reaction zone decouples from the lateral shock motion [1–3]. A similar situation appears in galloping detonations in narrow tubes [4]. Following a reformation of a detonation wave, the lateral losses to the tube walls do not permit the reaction zone to remain coupled. In the past, the dynamics of lead shocks have been modeled using point bast theory in a phenomenological manner, yielding relative success. At the other extreme, perturbations to the ZND structure to account for weak non-steady effects and losses also fail in the systems with sensitive chemistry where reactions truly decouple from the shock motion. The present paper discusses a very simple model for these transient problems using the shock change equations. These permit the dynamics of the lead shock to be determined once a partial derivative (or combination of them) behind the lead shock can be prescribed or modeled.

Diffracting detonation waves are shown to be well approximated by the quasi-steady rear piston support behind the lead shock, requiring $\partial u/\partial t \ll \dot{D}_w$. This leads to very simple analytical formulae for the shock dynamics. Galloping detonation waves with nearly instantaneous energy release followed by inert decay phases require $\partial u/\partial x \approx$ constant. This also leads to very simple analytical formulae for the shock dynamics. The present communication addresses these two problems, and reports on recent progress, summarizing and expanding on our recent publications on the subject [3, 5, 6].

2 Link between partial derivatives and the shock dynamics

Following the procedure of Fickett and Davis [7], Radulescu formulated the shock-change equations for any partial derivative of interest for a general fluid [6]. Here we focus on the expressions assuming a strong shock in a perfect gas, which are sufficiently simple and useful in practice.

We start with the Euler equations written for a stream-tube with varying area A(x); see Fig. 1. These describe the general motion of a compressible inert fluid.

$$\frac{1}{\rho}\frac{\mathbf{D}\rho}{\mathbf{D}t} = -\frac{\partial u}{\partial x} - \dot{\sigma}_A \quad \rho \frac{\mathbf{D}u}{\mathbf{D}t} = -\frac{\partial p}{\partial x} \quad \frac{\mathbf{D}p}{\mathbf{D}t} = c^2 \frac{\mathbf{D}\rho}{\mathbf{D}t} \tag{1}$$



Figure 1: Schematic of quasi-1D flow in a tube with enlarging cross-section.

where x and t are the coordinate along the stream tube and time, $D/Dt = \partial/\partial t + u\partial/\partial x$ is the rate of change along the motion of a fluid particle. The rate of strain of a fluid element in the transverse direction is $\dot{\sigma}_A = \frac{D\ln A}{Dt} = u d \ln A/dx = u\kappa$. This also is the product of the shock curvature and the flow speed, since $\kappa = d \ln A/dx$.

These partial differential equations (1) can be projected along the shock wave trajectory $x_w(t)$ such that partial derivatives appearing in (1) can be expressed in terms of time derivatives taken along the path $x_w(t)$. The speed of the observer being the shock speed $D_w = \dot{x}_w(t)$, convective derivatives taken along the path $x_w(t)$ satisfy

$$\left(\frac{d}{dt}\right)_{w} = \frac{\partial}{\partial t} + D_{w}\frac{\partial}{\partial x} \quad \text{and} \quad \frac{\mathbf{D}}{\mathbf{D}t} = \left(\frac{d}{dt}\right)_{w} + (u - D_{w})\frac{\partial}{\partial x} \tag{2}$$

If all variables appearing in (1) apply immediately behind the shock, the ratio $(du/dt)_w/(dp/dt)_w = \left(\frac{du}{dp}\right)_H$ becomes the variation of particle speed with pressure along the shock Hugoniot, the curve marking the loci of possible post shock states. This is a property of the material's equation of state. After some manipulations, using the mass conservation across the shock wave $\rho_0(D_w - u_0) = \rho(D_w - u)$ and the definition of the sonic parameter $\eta = 1 - \left(\frac{D-u}{c}\right)^2$, the desired shock-change equations can be obtained for any two partial derivatives, for example:

$$\frac{\partial u}{\partial x} = \eta^{-1} \left(-u\kappa - \frac{1}{\rho c^2} \left(\frac{dp}{dt} \right)_w \left(1 + \rho_0 (D_w - u_0) \left(\frac{du}{dp} \right)_H \right) \right)$$
(3)

$$\frac{\partial p}{\partial x} = \rho_0 (D_w - u_0) \eta^{-1} \left(-u\kappa - \frac{1}{\rho c^2} \left(\frac{dp}{dt} \right)_w \left(1 + \frac{\rho_0 (D_w - u_0)}{1 - \eta} \left(\frac{du}{dp} \right)_H \right) \right) \tag{4}$$

Expressions for other partial derivatives follow from (1). These shock change equations can be written in terms of a single variable characterizing the shock, for example the shock speed, Mach number, pressure, density, etc, since they are all linked through the Rankine-Hugoniot jump conditions. Choosing the shock speed for example, we can write $\left(\frac{dp}{dt}\right)_w = \left(\frac{dD_w}{dt}\right)_w \left(\frac{dp}{dD_w}\right)_H = \dot{D}_w \left(\frac{dp}{dD}\right)_H$ where $\left(\frac{dp}{dD}\right)_H$ is also a property of the shock Hugoniot. The right hand sides of all shock change equations listed can be re-written in terms of the wave speed D_w , its rate of change \dot{D}_w , shock Hugoniot properties and the upstream state. For a strong shock in a perfect gas, with $u_0 = 0$, the state behind the shock is given by very simple Rankine-Hugoniot jump conditions:

$$u = \frac{2}{\gamma + 1} D_w \quad \rho = \frac{\gamma + 1}{\gamma - 1} \rho_0 \quad p = \frac{2}{\gamma + 1} \rho_0 D_w^2 \quad c^2 = \gamma \frac{p}{\rho}$$
(5)

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from which we readily obtain

$$\left(\frac{dp}{dD_w}\right)_H = \frac{4}{\gamma + 1}\rho_0 D_w \tag{6}$$

Substituting (5) and (6) in (3) and (4), we obtain:

$$\frac{\partial u}{\partial x} = -\frac{6}{\gamma+1}\frac{\dot{D}_w}{D_w} - \frac{4\gamma D_w \kappa}{(\gamma+1)^2} \tag{7}$$

$$\frac{\partial p}{\partial x} = -\frac{4\rho_0 \dot{D}_w (2\gamma^2 + \gamma - 1)}{(\gamma - 1)(\gamma + 1)^2} - \frac{4\rho_0 \gamma D_w^2 \kappa}{(\gamma + 1)^2} \tag{8}$$

Expressions for other partial derivatives of interest can be easily obtained by substituting the last two expressions in (1), yielding, for example:

$$\frac{\partial u}{\partial t} = \frac{8D_w}{\gamma+1} + \frac{4\gamma D_w^2 \kappa}{(\gamma+1)^2} \tag{9}$$

3 Detonation diffraction

The *local* dynamics of diffracting shocks resulting from the diffraction of detonations can be argued to correspond to quasi-steady rear piston support [3], i.e.,

$$\frac{\partial u}{\partial t} \ll \dot{D}_w \tag{10}$$

A simple evolution equation for the lead shock can thus be obtained from (9), by neglecting the LHS, i.e.,

$$\frac{8D_w}{\gamma+1} + \frac{4\gamma D_w^2 \kappa}{(\gamma+1)^2} = 0 \tag{11}$$

This is an evolution equation for the shock dynamics of the form $D_w \propto A^{-1/n}$, since it can be re-written as:

$$\frac{D_w^2 \kappa}{\dot{D}_w} \equiv \frac{\mathrm{d}\ln A/\mathrm{d}x}{\mathrm{d}\ln D_w/\mathrm{d}x} = -2\frac{\gamma+1}{\gamma} \equiv -n \tag{12}$$

This simple power law dependence can readily be incorporated in the geometric theory of surface evolution of Whitham, known as Geometrical Shock Dynamics [8].

When the shock dynamics are of the form $D_w \propto A^{-1/n}$, the diffraction of a shock surface at a sharp corner has an analytical solution in terms of *n*, given by equations (8.95) in Whitham [8]:

$$\frac{X}{D_w t} = \sqrt{\frac{n+1}{n}} \exp\left(\frac{\theta}{\sqrt{n}}\right) \sin\left(\eta - \theta\right) \tag{13}$$

$$\frac{Y}{D_w t} = \sqrt{\frac{n+1}{n}} \exp\left(\frac{\theta}{\sqrt{n}}\right) \cos\left(\eta - \theta\right) \tag{14}$$

where η is given by $\tan \eta = \sqrt{n}$ and θ is the angle of the unit normal to the shock surface with the x-axis.

The prediction of shock shape evolution using (13) and (14), with n given from (12), was compared to experiments and simulations of hydrogen/oxygen/argon detonations and found in excellent agreement.

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Figure 2: Sequential Schlieren images a) to h) separated by 12.9 μ s of detonation diffraction in 2H₂+O₂+2Ar mixture at $T_0 = 295$ K and $p_0 = 17$ kPa, adapted from [3]; the distance between the bottom and top walls is 200 mm; overlaid in green is the shock shape predicted with the weakly supported shock assumption.

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An example is shown in Fig. xx for a critically diffracting detonation wave. Very good prediction of the shock shape evolution is apparent, until the re-amplification of new detonation kernels. The access to an analytical solution for the shock dynamics permitted us to formulate simple detonation transmission criteria [3].

Experiments in other reactive mixtures are under way and the model prediction capabilitity for these will be discussed at the conference.

4 Galloping detonations

Galloping detonations in narrow tubes consist in the quasi-periodic re-amplification of the detonation front through rapid DDT, followed by a period of decay of the lead shock [4]. As the limits are approached, the decay phase becomes longer than the re-amplification phase. In a recent study, an extreme model was considered in which the re-amplification phase is infinitely faster than the long decay phase. Under these conditions, energy is released periodically in the non-reacted gas accumulated behind the lead shock, as shown schematically in Fig. 3. Since the infinitely fast energy release corresponds to an energy addition at constant volume, the velocity and pressure gradients behind the shock after re-ignition are the same as those before re-ignition. It is not unreasonable to expect that the limit cycle oscillation will achieve constant gradients throughout the cycle, since they are constrained by their values at the start and end of each cycle, which are the same. This was empirically observed in our numerical calculations [5].

For 1D flows, the constancy of flow gradient $\partial u/\partial x$ behind the lead shock, through the shock change equation (7), signifies:

$$\frac{\partial u}{\partial x} = -\frac{6}{\gamma + 1} \frac{D_w}{D_w} \equiv b \tag{15}$$

where b is a constant. This integrates to

$$D_w = D_{w0} \exp\left(-\frac{\gamma+1}{6}bt\right) \tag{16}$$

and $D \propto -x$. This exponential decay in time is in very good agreement with experimental observations [4] and numerical simulations [5]. Further progress on the galloping problem will be communicated at the conference.

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