Modeling Detonation Reflection with Nonsteady Shock Change Equation

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1 Introduction

Previous models for the shock wave produced by planar detonation reflection have assumed flow gradients behind the shock to be zero, enabling simple computation of the trajectory [1, 2, 3]. However, the Taylor-Zeldovich expansion wave trailing the detonation transmits through the shock wave, establishing a nonsimple expansion wave between the shock wave and end wall. An accurate treatment of this problem requires including the variation in downstream flow gradients, which we achieve using a generalization of the shock change equation.

Versions of the shock change or acceleration wave formalism have been derived independently by a number of researchers over the past century as discussed by Becker [4] and Chen [5]. The results have been used to analyze the growth and decay of shock waves in inhomogeneous [6, 7] and chemically reacting flows [8, 9]. Fickett and Davis [10] discuss the application to detonations and the implications for steady flow in the reaction zone. Recently, Radulescu [11] derived expressions for shock propagation in quasi-one dimensional flows, gave explicit expressions for nonreactive perfect gases, and discussed the relationship to the shock dynamics approximation of Whitham. These derivations usually consider the upstream conditions to be uniform, with the exception of [6], and the flow to be at rest. In order to treat the interaction of a shock wave with an expansion wave, as occurs when a detonation wave reflects from an end wall, it is necessary to consider how both the upstream unsteadiness and spatial nonuniformity affect the shock wave acceleration and downstream flow gradients.

This article will describe an extension to the shock change equation that considers a general nonuniform and nonsteady upstream flow and apply the equation to the problem of planar detonation reflection. The result is a technique for predicting the trajectory of the ensuing reflected shock wave in one dimension for a general mixture and equation of state.

2 Nonsteady shock change equation

The shock change equation is derived by applying the equations of motion on either side of a shock discontinuity and using the Rankine-Hugoniot relations to connect the flows across the shock wave. A key step is to transform the equations of motion into a reference frame following the shock wave such that all quantities exist on a Hugoniot. The classic result for a uniform and steady upstream state describes the shock acceleration caused by chemical energy release and the velocity gradient behind the shock. Nonuniform and nonsteady upstream flows can also cause shock acceleration, and these effects can be evaluated by application of the chain rule to the post-shock derivatives. An abridged derivation of the full result is provided below; see a subsequent paper for further details and discussion.

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The equations of motion for a reacting flow, neglecting viscosity, diffusion, heat transfer, and considering only one dimension, are

$$\frac{\mathrm{D}\rho}{\mathrm{D}t} = -\rho\frac{\partial u}{\partial x} \tag{1}$$

$$\frac{\mathrm{D}u}{\mathrm{D}t} = -\frac{1}{\rho}\frac{\partial P}{\partial x} \tag{2}$$

$$\frac{\mathrm{D}P}{\mathrm{D}t} = a_f^2\frac{\mathrm{D}\rho}{\mathrm{D}t} + \rho a_f^2\dot{\sigma}\ , \tag{3}$$

where (3) is the adiabatic-change equation [10], which is obtained by combining the energy and species transport equations using a thermodynamic identity and equation of state. a_f is the frozen sound speed, and $\dot{\sigma}$ is the thermicity.

The material derivative used in the equations of motion describes the time rate of change of a quantity along a particle path. Consider instead the frame following the shock wave, then the corresponding "shock derivative" is

$$\left(\frac{\mathrm{d}}{\mathrm{d}t}\right)_{\mathcal{S}} = \frac{\partial}{\partial t} + U_s\frac{\partial}{\partial x}, \tag{4}$$

where U_s is the shock speed in the laboratory frame. The material derivative can then be expressed in terms of the shock derivative,

$$\frac{\mathrm{D}}{\mathrm{D}t} = \left(\frac{\mathrm{d}}{\mathrm{d}t}\right)_{\mathcal{S}} + (u - U_s)\frac{\partial}{\partial x}. \tag{5}$$

Substituting (1) into (3), and applying the transformation (5) to the result and (2) yields

$$\left(\frac{\mathrm{d}u}{\mathrm{d}t}\right)_{\mathcal{S}} + (u - U_s)\frac{\partial u}{\partial x} = -\frac{1}{\rho}\frac{\partial P}{\partial x} \tag{6}$$

$$\left(\frac{\mathrm{d}P}{\mathrm{d}t}\right)_{\mathcal{S}} + (u - U_s)\frac{\partial P}{\partial x} = -\rho a_f^2\frac{\partial u}{\partial x} + \rho a_f^2\dot{\sigma}. \tag{7}$$

Equations (6) and (7) can be combined to eliminate the pressure gradient. Following the shock wave, consider the quantities in (6) and (7) to be the post-shock state. After algebraic simplification, a general form of the shock change equation is obtained

$$\left(\frac{\mathrm{d}P_2}{\mathrm{d}t}\right)_{\mathcal{S}} + \rho_2 w_2\left(\frac{\mathrm{d}u_2}{\mathrm{d}t}\right)_{\mathcal{S}} = \rho a_{f,2}^2\left(\dot{\sigma} - \eta\left.\frac{\partial u}{\partial x}\right|_2\right), \tag{8}$$

where the sonic parameter, $\eta = 1 - w_2^2/a_{f,2}^2$, was introduced. $\left.\frac{\partial u}{\partial x}\right|_2$ is the velocity gradient behind the shock wave.

The shock derivatives on the left-hand side of (8) describe the time rate of change of the post-shock pressure and post-shock lab-frame velocity. The Rankine-Hugoniot shock jump equations relate the post-shock quantities to the upstream state,

$$P_2, \rho_2, w_2 = \mathcal{H}(P_1, \rho_1, \boldsymbol{Y_1}, w_1) \tag{9}$$

For frozen shock waves $\boldsymbol{Y_2} = \boldsymbol{Y_1}$, and for equilibrium post-shock states, $\boldsymbol{Y_2} = \boldsymbol{Y_2^{eq}}(w_1, \rho_1, P_1, \boldsymbol{Y_1})$. Lab-frame velocities are given by $u_2 = U_s - w_2$. Derivatives of the post-shock quantities can be expanded using the chain rule, and hence the shock derivatives are given by

$$\left(\frac{\mathrm{d}P_2}{\mathrm{d}t}\right)_{\mathcal{S}} = \sum_{\alpha\in\mathcal{U}}\left(\frac{\partial P_2}{\partial\alpha}\right)_{\mathcal{U}\setminus\alpha}\left(\frac{\mathrm{d}\alpha}{\mathrm{d}t}\right)_{\mathcal{S}} \tag{10}$$

$$\left(\frac{\mathrm{d}u_2}{\mathrm{d}t}\right)_{\mathcal{S}} = \frac{\mathrm{d}U_s}{\mathrm{d}t} - \left(\frac{\mathrm{d}w_2}{\mathrm{d}t}\right)_{\mathcal{S}} = \frac{\mathrm{d}U_s}{\mathrm{d}t} - \sum_{\alpha\in\mathcal{U}}\left(\frac{\partial w_2}{\partial\alpha}\right)_{\mathcal{U}\setminus\alpha}\left(\frac{\mathrm{d}\alpha}{\mathrm{d}t}\right)_{\mathcal{S}} \tag{11}$$

where $\mathcal{U} = \{w_1, P_1, \rho_1, \boldsymbol{Y_1}\}$.

If the upstream flow is uniform and steady, then the shock derivatives simplify to

$$\left(\frac{\mathrm{d}P_2}{\mathrm{d}t}\right)_{\mathcal{S}} = \left(\frac{\partial P_2}{\partial w_1}\right)_{\mathcal{U}\backslash w_1} \left(\frac{\mathrm{d}w_1}{\mathrm{d}t}\right)_{\mathcal{S}} = \left(\frac{\partial P_2}{\partial w_1}\right)_{P_1,\rho_1,\boldsymbol{Y_1}} \frac{\mathrm{d}U_s}{\mathrm{d}t} \tag{12}$$

$$\left(\frac{\mathrm{d}u_2}{\mathrm{d}t}\right)_{\mathcal{S}} = \frac{\mathrm{d}U_s}{\mathrm{d}t} - \left(\frac{\partial w_2}{\partial w_1}\right)_{\mathcal{U}\backslash w_1} \left(\frac{\mathrm{d}w_1}{\mathrm{d}t}\right)_{\mathcal{S}} = \left(1 - \left(\frac{\partial w_2}{\partial w_1}\right)_{P_1,\rho_1,\boldsymbol{Y_1}}\right) \frac{\mathrm{d}U_s}{\mathrm{d}t} \tag{13}$$

Substitution into (8) yields the shock change equation expressed in terms of the shock acceleration,

$$\frac{\mathrm{d}U_s}{\mathrm{d}t} = \frac{\rho_2 a_{f,2}^2 \left(\dot{\sigma} - \eta \left.\frac{\partial u}{\partial x}\right|_2\right)}{\left(\frac{\partial P_2}{\partial w_1}\right)_{P_1,\rho_1,\boldsymbol{Y_1}} + \rho_2 w_2 \left(1 - \left(\frac{\partial w_2}{\partial w_1}\right)_{P_1,\rho_1,\boldsymbol{Y_1}}\right)} \tag{14}$$

If the upstream flow is nonuniform and nonsteady, then the shock derivatives, (10) and (11), must be completely expanded. Factoring of the shock acceleration term, and then substituting into (8) yields the shock change equation for a generally nonuniform and nonsteady upstream flow,

$$\frac{\mathrm{d}U_s}{\mathrm{d}t} = \frac{\rho_2 a_{f,2}^2 \left(\dot{\sigma} - \eta \left.\frac{\partial u}{\partial x}\right|_2\right) - \Sigma_{\text{ns}}}{\left(\frac{\partial P_2}{\partial w_1}\right)_{P_1,\rho_1,\boldsymbol{Y_1}} + \rho_2 w_2 \left(1 - \left(\frac{\partial w_2}{\partial w_1}\right)_{P_1,\rho_1,\boldsymbol{Y_1}}\right)}. \tag{15}$$

The Σ_{ns} term contains all of the additional terms due to the nonuniform and nonsteady upstream flow,

$$\begin{aligned}
\Sigma_{\text{ns}} = &- \left[\left(\frac{\partial P_2}{\partial w_1}\right)_{P_1,\rho_1,\boldsymbol{Y_1}} - \rho_2 w_2 \left(\frac{\partial w_2}{\partial w_1}\right)_{P_1,\rho_1,\boldsymbol{Y_1}}\right] \left(\frac{\mathrm{d}u_1}{\mathrm{d}t}\right)_{\mathcal{S}} \\
&+ \left[\left(\frac{\partial P_2}{\partial P_1}\right)_{w_1,\rho_1,\boldsymbol{Y_1}} - \rho_2 w_2 \left(\frac{\partial w_2}{\partial P_1}\right)_{w_1,\rho_1,\boldsymbol{Y_1}}\right] \left(\frac{\mathrm{d}P_1}{\mathrm{d}t}\right)_{\mathcal{S}} \\
&+ \left[\left(\frac{\partial P_2}{\partial \rho_1}\right)_{w_1,P_1,\boldsymbol{Y_1}} - \rho_2 w_2 \left(\frac{\partial w_2}{\partial \rho_1}\right)_{w_1,P_1,\boldsymbol{Y_1}}\right] \left(\frac{\mathrm{d}\rho_1}{\mathrm{d}t}\right)_{\mathcal{S}} \\
&+ \sum_{k=1}^{K} \left[\left(\frac{\partial P_2}{\partial Y_{1,k}}\right)_{w_1,\rho_1,P_1,Y_{1,i\neq k}} - \rho_2 w_2 \left(\frac{\partial w_2}{\partial Y_{1,k}}\right)_{w_1,\rho_1,P_1,Y_{1,i\neq k}}\right] \left(\frac{\mathrm{d}Y_{1,k}}{\mathrm{d}t}\right)_{\mathcal{S}}.
\end{aligned} \tag{16}$$

In some situations, reactions proceed sufficiently rapidly behind the shock front such that an equilibrium state is reached a short distance δ behind the shock front. If δ is much smaller than any other length scale L, i.e., $\delta \ll L$, then the downstream state at chemical equilibrium can be idealized as the post-shock state. The shock change equation for equilibrium shocks is then

$$\frac{\mathrm{d}U_s}{\mathrm{d}t} = \frac{-\rho_2 a_{e,2}^2 \eta \left.\frac{\partial u}{\partial x}\right|_2 - \Sigma_{\text{ns}}}{\left(\frac{\partial P_2}{\partial w_1}\right)_{P_1,\rho_1,\boldsymbol{Y_1^{eq}}} + \rho_2 w_2 \left(1 - \left(\frac{\partial w_2}{\partial w_1}\right)_{P_1,\rho_1,\boldsymbol{Y_1^{eq}}}\right)}. \tag{17}$$

where all post-shock states and derivatives are computed assuming complete chemical equilibrium. The sonic parameter $\eta = 1 - w_2^2/a_{e,2}^2$ is based on the equilibrium sound speed, a_e, rather than frozen sound speed.

3 Application to detonation reflection

The planar detonation wave structure traveling along a pipe in one-dimension can be modeled by a shock wave, a reaction zone, and a nonsteady expansion wave. The first two are described by Zeldovich-von-Neumann-Döring (ZND) theory, and the latter is the Taylor-Zeldovich (TZ) expansion wave. The idealized structure is that the ZND reaction zone and TZ wave are joined at the Chapman-Jouguet (CJ) state. Upon reflection from the closed end of the pipe, the flow behind the detonation is brought to rest by a shock wave, which travels upstream first through the reaction zone and then into the TZ wave. The TZ wave is self-similar, scaling with the length of pipe over which the detonation has travelled, L. Consider the detonation reaction zone just prior to reflection to have size Δ. We argue that the reflected shock wave trajectory is asymptotic to the trajectory of the shock reflected by the CJ state directly into the TZ wave as $\Delta/L \to 0$, i.e. the detonation reaction zone is negligible for $\Delta \ll L$. Close to the point of the reflection, the interaction of the reflected shock through the reaction zone will have an additional influence on the trajectory [12] but we neglect this in the present treatment.

By neglecting the additional time scales associated with chemical reaction, the problem becomes self-similar. All properties in the TZ wave are given by unique values of the similarity parameter $\xi = x/t$, where $x = 0$ and $t = 0$ correspond to the initiation of the detonation in space and time. Values of ξ represent different characteristics in the TZ wave. The flow upstream of the reflected shock wave is then instantaneously described by $\xi = X_s(t)/t$, where $X_s(t)$ is the reflected shock position. So, the upstream properties are given by

$$u_1, P_1, \rho_1, \boldsymbol{Y_1} = f(\xi). \tag{18}$$

The post-shock quantities are then

$$w_2, P_2, \rho_2 = \mathcal{H}(U_s, \xi), \tag{19}$$

and the post-shock state is assumed to be at equilibrium, $\boldsymbol{Y_2} = \boldsymbol{Y_2^{eq}}(U_s, \xi)$.

The shock derivatives can be obtained simply by applying the chain rule for the two independent variables,

$$\left(\frac{\mathrm{d}P_2}{\mathrm{d}t}\right)_{\mathcal{S}} = \left(\frac{\partial P_2}{\partial U_s}\right)_{\xi} \frac{\mathrm{d}U_s}{\mathrm{d}t} + \left(\frac{\partial P_2}{\partial \xi}\right)_{U_s} \left(\frac{\mathrm{d}\xi}{\mathrm{d}t}\right)_{\mathcal{S}} \tag{20}$$

$$\left(\frac{\mathrm{d}u_2}{\mathrm{d}t}\right)_{\mathcal{S}} = \left(\frac{\partial u_2}{\partial U_s}\right)_{\xi} \frac{\mathrm{d}U_s}{\mathrm{d}t} + \left(\frac{\partial u_2}{\partial \xi}\right)_{U_s} \left(\frac{\mathrm{d}\xi}{\mathrm{d}t}\right)_{\mathcal{S}}. \tag{21}$$

Substituting (20) and (21) into (17) yields the desired version of the shock change equation

$$\frac{\mathrm{d}U_s}{\mathrm{d}t} = \frac{-\rho_2 a_{e,2}^2 \eta \left.\frac{\partial u}{\partial x}\right|_2 - \left(\left.\frac{\partial P_2}{\partial \xi}\right|_{U_s} + \rho_2 w_2 \left.\frac{\partial u_2}{\partial \xi}\right|_{U_s}\right)\left(\frac{\mathrm{d}\xi}{\mathrm{d}t}\right)_{\mathcal{S}}}{\left.\frac{\partial P_2}{\partial U_s}\right|_{\xi} + \rho_2 w_2 \left.\frac{\partial u_2}{\partial U_s}\right|_{\xi}}. \tag{22}$$

We have assumed the equilibrium limit as this is consistent with the full solution to the non-steady reactive flow simulation for the example we have considered.

An additional consequence of the flow's self-similarity is that the velocity distribution is of the form $u(x,t) = x\Phi(t)$, where $\Phi(t)$ is some function of time with a jump discontinuity at the reflected shock wave. Problems of this type were described by Sedov [13] and with particular attention by Pert [14].

The post-shock velocity distribution must satisfy both the shock jump relations at the shock wave and the zero velocity boundary condition at the wall, hence the velocity gradient in (22) can be expressed as

$$\left.\frac{\partial u}{\partial x}\right|_2 = \frac{u_2}{X_s - L}. \tag{23}$$

This model (23) is applicable while the reflected shock is within the TZ wave. Upon emerging from the TZ wave, there are two distinct expansion waves connecting the reflected shock wave to the wall, and hence there is a kink in the velocity profile. Only the shock trajectory within the TZ wave is considered.

Initial conditions are given by

$$\begin{aligned} X_s(t=0) &= L \\ U_s(t=0) &= U_R, \end{aligned} \tag{24}$$

where U_R is the shock speed given by the well-described detonation reflection solution assuming equilibrium post-shock state at zero velocity [3].

Upon specifying the initial mixture of the predetonation gases, with an equation of state, (23), and (24), equation (22) can be integrated as an initial value problem for the trajectory of the reflected shock wave, $X_s(t)$.

This calculation is demonstrated for a detonation in stoichiometric hydrogen-oxygen with 25% argon dilution, an initial pressure of 1 bar, and a temperature of 300 K. Equation (22) was integrated using a second-order Runge-Kutta solver [15, 16] with thermodynamic and post-shock calculations performed using Cantera [17] and the Shock and Detonation Toolbox [18]. Thermodynamic properties were computed using the NASA7 polynomials [19]. The gradients on the Hugoniot in (22) were computed numerically by looping through a range of U_s and ξ values, respectively, and computing the resulting post-shock state. The post-shock pressures and velocities were fit to a spline and differentiated to obtain the desired gradients. The velocity gradient given by (23) is not defined at $t = 0$, hence the numerical integration was begun using an artificial initial velocity gradient and subsequently switched to (23).

The same problem was numerically simulated using the finite-volume CFD toolbox, OpenFOAM [20], with an additional library, blastFoam [21]. The reactive Euler equations were solved in one-dimension using an ideal gas equation of state and a detailed chemical mechanism [22]. The simulation was initiated at $t = L/U_{CJ}$ with the CJ state at the wall, followed by the TZ wave. The initial condition was calculated using the Shock and Detonation Toolbox. The resulting trajectory of the reflected shock was determined from the maximum gradient in the pressure variable at each time step.

The resulting trajectories of the reflected shock wave from the simulation and the shock change model are plotted together in Figure 1. The two results have good agreement with maximum error of approximately 0.1%, which can be attributed to numerical error in both calculations.

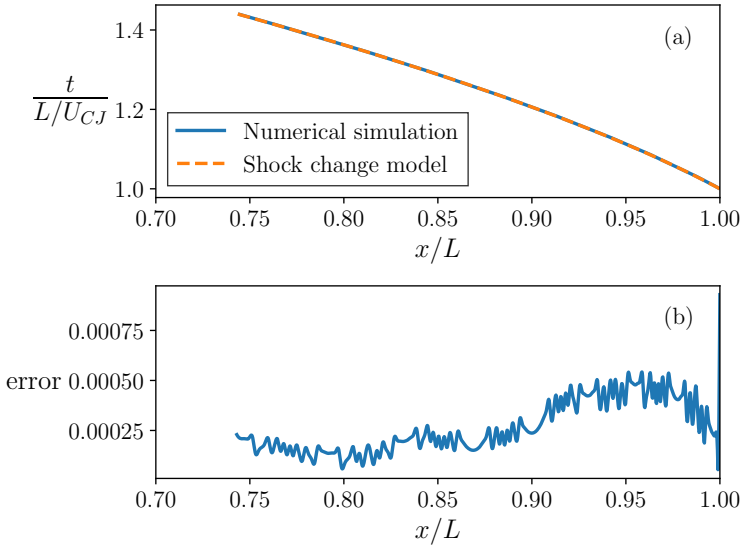

Figure 1: (a) Overlay of space-time trajectories of reflected shocks computed by numerical simulation of reactive Euler equations and integration of nonsteady shock change equation. (b) Normalized absolute error between calculations. Mixture: 50% H_2, 25% O_2, 25% Ar, 1 bar, 300 K.

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