UNDERSTANDING CURVED DETONATION WAVES

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The reaction zone of a detonation wave is very small compared to the hydrodynamic length scale for a typical application. Consequently, it is impractical for numerical calculations to fully resolve the reaction zone. A non-zero reaction zone width is critical to describe curved detonation waves because it affects the wave speed. The curvature effect is the result of an interaction between the rate of energy release and geometric source terms within the reaction zone. When the reaction zone width is determined by the computational cell size rather than the physical scale, the numerics introduces an artificial curvature effect which frequently dominates the physical effect and leads to mesh dependence of simulations. Modified Hugoniot jump conditions are derived which characterize the curvature effect. They express the conservation laws and are not sensitive to the detailed reaction dynamics but instead depend only on the reaction zone width, and averages of pressure and of mass, momentum and energy densities.

INTRODUCTION

The reaction zone of a detonation wave is very small compared to the hydrodynamic length scale for a typical application. Consequently, it is impractical for numerical calculations to resolve the reaction zone. In contrast to a shock wave, small changes in the dynamics of the reaction zone affect the detonation shock Hugoniot while the large energy release has a significant effect on the subsequent flow. Here, we focus on understanding the detonation jump conditions as a necessary step to incorporating the correct detonation dynamics into hydrodynamic calculations in which one cannot afford to resolve the reaction zone.

Detonation waves may be modeled using the reactive Euler equations. In planar geometry, with one irreversible exothermic reaction this leads to a large class of reaction rates to the Zel'dovich–von Neumann–Doering (ZND) model in which a detonation wave consists of a zero width shock wave followed by an extended reaction zone. The ZND model predicts that the state behind a steady detonation wave is determined by the strong branch of the detonation shock Hugoniot equations independent of the reaction rate or the reaction zone width. Moreover, there is a unique Chapman–Jouguet (CJ) wave with the minimum detonation velocity and some state behind the detonation front that corresponds to an underdriven detonation. Furthermore, the reactive flow equations determine the reaction zone dynamics and with sufficient resolution, non steady planar flows with detonation waves can be accurately computed.

More complicated detonation dynamics than predicted by the ZND model arise when other length scales are present. For example, when the shock width is comparable to the reaction zone length, the state behind the detonation front can be on the weak branch of the detonation shock Hugoniot. The shock width may have a physical origin or may be numerical artifact due to artificial viscosity or other de-
spatiotemporal mechanisms introduced by shock capturing algorithms.

In more than one spatial dimension, detonation waves are subject to an instability involving transverse waves within the reaction zone. This phenomenon has been observed experimentally (e.g., Ref. 1, Ch. 7), and an analysis of the reactive Euler equations shows this instability and it also has been studied in numerical calculations with a well-resolved reaction zone. Both the experiments and the simulations show that the amplitude of the instability saturates. On a scale large compared to both the width of the reaction zone and the wavelength of the instability, the detonation front is well defined. Moreover, heterogeneous explosives have an additional length scale set by the grain size. In effect, the reaction rate used in a numerical model can only account for the instabilities and the heterogeneities in an average sense and thus is phenomenological. By neglecting the instability, the simplified model of the detonation wave dynamics allows one to identify the relevant parameters describing the propagation of the detonation waves. However, the effective rate law cannot be simply related to the kinetics of the underlying chemical reaction and must be deduced from wave propagation data. Quantities which are sensitive to the details of the phenomenological model, such as the failure diameter, are not captured by the simplified flow equations.

For many applications, burn models are used to avoid the computational expense of resolving the small spatial and time scale within the reaction zone. Similar to a shock capturing algorithm, a burn model gives a detonation wave an artificial width which for a good model is a few cells. With crude resolution, even well-designed and physically motivated rate equations will at best deteriorate to such capturing algorithms. Furthermore, in multi-dimensional simulations great care must be taken to avoid having the effective reaction rate introduce an artificial transverse instability on the scale of the mesh. Typically, this smoothing is achieved with sufficient numerical dissipation.

Programmed burn is a particularly simple model in which a detonation wave is propagated in multiple spatial dimensions using a Hopfian wave generation with the planar CJ detonation velocity. Rather than explicitly tracking the wave, the wave front from the equation of state is switched from the reactant to the reaction products. The concurrent energy release increases the pressure and drives the wave. One numerical difficulty with this model is that the reaction front and the hydrodynamic front may separate because they are not calculated self-consistently. Such a model clearly is not adequate for overdriven detonation waves and as we will show does not correctly describe multi-dimensional effects.

A rate-stick experiment provides a good example of an important multi-dimensional effect on propagating detonation waves that is not modeled in the 2-D model or programmed burn. In a rate-stick the steady state consists of a curved detonation wave propagating at a velocity lower than the minimum planar CJ detonation velocity. The change in the detonation velocity is caused by the interaction within the reaction zone between the geometric source term due to the curvature of the detonation front and the source term for energy release from the chemical reaction. An analysis of a curved detonation wave shows that the detonation velocity of an underdriven diverging wave is a function of the mean front curvature. To first order the effect is proportional to the product of the reaction zone width and the front curvature. The fact that the detonation wave fails to propagate when this ratio is still small emphasizes the importance of the curvature effect. In addition to the curvature effect, the failure radius also depends on 2-D instabilities and heterogeneities in the explosive.

For numerical calculations, burn models are important for both initiation and propagation of detonation waves. Here we focus entirely on wave propagation. In this case, the burn model plays a role similar to artificial viscosity for non-reactive shock waves. It gives the detonation wave an artificial thickness determined by the cell size rather than the physical length scale of the reaction zone. Because of the artificial reaction zone width, one expects curvature effects in numerical simulations. However, with finite curvature effect may have the wrong functional form and be quantitatively inaccurate. Since the numerical width of the detonation front is proportional to the cell size, the artificial curvature effect is one cause of mesh size and mesh orientation dependence of the results of numerical computations.

An example of this common numerical effect is seen in the calculation of a rate-stick experiment in Ref. 10 using a burn model similar to Forest Line. The steady-state detonation velocity is a function of tube radius approaches the experimental value as finer meshes are used, Ref. 10, Fig. 7. As expected from theory, the detonation velocity increases as the reaction zone width decreases with a smaller effect. A very fine mesh, in this case 0.05 mm, is needed to obtain good agreement with the experiments. Furthermore, sufficient resolution was not available to verify convergence with mesh resolution. At extremely high resolution, the model will not resolve the reaction zone and then the computation should converge to the curvature effect which corresponds to the reaction rate used in the simulation.

An improved version of programmed burn which accounts for the curvature effect of an underdriven diverging detonation wave is known as detonation shock dynamics. It can be thought of as a Hopfian-like construction in which the flat wave is a function of front curvature. In
Planar Detonations

Planar detonation waves may be modeled using the reactive Euler equations which represent the conservation of mass, momentum, and energy. A fourth equation describes the progress of the chemical reaction taking place in the reaction zone. The conservation form of the equations are

\[ \rho \frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial x} = -\rho \frac{\partial E}{\partial x} \]

\[ \rho \frac{\partial E}{\partial t} + \rho u \frac{\partial E}{\partial x} = -P \frac{\partial u}{\partial x} \]

\[ \frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u^2 + P) = -\rho \frac{\partial E}{\partial x} \]

\[ \frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u^2) = \rho \frac{\partial E}{\partial x} \]

where \( \rho, u, P \) and \( \rho u, E \) are the fluid density, particle velocity, specific internal energy (thermal + chemical), and pressure, \( V = 1/\rho \) is the specific volume, \( E = (1/2)u^2 + \rho \) is the specific total energy, \( \rho \) is the mass fraction of the reaction products and \( R, A \) is the specific reaction rate.

The state behind a steady state detonation wave is determined by the Hugoniot jump relations

\[ J(\rho u - D) = 0 \]

\[ J(\rho u(D^2 + P)) = 0 \]

\[ J(\rho u(D^2 + P) + P) = 0 \]

where \( J([f] : f_0 - f_1) \) is the jump across the detonation wave from the ahead state \((\lambda = 0)\) to the behind state \((\lambda = 1)\), denoted by the subscripts 0 and 1 respectively. It follows that the detonation velocity \( D \) is given by

\[ J(\rho u(D^2 + P)) = 0 \]

when \( u_0 = 0 \).

For a given ahead state, these algebraic equations have a one parameter family of solutions. The CJ state corresponds to the minimum detonation velocity. The solutions with \( P' = P_0 \) are called strong detonations and those with \( P' = P_1 \) weak detonations. In the ZND model, the strong branch corresponds to overdriven detonation waves and the weak branch represents unphysical solutions.

The wave curve formed by the union of strong detonations plus the composite waves connecting a CJ detonation followed by a rarefaction or Taylor wave can be used to define the dynamics to propagate a detonation wave using the front tracking method. This represents a well consistent extension of programmed burn that is applicable to both underdriven and overdriven detonation waves. However, it corresponds to the limit of an infinite reaction rate or zero width reaction zone. In this limit the curvature effect is absent.
**CURVED DETONATION WAVE CURVE**

In contrast to a planar detonation wave, a non-zero reaction zone width has an important effect on the dynamics of a curved detonation wave. In order to model the reaction zone we introduce the natural coordinate frame formed by the detonation front and the stream lines. Within a local stream tube, the reactive Euler equations reduce to the reactive duct equations

\[
\frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho u^2)}{\partial x} = 0, \quad (9)
\]

\[
\frac{\partial (\rho u^2)}{\partial t} + \frac{\partial (\rho u^2 + P)}{\partial x} = P \frac{A}{\partial x}, \quad (10)
\]

\[
\frac{\partial (\rho u^2)}{\partial t} + \frac{\partial (\rho u (\rho u^2 + P))}{\partial x} = \rho \frac{A}{\partial x}, \quad (11)
\]

\[
\frac{\partial (\rho U^2)}{\partial t} + \frac{\partial (\rho U^2 + P)}{\partial x} = P \frac{\partial A}{\partial x}, \quad (12)
\]

The cross-sectional area of the stream tube is \(A\), the coordinate in the stream direction is \(x\) and the stream velocity is \(u\). In the limit that the diameter of the stream tube shrinks to zero, the only geometric term that the reaction zone dynamics depends on in the mean front curvature, \(\kappa = (dA/dx)/A\).

When the spatial and time scales of the reaction zone are smaller than those of the hydrodynamic flow in the reaction product, a detonation wave can be approximated as quasi-steady with the reaction rate equilibrating adiabatically to changes in the flow behind the wave. The quasi-steady approximation reduces the system of PDEs Eqs. (9-12) to a system of ODEs which represent the generalization of the planar equations for the reaction zone profile to include the curvature effect leading order on the product of the reaction zone width and the curvature of the front.

For a given \(\kappa\), these ODEs can be used to determine the quasi-steady detonation wave geometry. Illustrate the curvature effect, Fig. 1 shows the locus of reaction zone states in the \(P-V\) plane of quasi-steady detonation waves for the simple example calculated in Ref. 16. The planar case corresponds to the standard detonation shock Hugoniot which is determined entirely from the equation of state by the usual pump conditions Eqs. (5-7). As a consequence of the non-zero reaction zone width, neither a converging nor diverging detonation wave satisfy the standard pump conditions. Moreover, there is a qualitative difference between the detonation locus for the converging and diverging case. The diverging detonation locus has an isolated point which corresponds to an underdriven detonation wave. This is a consequence of the structure of the ODEs because only the diverging case has a critical point within the physical region, \(0 < \kappa < 1\). Converging geometry forces a detonation into the overdriven regime.

The underdriven diverging detonation wave is determined by solving an eigenvalue-like problem for the separatrix, the trajectory through the critical point, by using a shooting algorithm. This leads to a singular point within the reaction zone. As a consequence, an underdriven detonation wave decouples from the flow behind. This is the basis for detonation shock dynamics, It uses the relation between the detonation velocity and the front curvature, \(D(u, \kappa)\), to propagate an underdriven detonation wave. For the same example as in Fig. 1, the minimum detonation velocity as a function of curvature is shown in Fig. 2. Increasing curvature decreases the detonation velocity in diverging geometry while increasing it in converging geometry. Though the minimum detonation velocity jumps up continuously between the diverging and converging case, using detonation shock dynamics in converging geometry would cause numerical problems since acoustic waves from behind the detonation would cause the reaction front and the hydrodynamic front to separate in a similar manner to what occurs with programmed burn.

From the results in Figs. 1 and 2, which have been derived from the reactive Euler equations, it is clear that the Hugoniot pump conditions, Eqs. (6-7), are not satisfied for a curved detonation wave with non-zero width. In particular, the state behind the underdriven detonation, wave lies above the Rayleigh line in the \(P-V\) diagram of Fig. 1. Based on this, Eq. (8) would imply that the detonation velocity is higher than the planar CJ velocity. Nevertheless, Fig. 2 shows that it is lower.

The dynamics of the detonation front is affected by the interaction of the geometric source term with the rate of chemical energy release. This can be seen by comparing the loci of the sample points.
of underdriven diverging waves in the $P\,V$ plane parametrized by the curvature with the locus of planar CJ states corresponding to a partially burned Hugoniot parametrized by $\lambda$. From Fig. 3 it is clear that the family of partially burned planar CJ states is a bad approximation for the sonic states in an underdriven diverging detonation wave even though they too can be characterized by their value of $\lambda$. Unlike the planar detonation Hugoniot which is determined from the equation of state alone, the curved detonation Hugoniot depends on some aspects of the reaction dynamics and cannot be derived solely from the equation of state. This shows that the introduction of a new length scale, even if small compared to the mesh size, can significantly modify the large scale flow.

In a tracking algorithm the question arises whether the end state of an underdriven detonation should be the sonic point or the fully burned state. Figure 3 shows that the loci of some points and end states for the underdriven diverging detonation almost overlap. However, the end states are displaced to lower pressures as can be seen from the difference in the end points of the two lines. The end points correspond to the same front curvature.

**MODIFIED JUMP CONDITIONS**

The curved detonation shock Hugoniot must be insensitive to the uncertainties in the reaction rate if it is to be useful for propagating detonation waves. Here we use the conservation laws to derive jump conditions that account for the width of the detonation wave and use only integral quantities within the reaction zone. By determining these integral quantities empirically from wave propagation experiments we expect to capture the important wave properties in a manner that is insensitive to the detailed reaction dynamics.

Suppose the detonation wave speed is slowly varying in time and that the reaction zone is quasi-steady. This motivates the assumption that leading order $\partial_x D$ can be neglected, and the state variables depend on $x - Dt$. Under these assumptions, integrating Eqs. (9-11) through the reaction zone from $x_j$ (the end of the reaction region) to $x_i$ (the unburned state) leads to the equations for mass, momentum, and energy fluxes through the reaction zone:

$$J[\rho(u - D)] + sw(\rho)D_{,z} = 0 \quad (13)$$
$$J[\rho(u - D) + AP + sw(\rho)D - (P)]_{,z} = 0 \quad (14)$$
$$J[\rho(u - D) + Ap + sw(\rho)D]_{,z} = 0 \quad (15)$$

where $\rho = x_0$, $x_j$ is the reaction zone length, and the average quantities within the reaction zone are defined by

$$\overline{(\rho)}_{,z} = \int_{x_j}^{x_i} A dx \rho,$$
$$\overline{(\rho u A)}_{,z} = \int_{x_j}^{x_i} A dx \rho u,$$
$$\overline{(\rho u^2 A)}_{,z} = \int_{x_j}^{x_i} A dx \rho u^2,$$
$$\overline{(P)}_{,z} = \int_{x_j}^{x_i} A dx P.$$
In deriving these equations we have used the approximation
\[ \frac{dA}{dx} / A = \kappa \approx \text{constant} \]

Previously, we had approximated the integrals as the average of the end points, which is equivalent to the trapezoidal rule. For example, the mass in the reaction zone is given by
\[ \int_{x_l}^{x_r} \rho \, dx = \frac{1}{2} (\rho_{x_l} A_{x_l} + \rho_{x_r} A_{x_r}) \left[ 1 + O(w^2) \right]. \]
However, the coefficient of the error is proportional to \( d^2\rho / dx^2 \). Since the end points \( \rho(x_0) \) and \( \rho(x_1) \) are almost constant, the shape of the profile causes \( d^2\rho / dx^2 \) to increase as \( w \) gets small. Thus, the approximation does not give the leading order correction to the jump conditions.

Suppose the average densities are known. Then we can express the fluxes through the reaction zone by the following modified jump equations
\[ \begin{align*}
J[\rho(u - D)] & = \kappa \left[ \rho_1 \left( u_1 - D \right) + \left( \rho \right) D \right], \quad (16) \\
J[\rho \left( u - D \right) + P] & = \kappa \left[ \rho_1 \left( u_1 - D \right) + P_1 + \rho \left( u - \left( P \right) \right) \right], \quad (17) \\
J[\rho \left( u_1 - D \right) + u P] & = \kappa \left[ \rho_1 \left( u_1 - D \right) + u_1 P_1 + \left( \rho \right) D \right], \quad (18)
\end{align*} \]
where we have used the approximation
\[ A_0 - A_1 \approx w \frac{dA}{dx} / x = \kappa \omega A_0. \]

The right hand side of the flux equations is proportional to the dimensionless quantity \( \kappa \omega \) which is positive for a diverging wave and negative for a converging wave. For \( \kappa \omega = 0 \), they reduce to the planar jump conditions, Eqs. (5.7). The modified jump equations use the same approximation and are valid to the same order as the quasi-steady ODEs for the reaction zone profile discussed in the previous section. Equations (16-18) represent the leading order correction to the Hugoniot jump relations that accounts for the interaction between the geometric source terms from the front curvature and the rate of which chemical energy is released. For a fixed front curvature \( \kappa \), as the reaction rate increases the reaction zone length decreases. Consequently, the correction terms to the jump relations decrease and hence the curvature effect diminishes. In a numerical simulation with a capturing algorithm, decreasing the cell size has the same effect.

The correction terms have a physical interpretation. The first term on the right hand side of Eq. (16-18) corrects the outgoing integrated flux for the change in cross sectional area of the stream tube through the reaction zone. The term proportional to \( \kappa \omega \) in Eq. (17) represents a transverse momentum transfer within the reaction zone. The terms proportional to the product of the detonation velocity and the average densities represent the increase in the total of the conserved quantities within the reaction zone as the radius of curvature of the front and hence the volume of the reaction zone increases. Though the sum of these corrections is frame independent, their relative magnitudes are not. For a rate stick, it is natural to use the frame in which the reaction zone is stationary. In this case, the wave speed vanishes and the conserved quantities within the reaction zone are time independent. For an expanding detonation wave the natural frame is the one in which the origin is at rest. In this frame the increase of the reaction zone volume is a significant term.

The modified jump relations depend on five parameters: the reaction zone width and the volume averages over the reaction zone of the pressure and of the mass, momentum and energy densities. Once these parameters have been determined experimentally, as a function of wave strength, the curvature effect can be determined by solving algebraic equations. Rather than requiring a detailed understanding of the reaction zone dynamic this procedure would use a small number of integral quantities. It therefore provides the framework for a simple phenomenological description of wave propagation of curved detonations.

We have checked the plausibility of this idea with the simple model explosive used in the previous section as follows:

1. The reaction zone length and the average densities are calculated for a planar detonation;
2. For a given \( \kappa \) the quasi-steady ODEs are solved to determine the end state of the detonation shock Hugoniot;
3. The modified jump conditions are tested using the end states from (2) and the integral quantities from (1) with the corresponding detonation velocity.

The results of this test are shown in Fig. 1 and 3 for the diverging and converging cases respectively. As a dimensionless measure of the error we use the (left hand side - right hand side) of Eqs. (16-18) divided by the flux into the detonation front. From the figures we see that the error is \( \mathcal{O}(\kappa\omega) \) until limited by numerical roundoff errors. Because the quasi-steady approximation is only valid to first order in \( \kappa \omega \), it is consistent with the accuracy of the approximation to use the volume averages obtained from the planar wave for small values of \( \kappa \). In effect this shows that the curved detonation wave can be determined as a perturbation of the planar detonation wave with the same detonation speed.
SUMMARY

In order for a simulation of the reactive flow equations to predict the behavior of an explosive, a numerical algorithm must accurately propagate detonation waves. As with a non-reactive material the dominant wave behavior of an explosive is determined by its equation of state. However, in contrast to a shock wave, the width of a detonation wave cannot be neglected. This gives rise to a significant correction to the propagation of a detonation wave known as the curvature effect. The numerical width of a detonation wave in computing algorithms gives rise to an artificial curvature effect which results in a mesh dependence of numerical simulations.

Analysis of the dynamics of the reaction zone has led to an understanding that the curvature effect is due to the interaction between geometric source terms from the curvature of the detonation front and the rate at which energy is released by the chemical reaction. Underdriven detonation waves decouple from the flow behind and the wave front can be correctly propagated with detonation shock dynamics. However, the state behind the front must be carefully chosen such that the reactive front and the hydrodynamic front are propagated consistently.

We are studying a unified approach that can be used with a front tracking algorithm to propagate both underdriven and overdriven detonation waves. The subgrid structure reaction zone dynamics needed to propagate a detonation wave can be characterized analytically by the curvature dependent detonation shock Hugoniot. Given an equation of state and a reaction rate law, the curved detonation shock Hugoniot can be determined by integrating the ODEs for the quasi-steady reaction zone profile.

Numerical calculations use effective rate laws which averages over complicated and frequently not completely understood chemistry, and over length scales associated with material heterogeneities and transverse wave instabilities. At present, it is not possible to derive an averaged reaction rate from macroscopic chemical data. It is therefore necessary to use macroscopic data, such as a Pop Plot or the front curvature and detonation velocity in a rate stick, in order to empirically determine the effective rate law. Because of the difficulty of determining the functional form of a rate law, we have identified integral quantities which completely determine the curvature effect on wave propagation.

Constraints on the curvature effect from the conservation laws can be expressed as modified Hugoniot jump relations. The reaction zone dynamics enters the jump relations only through the reaction zone width and average values of pressure and of the mass, momentum and energy fluxes. At least for a simple rate law and equation of state we have shown that the curved detonation shock Hugoniot can be obtained from the modified jump conditions as a perturbation of a planar detonation.
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