Geometric Scaling for a Detonation Wave Governed by a Pressure-Dependent Reaction Rate and Yielding Confinement

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1 Introduction

The study of how detonation waves respond to losses is the primary experimental and theoretical means of understanding detonation dynamics. Specifically, for condensed explosives, quantifying the relationship between the diameter of a cylindrical charge with yielding confinement, propagation velocity, and front curvature is the principal technique used to develop models for detonation propagation for a given explosive. Likewise, for gaseous explosives, the response of the detonation velocity to losses in a finite diameter channel or tube due to heat transfer and friction reveals the link between the dynamic parameters (e.g., detonation cells) that characterize its structure and its global propagation behavior as quantified by the propagation velocity.

Recently, experimental results have been reported that appear to dispute the predictions of classical front curvature for both gas phase [1, 2] and condensed phase explosives [3, 4]. In classic, front-curvature-governed detonation waves, the propagation velocity deficit and critical velocity at failure should scale between axisymmetric (diameter d) and two-dimensional (slab thickness t) geometries according to d:$t \approx 2$:1. [5] The experimental results above report a scaling between these two geometries of approximately d:$t \approx 1$:1 for gaseous detonations in thin channels and d:$t \approx 3-4$:1 for gaseous and condensed phase detonations in wide rectangular slabs. Other studies, however, have verified an approximate 2:1 scaling as predicted by classic front curvature models. [6, 7] The difference between these results is hypothesized to be the heterogeneity of the systems studied: In systems with smooth, laminar-like reaction zones, the classic scaling relation is expected to be valid. Systems of this type would include highly-argon diluted gaseous explosives or plastic-bonded condensed explosives (PBX's) with very fine grain size in comparison to their critical diameter. In systems where the scaling breaks down, the wave is characterized by very rough, randomized and heterogeneous structures, such as seen in hydrocarbon

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gaseous detonations without noble gas dilution and condensed explosives with heterogeneities having a scale that are comparable to their critical diameter (e.g., blasting slurries, TBX's, etc.).

This paper outlines a program to systematically investigate detonation propagation while interacting with yielding confinement in different dimensionalities (axisymmetric, two-dimensional, and three-dimensional). For convenience, an ideal gas equation of state will be assumed, but the specific geometry considered (an explosive layer bounded by an inert layer of comparable density) is, in many ways, more similar to rate stick and slab experiments widely used for condensed phase explosives. Both steady, ZND-type analytic models and multidimensional and unsteady computational simulations will be examined. We begin, in the present study, by examining a perfect gas system which is expected to exhibit near-classical scaling due to its smooth wave structure. Specifically, a pressure-dependent reaction rate is selected with a reaction order of $n = 2$. This system appears to be stable, resulting in a laminar reaction zone structure, but still results in a critical dimension at which the detonation fails. This reaction model avoids the stability issues associated with using Arrhenius-type reaction mechanisms, which result in unconditionally unstable modes in multidimensional simulations. Extensions of this study will examine increasing reaction order and, eventually, Arrhenius-based kinetics with increasing activation energy, in which instability-generated transient dynamics are encountered. By systematically varying the degree of instability in the detonation wave and measuring the scaling between geometries, the point at which detonation dynamics is no longer governed by front curvature and instead becomes dominated by local mechanisms of propagation can be identified. In addition, detailed computations can be compared to analytic models to determine the domain of appropriate application of models based on weakly divergent flow or weakly curved shock fronts.

2 Modeling

2.1 Analytic Modeling

The detonation of a layer (two-dimensional) or column (axisymmetric) of explosive gas mixture bounded by an inert gas can be treated via a quasi-one-dimensional stream tube analysis. This approach was originally developed by Tsuge [8] and Fujiwara [9] to model the experiments of Sommers and Morrison [10]. The one-dimensional steady Euler equations with area change are numerically integrated along the central axis of the explosive layer, starting from the post-shock state. The shock velocity is iterated upon until a solution that passes smoothly through the sonic plane is identified (i.e., the eigenvalue solution satisfying the generalized Chapman Jouguet condition). The details of this procedure can be found in [11]. In order to couple the diverging flow area through the reaction zone to the yielding confinement of the bounding inert gas, the flow of inert gas past the expanding detonation products is modeled using Newtonian impact theory, as first proposed by [8, 9]. This technique provides a simple, analytic, but physics-based model to specify the rate of area divergence through the reaction zone.

For the calculations presented here, the reaction rate is assumed to follow the form

$$\frac{d\lambda}{dt} = k\,(1-\lambda)\left(\frac{p}{p_{\mathrm{CJ}}}\right)^{n}. \tag{1}$$

This weakly state dependent model for reaction rate is used (rather than the more familiar Arrhenius rate) because the resulting wave is stable and thus can be verified via computational fluid dynamic simulations of the unsteady, multidimensional Euler equations (see next section). The reaction order of $n = 2$ was used; use of values of $n < 2$ does not appear to result in critical behavior, meaning that the layer thickness can be decreased indefinitely, resulting in a monotonic decrease in detonation velocity. [12] This type of pressure-dependent reaction rate model has recently been used to model condensed-phase

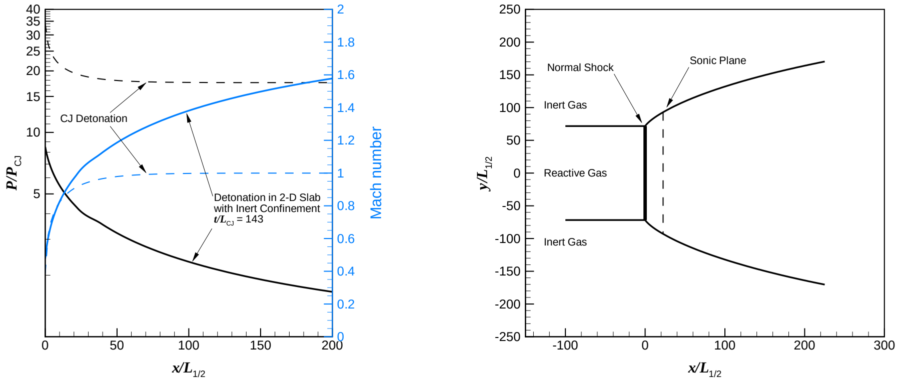

Figure 1: Pressure and Mach number (left) and stream tube area (right) for detonation in a thin layer of reactive gas surrounded by an inert layer, as calculated by quasi-1-D stream tube model. The ideal CJ detonation presssure and Mach number profile is also shown (thin lines).

explosives. [13, 14] The value of k is arbitrary, and the results here will be reported in terms of half-reaction zone length of the ideal CJ detonation. The ratio of specific heats $\gamma = 1.333$ and heat release $\frac{q}{RT_1} = 24$ were used as values representative of a hydrogen/oxygen detonation.

2.2 Computational Modeling

The unsteady, two-dimensional Euler equations with the same pressure-dependent reaction rate term described above are solved using a second-order accurate algorithm. Generally, the chemical reactions have much shorter time scales than those associated with the flow, resulting in stiffness due to coupling the fluid dynamics and the chemical kinetics. In order to isolate this stiff source term, a second-order accurate Strang operator splitting method [15] is employed in this study. The Euler equations with a reactive source term is thus split into a homogeneous partial differential equation for the fluid dynamics and an ordinary differential equation for the chemical reaction. The AUSM+ scheme [16] is used to deal with the inviscid flux as a sum of the convective and pressure terms due to recognizing the convection and acoustic waves as two physically distinct processes. A third-order TVD Runge-Kutta method [17] is used for the temporal discretization. The boundary condition along the x-axis is a mirror boundary condition (axis of symmetry), so that only the upper half of the layer is simulated in the case of a two-dimensional slab. The upper boundary of the computational domain (above the inert layer) is a supersonic outflow condition to ensure that no reflected waves return into the computational domain.

The simulations were initialized with a region on the left end of the computational domain where the initial pressure was set to twice the Chapman Jouguet pressure in order to initiate a detonation. The wave was initially overdriven and then allowed to propagate a distance sufficient to reach a steady velocity. We do not believe the details of the initiation process influenced the final velocities reported below.

3 Results

Figure 1 shows the reaction zone structure as calculated using the quasi-one-dimensional (Q1D) stream tube model described in Section 2.1. This calculation was done for the near-critical case where the explosive layer has a thickness of $143L_{\frac{1}{2}}$, where $L_{\frac{1}{2}}$ is the half reaction zone thickness of the ideal CJ detonation. The eigenvalue velocity in this case is about 50% of the ideal CJ detonation velocity.

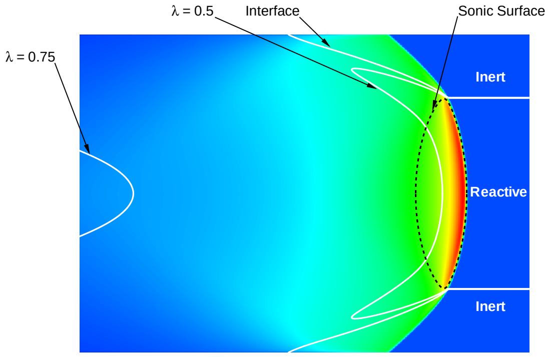

Figure 2: Detonation wave structure for a two-dimensional layer of reactive gas bounded by inert gas. The color scale represents pressure. White contours show values of the reaction progress variable, and the black dashed line is the sonic surface.

The reaction zone structure predicted by the Q1D model is also compared to the reaction zone structure for an ideal CJ detonation (i.e., without lateral expansion). Interestingly, the reaction is only about 1/3 complete at the location of the sonic plane (reaction progress variable $\lambda = 0.33$), which is a significant contribution to the large velocity deficit of about 50%. This result differs from that of detonations governed by Arrhenius reaction rates with divergent flow, for which the velocity deficit is predominately attributed to momentum losses and not due to incomplete reaction at the sonic plane. [11]

The two-dimensional computations are shown in Fig. 2, where the reaction progress variable is shown in color and the sonic line is shown as a thick dashed line. The structure obtained is in good qualitative agreement with the reaction zone structure proposed by Bdzil [5] and recently verified in computational simulations by Sharpe and Braithwaite. [14]

In Fig. 3, the propagation velocity of the detonation is plotted, as obtained after the wave had propagated a distance sufficient to result in a steady wave velocity. The velocity is plotted as a function of the inverse of the diameter ($L_{\frac{1}{2}}/d$) or twice the thickness of the explosive layer ($L_{\frac{1}{2}}/2t$) and nondimensionalized by the half-reaction thickness of the ideal CJ detonation. The wave velocity is plotted in this fashion, following the convention of the condensed phase detonation literature, so that extrapolation to the y-axis should yield the ideal CJ velocity. The factor of two applied to the thickness is in anticipation of the expected 2:1 scaling between diameter and thickness. As the thickness of the layer decreases, the velocity predicted by the Q1D stream tube model progressively decreases until, for an inverse diameter or thickness of $L_{\frac{1}{2}}/\left(d \text{ or } 2t\right) \approx 0.003$, the slope reaches infinite. Continuing to iterate upon even lower values of the shock velocity reveals a lower branch of the solution that approaches the sound speed, which is usually considered to be nonphysical. Thus, the turning point found in the steady solution is associated with failure of the detonation wave. The computational results exhibited a similar behavior, with the steady velocity of propagation decreasing until the wave is no longer able to propagate and fails (note only steady propagation velocities found in the simulations are reported in this figure). In the computational simulations, the critical diameter and thickness were found to be about a factor of 3 smaller than those predicted by the Q1D model. Ongoing analysis is attempting to identify the magnitude of different sources of discrepancy between the Q1D and 2D calculations. We conjecture that the likely explanations are: (1) The detonation flow-field in the case of weak confinement (the case considered here) is inherently multidimensional and cannot be effectively treated with a quasi-one-dimensional model and (2) the interaction with confinement has been treated using highly idealized Newtonian impact theory, which neglects the actual shock physics of the interaction with the boundary.

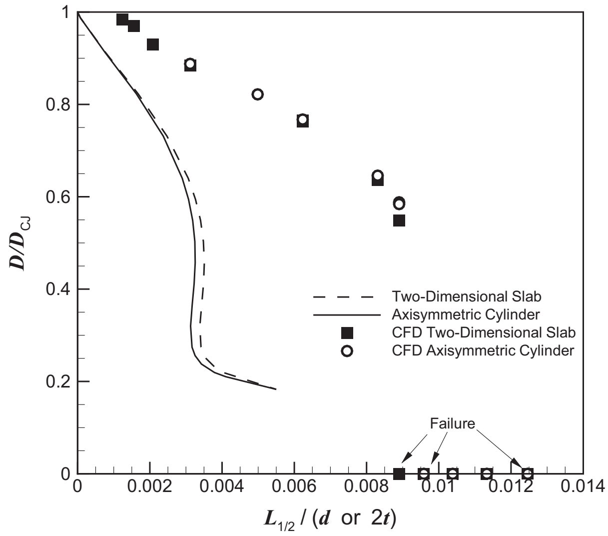

Figure 3: Detonation velocity (normalized by ideal CJ velocity) as a function of layer thickness or diameter (nondimensionalized by the half reaction length of the ideal CJ detonation) for the quasi-one-dimensional stream tube model (curves) and CFD simulations (points).

Although the Q1D model does not explicitly treat the shock front curvature, divergent flow along the central axis can be shown to be equivalent to shock front curvature [11, 18] Thus, if the correct physics can be incorporated into determine the flow divergence, the model should be able to be brought into agreement with the numerical simulations. The observed critical velocity at which failure occurs is in fairly good agreement between the model and simulation, however. In both the Q1D model and the 2D and axisymmetric computational simulations, the results obtained appear to scale approximately as predicted by theory; the diameter/thickness ratio at the failure point is approximately 2:1.

4 Conclusions

The results of this study verify that a detonation wave governed by a pressure dependent reaction rate, which generates a stable detonation wave structure, exhibits the 2:1 scaling between (*i*) the critical diameter and critical thickness and (*ii*) the velocity deficit as these critical velocities are approached for the two different geometries considered. While the stream tube model of Tsuge and Fujiwara over predicts the critical diameter and thickness by a factor of approximately 3, the qualitative behavior of their model and the critical velocity at which failure occurs agree well with the more detailed, multidimensional simulations. This work lays a foundation for further studies that will computationally examine increasingly complex wave dynamics, including detonations governed by Arrhenius kinetics, which exhibit a transient cellular structure, in order to determine if and when a breakdown in the classic scaling relationship occurs.

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