

# Detonation Properties Of A Model Condensed-Phase Explosive With A Pressure Sensitive Rate Law

Tariq D. Aslam \*

Los Alamos National Laboratory

Los Alamos, NM, USA

e-mail: aslam@lanl.gov

## 1 Background

During the course of modeling detonations in condensed-phase explosives, one typically resorts to empirical models for describing both the rate of chemical energy release and the equation of state of the explosive. At a minimum, the models are calibrated to one-dimensional shock initiation experiments, where samples of the explosive are struck with an inert flyer, causing an initial shock in the explosive. This lead shock will cause reaction to occur in the explosive which eventually builds to a detonation. During this build-up process, one can measure the shock speed in the explosive, as well as the particle velocity and/or pressure in the reacting flow [2] [5]. Often, the models will also be calibrated to a diameter effect curve, which shows the dependence on detonation propagation speed versus charge size of an unconfined explosive cylinder. The focus of this work is to examine some properties of one simple model, described next.

## 2 Mathematical Model

The model examined here [1] incorporates a pressure sensitive rate law, and an ideal equation of state, with  $\gamma = 3$ , appropriate for a condensed-phase explosive [4]. These complete the reactive flow model:

$$\frac{\partial \rho}{\partial t} + \bar{\nabla} \cdot (\rho \bar{u}) = 0, \quad (1)$$

$$\frac{\partial \rho \bar{u}}{\partial t} + \bar{\nabla} \cdot (\rho \bar{u} \bar{u} + \bar{I} P) = 0, \quad (2)$$

$$\frac{\partial \rho e}{\partial t} + \bar{\nabla} \cdot [(\rho e + P) \bar{u}] = 0, \quad (3)$$

where  $e = E + (\bar{u} \cdot \bar{u})/2$ ,  $\rho$  is density,  $\bar{u}$  is particle velocity,  $P$  is pressure and the the internal energy,  $E(P, \rho, \lambda)$  is taken as the polytropic form

$$E(P, \rho, \lambda) = \frac{P/\rho}{\gamma - 1} - q\lambda, \quad (4)$$

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with  $q$  the heat of detonation and  $\lambda$  the reaction progress variable ( $\lambda = 0$  is unreacted), which is governed by

$$\frac{d\lambda}{dt} \equiv R = k\sqrt{1-\lambda} \left( \frac{P}{P_{cj}} \right)^n, \quad (5)$$

Furthermore, we have chosen the following parameters:  $q = 4\text{mm}^2/\mu\text{s}^2$ ,  $\rho_o = 2\text{gm/cc}$ ,  $P_o = 1\text{bar}$ . This yields a Chapman-Jouget (CJ) detonation velocity of  $D_{cj} = 8\text{mm}/\mu\text{s}$ , and a CJ pressure of  $P_{cj} = 320\text{kbar}$ , typical of high explosives. Also, the rate multiplier,  $k$ , was chosen to give a total reaction-zone length,  $L_{rz}$ , of  $4\text{mm}$ . The reason for choosing this particular model is twofold. The rate law has a pressure sensitivity similar to many shock initiation models [6] [11]. Also, this particular model has been studied theoretically in [1], using a weakly-curved, quasi-steady asymptotic approach called detonation shock dynamics (DSD). We are interested in  $0 \leq n \leq 3$ , which are typical values used in pressure sensitive rate models [6] [11]. It has been demonstrated that the planar Zeldovich-von Neumann-Doring (ZND) detonation wave, for the above model with  $n \leq 2$ , is one- and two-dimensionally stable [10]. Note that for  $n$  large enough, instabilities are observed for the planar CJ wave.

### 3 Direct Numerical Simulations (DNS)

One of the primary focuses of this paper will be to carry out numerical parametric studies of the above model. This will include studying the diameter effect in unconfined charges of explosives (planar geometry) for various charge diameters,  $2R$ , and pressure sensitivity parameters,  $n$ . The typical setup is shown in Fig. 1. Note the disparity in scales,  $L_s \gg R \gg L_{rz}$ , that make such computations difficult on a uniform mesh, if one is to have fine resolution in the reaction zone. Note also that it is necessary to compute reacting flow with multiple materials (high explosive and inert).

To treat the multi-material flow, a level set method [8] is used in conjunction with the ghost fluid algorithm of [3]. The underlying numerical method is a third-order convex essentially non-oscillatory scheme [7]. This method has been shown to yield high fidelity solutions to multi-material compressible reacting flow.

Furthermore, an adaptive mesh refinement (AMR) strategy is used [9], to carry out computations efficiently. Since the propagation of a (non-overdriven) detonation typically contains a sonic surface in the reaction zone, disturbances from behind this surface can not influence the propagation of the detonation shock. And, since the upstream fluid state is quiescent, one can focus the computational effort on the detonation shock and thin reaction zone. This allows for a computational speed-up of  $O(L_s/L_{rz}) \approx O(100)$ . A plot of one such solution is given in Fig. 2.

### 4 Theory

The asymptotic theory presented in [1] yields an intrinsic propagation law for the detonation shock front. In particular, there will be a relation between the normal detonation shock speed,  $D_n$ , the acceleration of the normal detonation speed,  $\frac{DD_n}{Dt}$ , the second derivative (along the shock) of the detonation speed,  $D_{n,\xi\xi}$ , and the curvature of the shock,  $\kappa$ . From

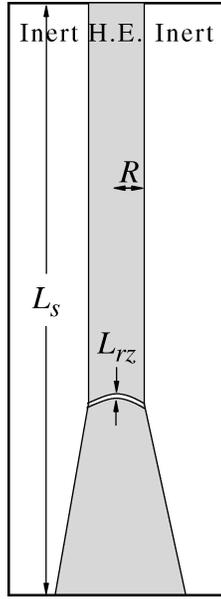


Figure 1: Schematic of the planar rate stick geometry, showing the stick radius,  $R$ , stick length,  $L_s$ , and reaction-zone length,  $L_{rz}$ .

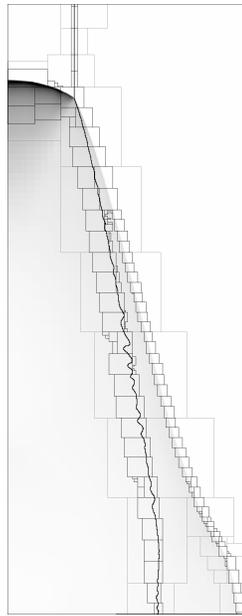


Figure 2: AMR pressure plot (darker color is higher pressure). Also shown are the various mesh patches used, and material interface (dark thick line). Symmetry is assumed on left boundary.

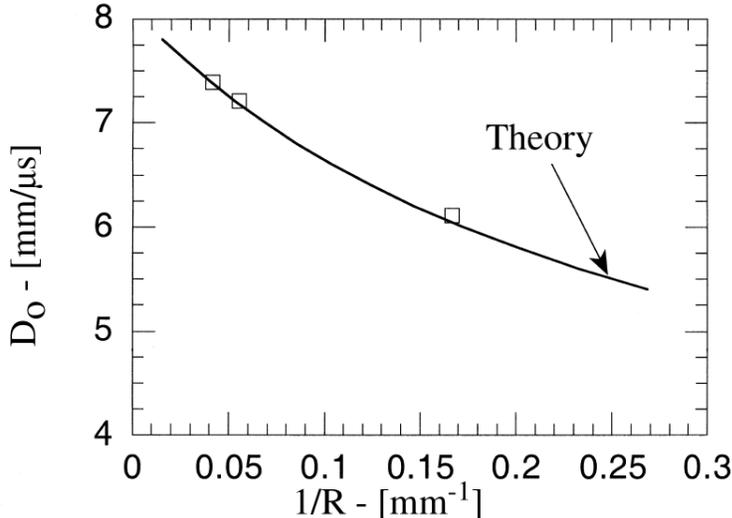


Figure 3: Diameter effect curve from theory ( $n=0$ ). The  $\square$  symbols represent the DNS.

the theory of [1], one can generate steady traveling detonation solutions to the rate stick geometry in Fig. 1. One finds that for  $n = 0$ , given a charge radius,  $R$ , one can find a unique detonation speed on axis (phase velocity up the stick),  $D_o$ . See Fig. 3. Likewise for  $n = 2$ , a similar relation exists, except that the steady solutions only exist for radii greater than some critical radius,  $R > R_c$ , see Fig. 4. Phenomenologically, we find that  $n = 0, 1$  can support a steady traveling wave for arbitrary stick radii, while for  $n = 2, 3$  we find that there is a critical radius, below which a steady traveling solution to the above intrinsic propagation law doesn't exist.

## 5 Discussion

The results from the numerical simulation agree with the theory, that for  $n = 0, 1$  arbitrary stick sizes can support a steady traveling detonation, while for  $n = 2, 3$ , there is a criticality at a certain radius. It is found from carrying out several numerical simulations that for  $n = 2$ ,  $R_c = 17.5mm \pm 0.5mm$ , while for  $n = 3$ ,  $R_c = 34mm \pm 2mm$ . The corresponding detonation phase velocity versus inverse radius are shown in Figs. 3 and 4. Furthermore, it is observed that the  $n = 2$  DNS appears to propagate a steady traveling detonation up the ratestick (even for  $R$  near  $R_c$ ), while for the  $n = 3$  case, the DNS appear to be unstable for  $R$  near  $R_c$ . Also, the DNS and theory agree well when one is not near the failure radius.

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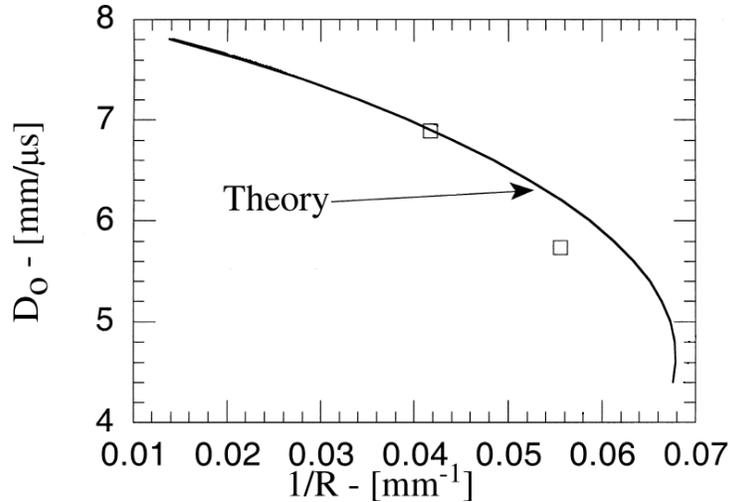


Figure 4: Diameter effect curve from theory ( $n=2$ ). The  $\square$  symbols represent the DNS.

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