# Analog System of Detonations with Losses and Pressure-Dependent Reaction Rate

XiaoCheng Mi[1], Yuanxiang Sun[2], Junqiu Zhang[2], Pengyan Hu[2], and Cheng Wang[2]

[1]McGill University
Montreal,Canada
and
[2]State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology
Beijing, China

## 1 Introduction

The existence of a critical condition (i.e., a condition at which detonation is no longer possible) when losses are present is one of the defining characteristics of detonation waves. In the presence of losses in mass, momentum, or energy as resulting from, for example, boundary layers on a tube wall for gaseous detonations or lateral expansion due to yielding confinement for solid explosives, there exists a critical degree of loss beyond which a detonation wave solution is no longer possible, and this feature is associated with the existence of detonation limits in experimental practice. By solving the eigenvalue problem for the detonation by numerically iterating upon the structure of the reaction zone, the detonation velocity vs. the loss parameter (e.g., friction, curvature, etc.) exhibits a turning point that can be defined as the critical condition for propagation. This approach was originally developed by Wood and Kirkwood [1] and then significantly expanded upon by Bdzil [2] and Cowperthwaite [3].

For a detonation reaction rate that does not exhibit extreme sensitivity to the local thermodynamic state, it may not be possible to find a critical condition. The use of a $p^n$ reaction rate model is popular in the modelling of condensed explosives, since they do not exhibit the exponential (Arrhenius) sensitivity to temperature in the burn-out of the explosive in the reaction zone. For a sufficiently low value of $n$ ($n \lesssim 2$), the detonation may not exhibit a turning point in the detonation velocity vs. front curvature relationship, meaning that a detonation solution always exists [3].

Attempts to compare the predictions of steady-state theory to full numerical simulations of detonation dynamics are complicated by the fact that the detonation wave may be unstable, exhibiting regular or chaotic oscillations. For example, in one-dimension with $\gamma = 1.2$ and $Q/\mathrm{R}T_0 = 50$, Chapman-Jouguet detonations in the case of activation energy greater than $E_\mathrm{a}/\mathrm{R}T_0 = 25.26$ result in an unstable, oscillating wave. [4, 5] In two dimensions, detonation waves are even more susceptible to instability, with all detonations for any value of activation energy being unstable to transverse perturbations. [6] For a pressure-dependent reaction rate, Short et al. [7] showed that for sufficiently small values of $n$ ($n < 2.168$ for $\gamma = 3$), it is possible for the detonation wave to be stable in two dimensions. It is intriguing that this value of $n$ is near the value required to exhibit a critical point in the detonation velocity/curvature relation. This paper seeks to explore the relation between these two phenomena, namely, can a detonation that is stable exhibit a critical velocity for propagation?

Instead of the reactive Euler equations, a one-dimensional analog system, which mimics the dynamics of detonations with losses and a pressure-dependent reaction rate law, is considered in this present work.

The existence of a minimal $n$ (denoted as $n_{\mathrm{crit}}$) required for this analog system to exhibit a critical point in the relationship of detonation velocity vs. loss parameter will be first examined. As a preliminary study, a linear stability analysis will be performed to investigate whether the ideal steady state detonation structure modeled by this analog system is stable to small one-dimensional perturbations.

## 2 Description of the Analog System

This one-dimensional analog system is constructed in an Eulerian reference frame as Fickett's model [8], while the energy released by reaction is treated as that in Majda's model [9]. The losses due to divergent flow are modeled as a state-dependent loss term, which was proposed by Faria and Kasimov [10]. The coefficient associated with the loss term represents the curvature of the detonation wave front, so it is denoted as $\kappa$. By setting $\kappa = 0$, the system reverts to an ideal detonation. This analog system is governed by a reactive Burgers equation as follows,

$$\frac{\partial \rho}{\partial t} + \rho \frac{\partial \rho}{\partial x^{\mathrm{L}}} = q \frac{\partial Z}{\partial t} - \kappa \left( \frac{\rho}{\rho_{\mathrm{CJ}}} \right)^m \tag{1}$$

where $\rho$ is a scalar quantity representing some features of an intensive property in compressible flow, $Z$ is the reaction progress variable ($Z = 0$ for unreacted and $Z = 1$ for fully reacted), $q$ represents the spatial density of energy released by the explosive medium, $m$ is the state dependence of loss rate, and superscript "L" indicates the coordinate in a lab-fixed reference frame. It can be shown that the ideal Chapman-Jouguet detonation velocity for this system is as follows,

$$\rho_{\mathrm{CJ}} = D_{\mathrm{CJ}} = 2q \tag{2}$$

The reaction rate law is specified as the following equation to mimic a pressure-dependent reaction rate, which is commonly used to model detonations in condensed phase explosives,

$$\frac{\partial Z}{\partial t} = (1 - Z)^{\nu} \left( \frac{\rho}{\rho_{\mathrm{CJ}}} \right)^n \tag{3}$$

Via $x = x^{\mathrm{L}} - Dt$, Eqs. 1 and 3 can be transformed into a wave-attached reference frame,

$$\frac{\partial \rho}{\partial t} + (\rho - D) \frac{\partial \rho}{\partial x} = q \left( \frac{\partial Z}{\partial t} - D \frac{\partial Z}{\partial x} \right) - \kappa \left( \frac{\rho}{\rho_{\mathrm{CJ}}} \right)^m \tag{4}$$

$$\frac{\partial Z}{\partial t} - D \frac{\partial Z}{\partial x} = (1 - Z)^{\nu} \left( \frac{\rho}{\rho_{\mathrm{CJ}}} \right)^n \tag{5}$$

Assuming the strong shock limit, the jump condition at a nonreacting shock (i.e., Rankine-Hugoniot relation) is

$$\rho(x = 0) = 2D, \quad Z(x = 0) = 0 \tag{6}$$

### 2.1 Steady State Solutions

Steady state solutions $\rho_0(x)$ and $Z_0(x)$ satisfy the following equations,

$$(\rho_0 - D_0) \frac{\mathrm{d}\rho_0}{\mathrm{d}x} = -q D_0 \frac{\mathrm{d}Z_0}{\mathrm{d}x} - \kappa \left( \frac{\rho_0}{\rho_{\mathrm{CJ}}} \right)^m \tag{7}$$

$$-D_0 \frac{\mathrm{d}Z_0}{\mathrm{d}x} = (1 - Z_0)^{\nu} \left( \frac{\rho_0}{\rho_{\mathrm{CJ}}} \right)^{n} \tag{8}$$

Applying the jump condition at the shock, Eqs. 7 and 8 can be integrated numerically. To close Eqs. 7 and 8, the generalized Chapman-Jouguet condition, i.e., the rate of energy release is exactly balanced by the loss rate at the sonic locus relative to the leading shock (where $\rho_0 - D_0 = 0$), is required. For a given steady state detonation velocity, $D_0$, a unique value of $\kappa$, which satisfies the generalized CJ condition, can be obtained by a numerical "shooting" procedure.

### 2.2 One-Dimensional Linear Stability Analysis

Stability analysis begins by introducing small (linear) perturbations to the steady state solutions via

$$D = D_0 + \epsilon\alpha \exp{(\alpha t)} \tag{9a}$$

$$\rho = \rho_0 + \epsilon\rho_1(x) \exp{(\alpha t)} \tag{9b}$$

$$Z = Z_0 + \epsilon Z_1(x) \exp{(\alpha t)} \tag{9c}$$

where $\rho_1(x)$ and $Z_1(x)$ are the spatially dependent eigenfunctions of linear perturbations to $\rho_0$ and $Z_0$, and $\alpha$ is a complex growth rate of the perturbations. The magnitudes of these linear perturbations are of order $\epsilon$ where $\epsilon \ll 1$. Inserting Eq. 9 into the unsteady governing equations (Eqs. 4 and 5), canceling out the steady state solutions on both sides of the equations, and only retaining the terms of order $\epsilon$, the governing equations of one-dimensional linear stability can be derived,

$$\begin{pmatrix} \rho_0 - D_0 & qD_0 \\ 0 & -D_0 \end{pmatrix} \begin{pmatrix} {\rho_1}' \\ {Z_1}' \end{pmatrix} + \begin{pmatrix} \alpha + {\rho_0}' + \frac{\kappa m}{\rho_{\mathrm{CJ}}} \left( \frac{\rho_0}{\rho_{\mathrm{CJ}}} \right)^{m-1} & -q\alpha \\ -\frac{n(1-Z_0)^{\nu}}{\rho_{\mathrm{CJ}}} \left( \frac{\rho_0}{\rho_{\mathrm{CJ}}} \right)^{n-1} & \nu(1-Z_0)^{\nu-1} \left( \frac{\rho_0}{\rho_{\mathrm{CJ}}} \right)^{n} \end{pmatrix} \begin{pmatrix} \rho_1 \\ Z_1 \end{pmatrix} = \begin{pmatrix} \alpha{\rho_0}' - q\alpha{Z_0}' \\ \alpha{Z_0}' \end{pmatrix} \tag{10}$$

where prime denotes the derivative with respect to $x$. By inserting Eq. 9 into Eq. 6, the shock relations for the perturbation variables are obtained

$$\rho_1(x = 0) = 2\alpha, \quad Z_1(x = 0) = 0 \tag{11}$$

To determine the eigenvalue of the complex growth rate, $\alpha$, a rear boundary condition, which ensures the perturbations to be spatially bounded within the steady reaction zone and not influenced by the disturbances from the far field, must be applied at the CJ point (where $\rho = D$) to close Eq. 10. This condition can be derived by constructing asymptotic solutions for Eq. 10 at the CJ point and eliminating the component of the characteristics propagating forward. For an ideal detonation ($\kappa = 0$) with $0.5 < \nu < 1$, where the CJ point is at the end of the reaction zone, and $\rho_0'$ and $Z_0'$ are zero [7], the simplest form of this closure condition can be obtained,

$$H(\alpha) = \rho_1 + Z_1 \left\{ \frac{q\left[\nu\,(1 - Z_0)^{\nu-1} \left(\frac{\rho_0}{\rho_{\mathrm{CJ}}}\right)^{n} - \alpha\right]}{\frac{\rho_0 - D_0}{D_0}\left[\nu\,(1 - Z_0)^{\nu-1} \left(\frac{\rho_0}{\rho_{\mathrm{CJ}}}\right)^{n}\right] + \alpha} \right\} = 0 \qquad \text{at} \quad x = x_{\mathrm{CJ}} \tag{12}$$

## 3 Results and Discussion

The eigenvalue $D$-$\kappa$ relations for the steady state solution of Eqs. 7 and 8 with $m = 2$, $\nu = 0.75$, and $n = 1.8$ - $2.3$ are plotted in Fig. 1. The value of $\nu$ is chosen to be between $0.5$ and $1$ so the ideal steady state detonation structure of this system has a finite reaction zone length and a zero spatial gradient at the end of the reaction zone. As shown in Fig. 1, the $D$-$\kappa$ curve exhibits a critical turning-point behavior for $n \geq 2.2$. Hence, $n_{\text{crit}}$ can be roughly determined as $2.2$ for a system with $q = 0.5$, $m = 2$ and $\nu = 0.75$.

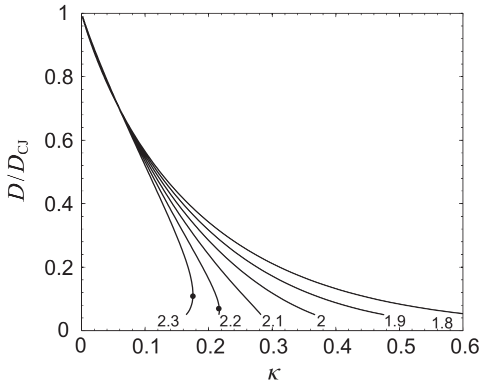


Figure 1: Eigenvalue $D$-$\kappa$ relation for $q = 0.5$, $m = 2$, and $\nu = 0.75$. The value of $n$ is labeled next to each curve. The black dot indicates the critical turning point where detonation fails to propagate.

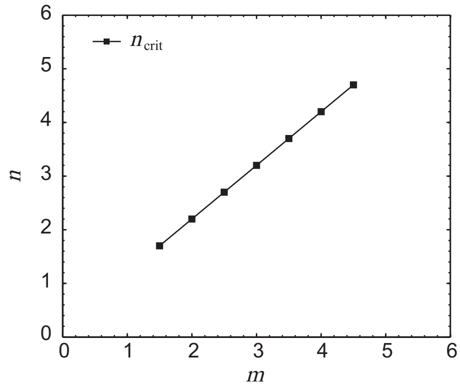


Figure 2: Plot of $n_{\text{crit}}$ as a function of $m$ for $q = 0.5$ and $\nu = 0.75$.

While keeping $q = 0.5$ and $\nu = 0.75$ but varying $m$ in a range from $m = 1.5$ - $4.5$, $n_{\text{crit}}$ is determined in the same manner as shown in Fig. 1. A linear relationship between $n_{\text{crit}}$ and $m$, i.e., $n_{\text{crit}} = m + 0.2$, is found and plotted in Fig. 2.

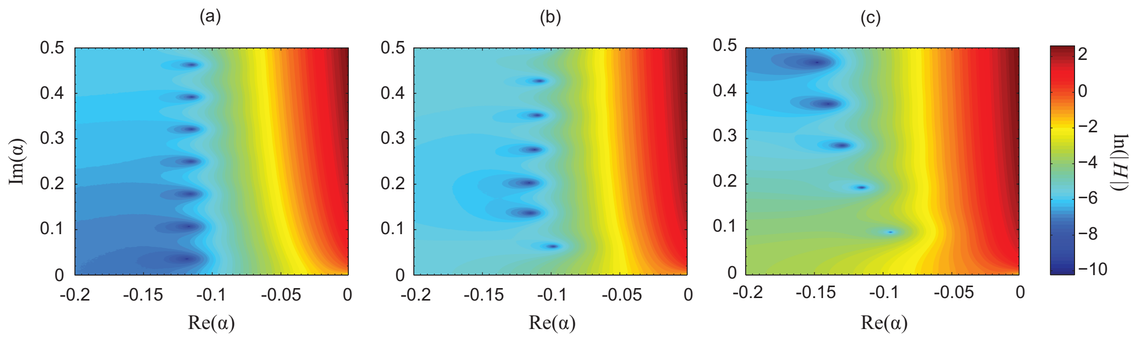


Figure 3: Contour plot of $\ln(|H|)$ showing the locations of the eigenvalues of $\alpha$ for an ideal detonation with $q = 0.5$, $\nu = 0.75$, and (a) $n = 2$, (b) $n = 5$, and (c) $n = 20$.

To determine the eigenvalues of $\alpha$ in Eq. 10, which satisfy the closure condition (Eq. 12), the absolute value of $H(\alpha)$ is evaluated for different real and imaginary parts of $\alpha$, and plotted as logarithmically scaled contours in the complex plane of $\alpha$ as shown in Fig. 3. Each local minimum (dark blue spot) in the contour plots indicates an eigenvalue $\alpha$ satisfying Eq. 12. For $q = 0.5$, $\nu = 0.75$, and $\kappa = 0$, as $n$ is varied from 2 to 20, all the eigenvalue $\alpha$'s are in the negative domain of $\text{Re}(\alpha)$. A slightly rightward migration of the most dominant perturbation mode (i.e., the eigenvalue $\alpha$ with the greatest real part) can be observed as $n$ increases. Hence, although a more sensitive dependence of the reaction rate on the local state property has a destabilizing effect, the ideal steady state solution of this detonation analog system is found to be stable to one-dimensional linear perturbations at least up to $n = 20$.

From the preliminary examinations of the detonation analog system reported in this paper, it was shown that, as the dependence of the reaction rate on the local state property is more sensitive than that of the rate of losses, the detonation system is expected to exhibit a critical point in the $D$-$\kappa$ relation, while this state dependence of reaction rate is not sufficiently sensitive for the ideal steady state detonation structure to be unstable to small one-dimensional perturbations.

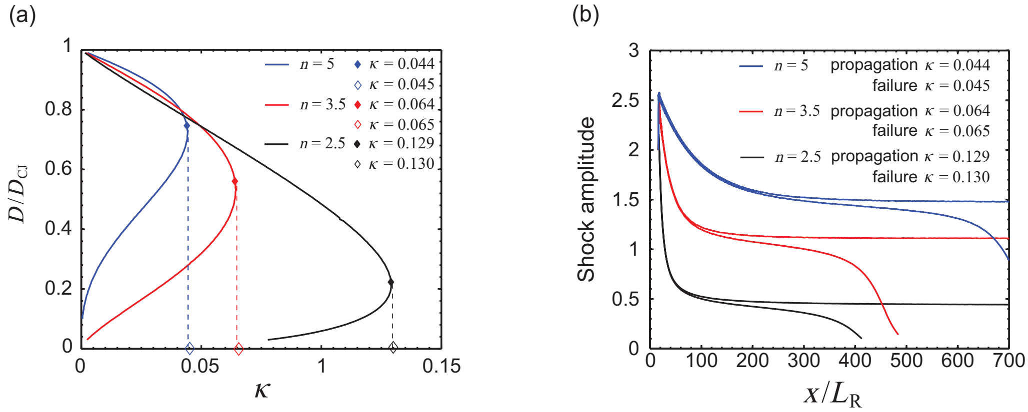


Figure 4: For $q = 0.5$, $m = 2$, and $\nu = 0.75$, the simulation results of (a) the steady detonation velocity compared to the analytically solved eigenvalue $D$-$\kappa$ relation, and (b) the evolution of the leading shock amplitude (i.e., $\rho$ at the shock front) plotted against the propagation distance normalized by the reaction zone thickness, $L_R$. In (a), the analytic solutions are plotted as solid curves, and simulation results as "diamonds". Simulations resulted in detonation failure are denoted as empty diamonds along $x$-axis. The boundary between propagation and failure determined from the simulations are plotted as vertical dashed lines.

As shown by Zhang and Lee [11] for friction and by Sharpe for the case of curvature [12], losses can result in an otherwise stable detonation wave becoming unstable. Therefore, the analog of non-ideal detonations was investigated by direct numerical simulation. A second-order finite volume and second-order source splitting method with an exact Riemann solver and a min-mod slope limiter was used to numerically solve Eqs. 1 and 3. For $q = 0.5$, $m = 2$, $\nu = 0.75$, and 3 different values of $n$ ($n = 2.5$, 3.5, and 5) which all result in a critical point in the $D$-$\kappa$ relation, the loss parameters ($\kappa$) were selected to be slightly smaller or greater than its critical value. As shown in Fig. 4 (b), after being initiated by a high-pressure region, detonations with $\kappa$ smaller than its critical value eventually reach steady state, while those with $\kappa$ greater than its critical value fail to propagate. The steady state detonation velocity is obtained by calculating the average velocity of the leading shock propagating from $x/L_R = 650$ to 700, and, as shown in Fig. 4 (a), agrees well with the analytic solution of the $D$-$\kappa$ relation. All the simulations reported above are performed at a resolution of 50 computational cells per reaction zone length.

The preliminary simulation results show only steadily propagating detonations or quenching, but no oscillatory or chaotic behaviour in the detonation propagation, even with a loss parameter near its critical value. Hence, the presence of losses and a sufficiently sensitive dependence of reaction rate on the local state property as the key mechanism responsible for the critical behaviour of detonation propagation can be successfully captured by this analog system based on the Burgers equation. The mechanism responsible for the instabilities of detonation might be unrelated to that for the propagation/failure criticality, and perhaps cannot be captured by this analog system due to the lack of backward propagating signals which are necessary to establish a feedback loop for the instabilities to persist.

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