Condensed-phase detonation stability for a
Tait equation of state

By MARK SHORT\textsuperscript{1}, JOHN B. BDZIL\textsuperscript{2}
and IANA I. ANGUELOVA\textsuperscript{3}

\textsuperscript{1} Theoretical and Applied Mechanics, University of Illinois, Urbana, IL 61801
\textsuperscript{2} Los Alamos National Laboratory, Los Alamos, NM 87545,
\textsuperscript{3} Department of Mathematics, University of Illinois, Urbana, IL 61801

(Received ?? and in revised form ??)

The linear stability analysis of a planar detonation wave is reformulated for an arbitrary
caloric equation of state in an attempt to better represent the stability properties of
detonations in condensed phase explosives. In this paper, we focus our attention on a
Tait equation of state which allows us to prescribe a finite detonation Mach number, and
simultaneously allows for a detonation shock pressure that is substantially larger than the
ambient pressure. We show that the effect of increasing the ambient sound speed in the
material, for a given detonation speed, has a stabilizing effect on the detonation. We also
show that the slow reaction stage that is present in detonations in explosives like liquid
nitromethane, where the detonation structure is characterized by a fast reaction stage
behind the detonation shock followed by a slow reaction stage, tends to be destabilizing.

1. Introduction

A detonation is a destructive form of propagating wave front, consisting of a lead
shock sustained by chemical reaction in a following reaction zone, which can occur in
gaseous, liquid or solid explosives. The idealised detonation structure in any explosive
is a one-dimensional wave front, the Zeldovich-Von Neumann-Döring, or ZND, wave
(Fickett & Davis 1979), which in most cases propagates at a minimum speed defined
by the presence of a sonic flow point (relative to the detonation wave speed) within the
reaction zone, known as the Chapman-Jouguet, or CJ, detonation. However, in gases, this
idealized structure is invariably unstable, and detonation fronts tend to propagate in a
highly unsteady multi-dimensional manner, leading to the formation of spectacular fish-
scale patterns on the walls of rectangular shock tubes lined with soot-covered aluminum
foil (Fickett & Davis 1979). Several experimental investigations (including schlieren and
PLIF imaging (e.g. Lee 1984, Kaneshige & Shepherd 1997, Austin, Pintgen & Shepherd
2004)) and analysis via direct numerical simulation (e.g. Sharpe 2001, Gamezo \textit{et al.}
2000), have lead to a reasonable understanding of the Mach stem, reflected and lead
shock triple-point interactions that underlie the cellular detonation structure in gases.

On the other hand, comparatively little information is known about the reaction wave
structure in detonating liquid and solid explosives, where the extreme high pressure envi-
noment (\textasciitilde 30-50GPa) and high wave speeds (\textasciitilde 6-8km/s) make experimental diagnostic
data collection and imaging difficult. While there is some evidence that detonations in
some forms of liquid explosives (such as nitromethane diluted with acetone) may exhibit
a cellular structure, it has not yet been established whether this is due to an inherent
reactive-hydrodynamic instability (as in gases) or due to the effects of explosive confinement (Fickett & Davis 1979). On the other hand, laser-based interferometry measurements of particle velocities in the reaction zone of detonations in pure and commercial grade liquid nitromethane (Sheffield et al. 2002), and in the solid explosives PBX9501 (Gustavsen, Sheffield & Alcon 2000) and PBX9502 (Seitz et al. 1989), appear to indicate that the idealized one-dimensional planar structure is stable. This conclusion is reinforced by velocity against curvature measurements of detonations propagating in cylindrical sticks of nitromethane (Hill et al. 1999) and PBX9502 (Hill, Bdzil & Aslam 2000). However, the rapid time resolution (< 1ns) required to experimentally resolve the very fine structure of the detonation front in liquid and solid explosives is currently unavailable. Consequently it seems likely at this point in time that several advances in our understanding of detonation structure and stability in condensed phase systems can be made from mathematical and numerical modeling.

To this end, Short et al. (2005) have examined the stability of planar detonations within the context of the idealized condensed-phase model. This reactive-Euler model consists of a constant-$\gamma$ ideal gas caloric equation of state having $\gamma = 3$, and assumes a one-step reaction with an algebraic pressure-dependent rate (with a sensitivity measured by an exponent $n$) and a non-integer reaction order ($\nu$). In the strong shock limit, and with $\nu = 1/2$, the planar CJ detonation is unstable to disturbances within a finite band of wavenumbers for $n > 2.16$, a value which characteristic of those used to mimic explosives like nitromethane (NM) and PBX9501/2 within the context of the idealized condensed-phase detonation model. Thus the use of this model tends to conflict with the experimental observations that detonations in condensed-phase systems are stable. One of the drawbacks of this model is the use of the ideal-gas caloric equation of state, which, for the typical ratios of detonation shock pressure to ambient pressure found in condensed-phase systems, results in extremely large detonation Mach number values, since the sound speed in the initial state is proportional to the initial pressure. In practice, for most condensed phase explosives the characteristic detonation Mach numbers are in the range 2-4. It seems natural, therefore, to examine the effect on the location of the neutral stability boundaries found in Short et al. (2005) for more realistic equations of state, where the ambient material sound speed can be specified from experiments at a given pressure.

In the following, the classical detonation linear stability problem is reformulated for a caloric equation of state in which the internal energy is specified as an arbitrary function of pressure, specific volume and reaction progress variable. We assume a one-step reaction as in Short et al. (2005), but now with an arbitrary reaction rate law. The extension to multiple reaction steps is trivial, but omitted here for reasons of clarity of the analysis. We then describe the extension of the idealized condensed phase detonation model to a Tait equation of state (Davis 1997), under which the stability of detonations with finite Mach numbers and large ratios of the post- to pre-shock pressures, found in explosives such as NM and PBX9501/2, can be better modelled. Subsequently, we describe the transition in the location of the one- and two-dimensional neutral stabilities that occurs as the detonation Mach number is systematically decreased from infinite values (Short et al. 2005) to finite values, within the Tait equation of state model.

A second question is also addressed in the current paper. It is apparent that detonations in liquid nitromethane and PBX9502 are characterized by reaction zones with dual length scales. These multi-length scale detonations likely occur due to a change in reaction mechanisms within the reaction zone, where one set of explosive components are consumed rapidly behind the detonation shock, and then a second set of components are consumed over a longer time scale (Sheffield et al. 2002). For example, detonation
particle velocity histories in nitromethane (Sheffield et al. 2002) indicate that 70-75% of the reaction occurs with 10ns of the passage of the shock, while the latter 25-30% of the reaction occurs over a time-scale of around 50ns. Similarly in PBX9502 (Seitz et al. 1989), 85% of the reaction occurs with 25ns of the passage of the detonation shock, while the latter 15% occurs over 300ns. Particle velocity histories in PBX9501 (Gustavsen, Sheffield & Alcon 2000) indicate a single length scale reaction zone. We address how the presence of a slow reaction stage, characteristic of detonations in NM and PBX9502, affects the location of the detonation stability boundaries.

The linear stability of detonation for a non-ideal equation of state (similar to that described by Wescott, Stewart & Davis (2004)) has also been examined by Kasimov et al. (2003 and Kasimov (2004), including one-step pseudo reaction models for NM and PBX9502 similar to those used in the current paper. However, their general equation of state stability formulation differs from that contained here, particularly in the form of the ordinary differential equation system that describes the normal mode eigenfunction structure, and in the nature of the shock and compatibility conditions used to provide the eigenfunction boundary conditions. Moreover, for one of the cases discussed in Short et al. (2005), i.e. for a CJ wave with a square root depletion reaction rate within the ideal condensed phase detonation model, where a comparison between the different formulations can be made, Kasimov et al. 2003 and Kasimov (2004) predict the presence of six one-dimensionally unstable modes for a reaction rate pressure exponent value of n = 3, whereas Short et al. (2005) predicts the detonation is only one-dimensionally unstable for n > 5.904. The latter result has been verified by direct numerical simulation (Short et al. 2005).

2. Model

2.1. Equations

The nondimensional equations of motion coupled with an equation for species conservation for the single-step reaction $\mathcal{F} \rightarrow \mathcal{P}$ are given by

$$\frac{DA}{Dt} - \lambda \left( \nabla \cdot \mathbf{u} \right) = 0, \quad \frac{D\mathbf{u}}{Dt} = -\lambda \nabla p, \quad \frac{De}{Dt} = -p \lambda \left( \nabla \cdot \mathbf{u} \right), \quad \frac{D\beta}{Dt} = r, \quad (2.1)$$

for specific volume $\lambda$, pressure $p$, specific internal energy $e$, laboratory frame velocity $\mathbf{u} = (u', v')$ and reaction progress variable $\beta$, where $\beta = 1$ represents unreacted fuel, and $\beta = 0$ is fully depleted fuel. At this stage we adopt the general caloric equation of state and reaction rate forms,

$$e = e(p, \lambda, \beta), \quad r = r(p, \lambda, \beta). \quad (2.2a,b)$$

The (chemically) frozen sound speed $c$ is related to (2.2a) via

$$c^2 = \Lambda^2(p + e, \lambda, \beta). \quad (2.3)$$

Equations (2.1)–(2.3) have been nondimensionalised such that $\Lambda = \tilde{\lambda}/\Lambda_0$, $\mathbf{u} = \tilde{\mathbf{u}}/\tilde{D}$, $p = \Lambda_0 \tilde{p}/\tilde{D}^2$, $x' = \tilde{x}/l$, $t = \tilde{D}t/l$, $e = \tilde{e}/\tilde{D}^2$, $c^2 = \tilde{c}^2/\tilde{D}^2$, where $\Lambda_0$ is the upstream specific volume and $\tilde{D}$ is the dimensional (ZND) planar steady detonation velocity. The length scale $l$ is set below.

3. Travelling wave solutions

The above model supports a one-dimensional steady, travelling wave solution consisting of a lead shock followed by a region of chemical reaction (the ZND structure). In a
reference frame attached to the wave, \( x = x^l - t \), where \( x = 0 \) is set by the location of the shock front, the thermodynamic states in the steady wave for a general caloric equation of state are connected by the conditions

\[
\Lambda = -u, \quad p = u + 1 + p_0, \quad e + p\Lambda + \frac{u^2}{2} = e_0 + p_0 + 1/2, \tag{3.1a,b,c}
\]

where \( p_0 = \tilde{\lambda}_0\tilde{p}_0/D^2 \), is the dimensional unshocked material pressure, and the ambient internal energy \( e_0 = \tilde{e}_0/D^2 \). Relations (3.1a,b) define the Rayleigh line variation, which holds regardless of the form of (2.2a), while (3.1c) defines the Hugoniot curves for any degree of reaction, which do depend on the form of (2.2a). The spatial structure of the ZND wave can be determined through the Master equation relation,

\[
u = \frac{u e^r}{\eta p}, \quad \eta = u^2 - c^2, \tag{3.2}
\]

which depends on the form of both \( e \) and \( r \). Here, \( \eta \) is a sonic parameter. The structure of the CJ wave, the slowest of all possible steady wave solutions, is defined by the appearance of a sonic point relative to the detonation wave speed either at a point of incomplete or complete reaction, and for general forms of (2.2a,b) may be determined as follows. If \( \tilde{D}_{CJ}, \tilde{p}_0 \) and \( \tilde{e}_0 \) are known initially, where \( \tilde{D}_{CJ} \) is the CJ speed, (3.1a,b,c) can be solved to determine the immediate post-shock state at which no reaction has occurred. Subsequently, (3.2) can be integrated from the shock \( (x = 0) \) into the region \( x < 0 \). A single value of the heat of reaction \( \tilde{q} \) will define a solution trajectory which passes through the critical point (where \( \eta \) and \( r \) vanish simultaneously), and it is this trajectory which defines the spatial structure of the CJ wave. Note that if the sonic point appears at the end of the reaction zone, then (3.1a,b,c) can be used to determine \( \tilde{q} \) algebraically, otherwise \( \tilde{q} \) must be determined iteratively by successive integrations of (3.2). If \( \tilde{q}, \tilde{p}_0 \) and \( \tilde{e}_0 \) are known initially, a similar procedure can be used to determine \( \tilde{D}_{CJ} \). Finally, once the CJ wave structure has been determined, it is straightforward to generate the spatial structure of the overdriven ZND wave, defined by a given overdrive factor \( f = D^2/D_{CJ}^2 \).

4. Linear analysis

4.1. Perturbation equations

The equations governing small (linear) perturbations to the steady traveling wave identified in §3 are constructed as follows. We transform to a new spatial coordinate system \( x = x^l - t - \Psi(y,t), y^l = y \), where \( x^l = t + \Psi(y^l,t) \) is the shock locus in laboratory frame, which now becomes \( x = 0 \). We seek a normal mode decomposition,

\[
\Psi = \Psi_0 \exp(\alpha t + ik y), \quad z = z^* + \Psi_0 z'(x) \exp(\alpha t + ik y), \tag{4.1}
\]

for the growth rate/frequency eigenvalue \( \alpha \) and wavenumber \( k \), where \( z = (\Lambda, \ u, \ v, \ p, \ \beta)^T \) represents the vector of dependent variables, the superscript "*" refers to the underlying steady wave solution, the ' quantities indicate the spatially \( x \) dependent eigenfunctions and \( \Psi_0 \ll 1 \). The system of equations that govern the linear stability of a detonation with the general caloric equation of state and reaction rate law (2.2a,b) is then determined to be

\[
\eta^* u^* z'_{xx} + A^* z' + a^* = 0, \tag{4.2}
\]
where the matrix $A^*$ is defined in terms of steady state quantities as,

$$
A^* = \begin{pmatrix}
\alpha \eta + u_x(c^2 - 2u^2) - u^2a_A & -\alpha u^2 + u_x(c^2 - 3u^2) \\
u_x(u_x + a_A) & \alpha u^2 + 2u^2u_x \\
0 & 0 \\
c^2u_x + u^2a_A & \alpha c^2 + u_x(c^2 + u^2) \\
-\eta r_A & \eta \beta_x \\
iu^3 & -u^2(\alpha + a_p) & -u^2a_\beta \\
-iuc^2k & u^2(\alpha + a_p) & u^2a_\beta \\
\alpha \eta & -iku \eta & 0 \\
-iuc^2k & u^2(\alpha + a_p) & u^2a_\beta \\
0 & -\eta r_p & \eta(\alpha - r_\beta)
\end{pmatrix}
$$

(4.3)

where

$$
a_p = (uu_x(e_{pp} - 1 - e_{A\beta}) + e_{,\beta}r_{,p} + e_{,p}r_\beta) / e_p
$$

$$
a_A = (uu_x(e_{pA} + c^2e_{,p}/u^3 - e_{,\Lambda A}) + e_{,\beta}r_A + e_{,\beta}\Lambda r)/e_p
$$

$$
a_\beta = (uu_x(e_{p\beta} - e_{A\beta}) + e_{,\beta}r_{,\beta} + re_{,\beta}) / e_p.
$$

(4.4)

The vector $a^*$ is

$$
a = \begin{bmatrix}
\alpha u_x(3u^2 - c^2), & -2\alpha u^2u_x, & i\kappa uu_x, & -\alpha u_x(c^2 + u^2), & -\alpha \eta \beta_x
\end{bmatrix}^T.
$$

(4.5)

4.2. Shock relations

The general conservation relations across the detonation shock surface $F(x^t, t) = 0$, are

$$
[m] = 0, \quad [mu^i + pn^i] = 0, \quad \left[ m \left( e + \frac{1}{2}u^i \cdot u^i \right) + p(u^i \cdot n^i) \right] = 0,
$$

(4.6)

where $m = \rho(u^i - V^i) \cdot n^i$, for shock normal $n^i = \nabla^T F / |\nabla^T F|$ and normal shock velocity $V^i \cdot n^i = -F^t / |\nabla^T F|$. This assumes no reaction occurs within the shock. Conditions (4.6) may be linearized, and the perturbation eigenfunctions $z^*$ shown to satisfy the shock relations

$$
u' = a_\nu \alpha, \quad p' = (a_p + 1 + u)\alpha, \quad \nu' = -(1 + u)ik, \quad \Lambda' = (-a_\nu + 1 + u)\alpha, \quad \beta' = 0,
$$

(4.7)

where

$$
a_\nu = (1 + u)(e_{,p} + e_{,\Lambda} + p_0) / (p + e_{,\Lambda} - e_{,p})
$$

(4.8)

and we have dropped the steady state index notation *. These conditions are valid for the general equation of state (2.2a) and are applied at $x = 0$.

4.3. Compatibility condition

4.3.1. Chapman-Jouguet waves

Steady, traveling Chapman-Jouguet waves have a bounding, forward facing sonic characteristic (where $u = -c$) which isolates the the region between the shock and sonic point from unsteady acoustic disturbances that may arise beyond the sonic point. Without approximation, an equation which describes any forward traveling plane wave in the
\[ L_{u+c}p + \frac{c}{\Lambda} L_{u+c}u = \Psi_{,t} \left( p_x + \frac{c}{\Lambda} u_x \right) - \frac{c}{\Lambda} L_y u - \nu L_y p - \frac{c^2}{\Lambda} L_y v - E_{,r}, \tag{4.9} \]

where \( L_{u+c} = \partial_t + (u + c) \partial_x \) and \( L_y = \partial_y - \Psi_y \partial_x \). When linearized about the sonic point (where \( u = -c \)) of the steady wave, we derive the compatibility condition

\[ p' + u' - \frac{ik}{\alpha} uu' + \frac{2u_x}{\alpha} (u' - \alpha) + b_p p' + b_A \Lambda' + b_{j\beta} \beta' = 0 \tag{4.10} \]

where

\[ b_p = (-uu_x(1 - e_{,pp} + e_{,p} \Lambda_p)/e_{,p} + e_{,\beta r_{,p}} + e_{,\beta p})/\alpha \]
\[ b_A = (-uu_x(e_{,\Lambda \Lambda} - e_{,p} \Lambda - 2e_{,p} c^2/u^3)/e_{,p} + e_{,\beta r_{,\Lambda}} + e_{,\beta r})/\alpha \tag{4.11} \]
\[ b_{j\beta} = (-uu_x(e_{,\Lambda \beta} - e_{,\beta p})/e_{,p} + e_{,\beta r_{,\beta}} + e_{,\beta r})/\alpha. \]

Equation (4.10) simply describes how disturbances are propagated along the steady sonic characteristic and is applied at the point in the steady wave where \( u = -c \). It again applies for general caloric equations of state and reaction rates (2.2a,b), and also regardless of whether the sonic point in the steady waves occurs at a point of incomplete reaction or at the point of complete reaction. For the Tait equation of state described below, it can be shown that condition (4.10) is equivalent to a boundedness condition on the perturbation eigenfunctions at the steady sonic point, as it has to be. A less specialized analysis that describes the propagation of any wave along an arbitrary “unsteady” sonic surface is given in Kasimov (2004).

### 4.3.2. Overdriven waves

The compatibility condition for supported overdriven waves assumes that the amplitude of the signal on all the characteristics in the equilibrium (fully reacted) zone that point toward the reaction zone is zero (Short et al. 2005). For the arbitrary equation of state (2.2a), this condition becomes

\[ u' - \frac{u_0 \omega}{c_b} p' - \frac{ik u_0}{\alpha} e' = 0, \quad \omega = \sqrt{1 - \eta k^2/\alpha^2}. \tag{4.12} \]

where the subscript \( b \) denotes steady conditions in the equilibrium zone.

Equation (4.2) can now be integrated for \( x < 0 \) subject to shock conditions (4.7). The eigenvalues \( \alpha \) are determined by enforcing (4.11) or (4.12) at the appropriate point in the steady wave.

### 5. Tait equation of state and reaction rate law

As discussed above, one of the drawbacks of the idealized condensed phase detonation model (Short et al. 2005) is that when the detonation shock pressure \( p_* \gg p_0 \), as it is in condensed phase explosives, the associated detonation Mach number is large. In practice, while \( p_* \gg p_0 \), the detonation Mach numbers are typically in the range 2-4 in condensed phase explosives due to the large ambient sound speed of the explosive. This limitation can be overcome by employing a more complex choice of the caloric equation of state that will allow \( p_* \gg p_0 \) for finite detonation Mach numbers. In the following, we will examine the Tait equation of state (Davis 1997),

\[ e = \frac{(p + a) \Lambda}{\Gamma_0} - \lambda q, \quad a = \delta - (\Gamma_0 + 1)p_0, \quad \delta = \frac{c_s^2}{D^2}, \quad p_0 = \frac{\tilde{p}_0}{\rho_0 D^2} \tag{5.1} \]
Non-ideal detonation stability

<table>
<thead>
<tr>
<th>Explosive</th>
<th>( \tilde{\rho}_0 ) (g/cm(^3))</th>
<th>( \tilde{c}_0 ) (km/s)</th>
<th>( \tilde{D}_{CJ} ) (km/s)</th>
<th>( \delta )</th>
<th>( p_0 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>NM</td>
<td>1.125</td>
<td>1.65</td>
<td>6.248</td>
<td>0.070</td>
<td>2.3 x 10(^{-6})</td>
</tr>
<tr>
<td>PBX9501</td>
<td>1.844</td>
<td>2.96</td>
<td>8.792</td>
<td>0.113</td>
<td>7.1 x 10(^{-7})</td>
</tr>
<tr>
<td>PBX9502</td>
<td>1.895</td>
<td>3.26</td>
<td>7.706</td>
<td>0.179</td>
<td>9.0 x 10(^{-7})</td>
</tr>
</tbody>
</table>

Table 1. Characteristic properties of the explosives liquid nitromethane (NM), PBX9501 (95% HMX (cyclotetramethylenetetranitramine) and 5% binder by weight) and PBX9502 (95% TATB (triaminonitrobenzene), 5% Kel-F 800 by weight). Here \( \tilde{\rho}_0 \) and \( \tilde{c}_0 \) are the ambient material density and sound speed, while \( \tilde{D}_{CJ} \) is the characteristic planar Chapman-Jouguet detonation speed. All values are taken from Marsh (1980). The values of \( p_0 \) are calculated assuming \( p_0 = 1 \text{atm} \).

where \( \delta^{-\frac{1}{2}} \) is the detonation Mach number with respect to the ambient sound speed, \( p_0 \) is the ratio of the ambient pressure \( \tilde{\rho}_0 \) to \( \tilde{\rho}_0 \tilde{D}^2 \), and \( \Gamma_0 \) is the Gruneisen gamma, which is assumed to be constant. Also, \( \lambda \) is the product mass fraction variable and \( q (= \tilde{q}/\tilde{D}^2) \) is the non-dimensional heat of reaction.

The value of \( a \) is in principle chosen to fit the experimentally determined sound speed in the material at a given pressure, where \( c^2 = (1 + \Gamma)\lambda(p + a/(1 + \Gamma)) \). The values of \( \delta \) and \( p_0 \) for the three condensed phase explosives NM and PBX9501/02 are listed in table 1 based on their material properties given in Marsh (1980). It can be seen that the contribution to \( a \) from \( p_0 \) is negligible, while the detonation Mach number \( \delta^{-\frac{1}{2}} \) ranges from 3.78 in NM to 2.36 for PBX9502. The idealized condensed phase detonation model can be recovered by setting \( a = 0 \).

As in Short et al. (2005) we also assume a one-step reaction, although the generalization to multiple reaction steps is trivial. Rather than working with the product mass fraction variable \( \lambda \), it proves convenient to transform to the reaction progress variable \( f \), which is typically chosen to facilitate the integration of the linearised system (4.2) near the sonic point (\( f = 1 \)) or equilibrium point (\( f > 1 \)), based on the asymptotic structure of the solution to (4.2) near these points (Short et al. 2005). For the present, we set

\[
\frac{D\lambda}{Dt} = \tilde{K}(1 - \lambda)^\nu, \quad \beta = (1 - \lambda)^\mu, \quad \frac{D\beta}{Dt} = r = -\mu\tilde{K}\beta^{(\nu + \mu - 1)/\mu}, \quad (5.2)
\]

where \( \nu \) is the reaction order, \( \beta = 1 \) represents the shock state, and \( \beta = 0 \) represents the product state. The rate constant \( \tilde{K} = \tilde{K}(p, \lambda, \beta) \) is chosen to mimic the ZND detonation structure of NM and PBX9501/02 described in §1 as determined by laser-based interferometry measurements of particle velocities (Sheffield et al. 2002, Gustavsen, Sheffield & Alcon 2000, Seitz et al. 1989). This is given by

\[
\tilde{K} = \tilde{K} [p^{n_1}(1 - \omega) + k_r p^{n_2} (1 + \omega)]/2, \quad \omega = \text{erf}((-\beta - \beta_c)/\epsilon), \quad (5.3)
\]

where \( \tilde{K} \) is a constant, set by choosing \( \tilde{l} \) so that \( x = -1 \) corresponds to \( \lambda = 1/2 \) in the steady ZND wave. The parameter \( k_r \) \((< 1)\) establishes the ratio of the rates of the slow to fast reaction stages that occur in detonations in NM and PBX9502 (Sheffield et al. 2002, Seitz et al. 1989). The parameters \( n_1 \) and \( n_2 \) are the pressure sensitivities in the fast and slow reaction stages respectively. For \( \epsilon \ll 1 \), the parameter \( \beta_c \) represents the transition point from the fast to slow reaction stage. When \( k_r = 1 \) and \( n_1 = n_2 \) the reaction rate form is identical to that used in Short et al. (2005), and is characteristic of the single length scale detonation structure found in PBX9501 (Gustavsen, Sheffield & Alcon 2000).

For the Tait equation of state (5.1) and for a one-step irreversible reaction (5.2), the
steady CJ detonation structure can be calculated exactly, and is given by
\[
\nu = -\frac{(1 + \Gamma)}{2 + \Gamma} \left( 1 + \tilde{p}_0 \right) + \frac{(1 - (1 + \Gamma)\tilde{p}_0)}{2 + \Gamma} \beta^{1/2}, \quad q = \frac{(1 - (1 + \Gamma)\tilde{p}_0)^2}{2\Gamma(2 + \Gamma)}, \quad (5.4)
\]
where \( \tilde{p}_0 = p_0 + a/(1 + \Gamma) \).

We now present an analysis of the linear stability characteristics of a CJ detonation for the Tait equation of state (5.1) and reaction rate law (5.2), highlighting the differences with the results found in Short et al. (2005). Based on the values given in table 1, in the following we have set \( p_0 = 0 \), so \( a = \delta \), and restricted our range of interest of \( a \) to \( 0 \leq a \leq 0.2 \). We have also set \( \nu = \mu = 1/2 \), \( \Gamma_0 = 2 \), and only considered the practically relevant cases of CJ detonations. For cases where \( k_r = 1 \), we use a single pressure exponent \( n = n_1 = n_2 \), so \( K = Kp^n \). When \( k_r \neq 1 \), we set \( \epsilon = 0.05 \).

6. Results

Figure 1a shows the variation in the neutral stability boundary that governs one-dimensional \((k = 0)\) stability as \( a \) varies for \( k_r = 1 \). For the strong shock limit \((a = 0)\), the neutral stability point occurs at \( n = 5.904 \). Increasing \( a \) has a three fold effect on the CJ wave structure: it reduces the effective heat release \( q \), decreases the shock pressure, while lowering the overall length of the CJ wave. Correspondingly, as \( a \) increases, the value of the pressure exponent \( n \) at the point of one-dimensional neutral stability increases rapidly. Thus for fixed \( n \), the CJ wave becomes more stable to one-dimensional disturbances as the detonation Mach number decreases. The neutral stability point based on table 1 for NM \((a = 0.07)\) occurs at \( n = 6.44 \), for PBX9501 \((a = 0.113)\) at \( n = 6.81 \) and for PBX9502 \((a = 0.179)\) at \( n = 7.44 \). Figure 1b shows the neutral stability boundaries that govern stability to two-dimensional disturbances for \( k_r = 1 \), and three values of \( a \), namely \( a = 0 \), \( a = 0.1 \), and \( a = 0.2 \). Again, increasing \( a \) raises the value of the reaction rate pressure sensitivity exponent \( n \) required for instability. Instability when \( a = 0 \) occurs for \( n > 2.168 \), when \( a = 0.1 \) for \( n > 2.552 \) and when \( a = 0.2 \) for \( n > 2.953 \). Thus assuming NM and PBX9501/02 all have the rate form (5.3) with \( k_r = 1 \) and identical rate pressure sensitivities, \( n_1 = n_2 \), detonations in PBX9502 would be the most stable.

Figures 2 and 3 concern the effect on stability of a dual length scale detonation reaction zone observed in NM and PBX9502, i.e. for \( k_r \neq 1 \). Figure 2a shows the two-dimensional neutral stability boundaries found when \( a = 0.1 \) and \( n_1 = n_2 = n \) for \( k_r = 1 \) and for
Non-ideal detonation stability

Figure 2. (a) Two-dimensional neutral stability boundaries for \( k < 2 \) for \( a = 0.1 \) and \( n = n_1 = n_2 \). Shown are the boundaries for \( k_r = 1 \) and for \( k_r = 0.5 \) with \( \beta_c = 0.274, 0.447 \) and \( 0.570 \). (b) Corresponding CJ wave profiles for \( n = 2.5 \).

Figure 3. (a) Two-dimensional neutral stability boundaries for \( k < 1.5 \), for \( a = 0.1 \) and \( \beta_c = 0.447 \). Shown are boundaries for \( k_r = 0.5 \) and \( n_2 = n_1, n_2 = 0.8n_1 \) and \( n_2 = 0.6n_1 \) and for \( k_r = 0.25 \) with \( n_2 = n_1 \). (b) Corresponding CJ wave profiles for \( n_1 = 2.5 \).

\( k_r = 0.5 \) with three different transition points between the fast and slow reaction stages. Figure 2b shows the corresponding CJ wave pressure profiles for the cases considered in fig. 2a when \( n = 2.5 \). Due to the second slow reaction stage the length of CJ wave for \( k_r = 0.5 \) is greater than that for \( k_r = 1 \), when the slow reaction stage is absent. As the transition point \( \beta_c \) moves closer to the detonation shock, more of the heat is released in the slow reaction stage, while the overall length of the CJ wave increases. The presence of a slow reaction stage \( (k_r < 1) \) has a destabilizing effect on the detonation, decreasing the value of \( n \) at which instability occurs compared with that when \( k_r = 1 \). However, there is a non-montonic behavior in the value of \( n \) above which the CJ wave is unstable as \( \beta_c \) increases. For \( \beta_c = 0.274 \), the rate pressure exponent above which instability occurs is \( n = 2.157 \), for \( \beta_c = 0.447 \), \( n = 2.069 \), and for \( \beta_c = 0.570 \), \( n = 2.192 \). Thus there appears to be a critical value of the ratio of the heat released in the fast reaction stage to that in the slow reaction stage that renders the lowest value of \( n \) for instability. Note that there is also a significant variation in the corresponding value of \( k \) at the instability onset values of \( n \) for the various cases.

Figure 3a shows the two-dimensional neutral stability boundaries for \( a = 0.1, \beta_c = 0.447 \), when \( n_2 = n_1, k_r = 0.5 \) and \( k_r = 0.25 \), and when \( n_2 = 0.8n_1, n_2 = 0.6n_1 \) with \( k_r = 0.5 \). Figure 3b shows the corresponding CJ wave pressure profiles for the cases considered in fig. 3a when \( n = 2.5 \). The effect of reducing \( k_r \), keeping the ratio of the heat released in the fast and slow stages constant, is to lower the instability onset value.
of $n$. Thus for $n_1 = n_2$, there is a band of instability for $k_r = 0.5$ when $n > 2.069$, and for $k_r = 0.25$ when $n > 1.978$. This trend has been verified for other values of $k_r$.

The final case examined concerns the effect of different rate pressure sensitivities in the fast and slower reaction stages. Figure 3a also shows the neutral stability boundaries for $n_2 = n_1$, $n_2 = 0.8n_1$, and $n_2 = 0.6n_1$ with $k_r = 0.5$. The decreased sensitivity in the slower reaction stage with $k_r$ fixed diminishes the difference in the rates of the fast and slower reaction stages, and consequently the value of $n$ which determines instability is greater for $n_2 < n_1$ than for $n_2 = n_1$. Again the effect is monotonic, since for $n_2 = 0.8n_1$ instability occurs when $n > 2.296$, but for $n_2 = 0.6n_1$ it occurs when $n > 2.237$.

In summary, we have examined the linear stability of a detonation in a condensed phase material under the assumption of a Tait equation of state, where the ambient pressure can be ignored relative to detonation shock pressure when the detonation Mach number is finite. We studied a single-step reaction, with a pressure-sensitive rate that has a single (as occurs in PBX5501) or dual (as occurs in NM or PBX9502) time scale. When the rate pressure sensitivity exponents $n_1 = n_2 = n$, $k_r < 1$, the presence of a fast reaction stage followed by a slow reaction stage in the CJ wave tends to decrease the value of $n$ at which instability occurs. For $n_1 = n_2 = n$, $k_r < 1$, the presence of a fast reaction stage followed by a slow reaction stage in the CJ wave tends to decrease the value of $n$ at which instability occurs relative to the value of $n$ for which instability occurs if the second slow reaction were absent. Finally, for cases where $n_2 < n_1$, $k_r < 1$, the value of $n_1$ for which instability occurs is higher that that when $n_2 = n_1$. In summary, it appears that the detailed underlying CJ detonation wave structures in NM and PBX5501/02 can have a major impact on their stability properties.

M.S. and I.I.A. were supported by DOE LANL and AFOSR, while J.B.B. was supported by DOE LANL.

REFERENCES


Non-ideal detonation stability


