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THE STRUCTURE AND STABILITY OF HIGH-EXPLOSIVE DETONATION WAVES

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1. INTRODUCTION

Since the pioneering works of Erpenbeck (e.g. [1]), the detonation stability theory contributed to the elucidation and explanation of many detonation phenomena. Careful and thorough calculations of pulsating [2], two- and three-dimensional [3, 4] instabilities have been performed relatively recently. All such calculations have been done for gaseous detonations, mostly for simple one-step Arrhenius kinetics. However, the important problem of stability of high-explosive detonations has not received attention it deserves. The absence of a simple equation of state and reaction rate law that would accurately describe the reaction zone thermodynamics and the heat-release kinetics has prevented researchers from addressing this fundamental problem carefully. Moreover, the stability formulation requires an additional condition in the far-field, the so-called radiation condition, that has not been understood well. All these necessary components have recently been significantly developed, see [5, 6, 7, 8], and the present work is based on these developments.

Below we describe the mathematical formulation of the linear stability problem for the high-explosive detonation wave that is based on the reactive Euler equations and constitutive model described in [7]. Calculations of the one-dimensional steady-state structure and the stability spectra for one- and two-dimensional perturbations are presented. The numerical method for solving the eigenvalue problem is based on the technique developed in the original work of Lee and Stewart [2] for calculation of the one-dimensional detonation instability.

2. GOVERNING EQUATIONS

2.1. **Reactive Euler equations.** Governing equations are the two-dimensional Euler equations for a reactive medium undergoing one-step chemical reaction,

$$\rho_t + \nabla\rho \cdot \mathbf{u} = 0, \tag{2.1}$$

$$\mathbf{u}_t + \mathbf{u} \cdot \nabla\mathbf{u} + v\nabla p = 0, \tag{2.2}$$

$$e_t + \mathbf{u} \cdot \nabla e + pv\nabla \cdot \mathbf{u} = 0, \tag{2.3}$$

$$\lambda_t + \mathbf{u} \cdot \nabla\lambda - \omega = 0. \tag{2.4}$$

Here $e = e(p, v, \lambda)$ is the specific internal energy as a function of pressure p, specific volume $v = 1/\rho$, and reaction progress variable λ, ω is the reaction rate, $\mathbf{u} = (u_1, u_2)$ is the velocity. The governing equations must be supplemented

by the equation of state $e = e(p,v,\lambda)$, rate law $\omega = \omega(p,v,\lambda)$, and the boundary conditions at the shock, that is the Rankine-Hugoniot conditions, and in the far field away from the lead shock, that is the radiation condition.

2.2. **The equation of state.** The functional form of the equation of state is given by the weighted superposition of the product and reactant terms [7],

$$e(p,v,\lambda) = \lambda\left[e_p^s(v_p) + \frac{v_p}{\Gamma_p}\left(p - p_p^s(v_p)\right)\right] + (1-\lambda)\left[e_r^s(v_r) + \frac{v_r}{\Gamma_r}\left(p - p_r^s(v_r)\right)\right], \tag{2.5}$$

where the subscript p is for products, r is for reactants, superscript s means that the quantity is evaluated along the expansion isentrope. The reaction progress variable λ goes from zero in the unreacted explosive to one in the completely reacted products. The internal energy function both for products and reactants is given in terms of the Grüneisen coefficients, Γ_p and Γ_r, which depend on the specific volume.

Various reference functions and parameters in equation 2.5 are given as follows [7, 5, 6]. For the products,

$$p_p^s(v) = p_c \frac{\left[\frac{1}{2}(v/v_c)^n + \frac{1}{2}(v/v_c)^{-n}\right]^{a/n}}{(v/v_c)^{k+a}} \frac{k-1+F(v)}{k-1+a},$$

$$e_p^s(v) = \frac{p_p^s v}{k-1+F(v)} = E_c \frac{\left[\frac{1}{2}(v/v_c)^n + \frac{1}{2}(v/v_c)^{-n}\right]^{a/n}}{(v/v_c)^{k-1+a}},$$

where

$$F(v) = \frac{2a(v/v_c)^{-n}}{\frac{1}{2}(v/v_c)^n + \frac{1}{2}(v/v_c)^{-n}}, E_c = \frac{p_c v_c}{k-1+a}, \Gamma_p = k-1+(1-b)F(v).$$

The parameters p_c, v_c, a, k, n, and b are specific for a given explosive and are found by calibrating to experimental data. Corresponding reference functions for the reactants are given by

$$p_r^s(v) = \hat{p}\sum_{j=1}^{4}\frac{(4By)^j}{j!} + C\frac{(4By)^5}{5!}, e_r^s(v) = e_0 + v_0\int_0^y p_r^s dy,$$

$$y = 1 - v/v_0,\ \hat{p} = \frac{\rho_0 A^2}{4B}, \Gamma_r(v) = \Gamma_r^0 + Zy.$$

The constants A, B, Γ_r^0, and Z are again determined by calibration with shock Hugoniot data, $\rho_0 = 1/v_0$ is the initial density of the explosive , e_0 is the heat of reaction.

To finalize the equation of state, we also need a relationship between v_p and v_r. Define $\Phi = v_r/v_p$. Then, if $v = (1-\lambda)v_r + \lambda v_p$ denotes the total specific volume of the mixture of products and reactants, we have

$$v_p = \frac{v}{\lambda + (1-\lambda)\Phi}, v_r = \frac{\Phi v}{\lambda + (1-\lambda)\Phi}.$$

Now $\Phi(\lambda)$ will be determined by fitting to the experimental data. Although constant value of Φ of about 1 gives good agreement with most of the experimental data, simple linear functions, for example, $\Phi = c_1 + c_2\lambda$, have also been used in the calculations, with fitting parameters c_1 and c_2.

2.3. **The heat release rate.** The reaction rate law used in the calculations is the following superposition

$$\omega = \frac{1}{2}\{1-\tanh[100(\lambda-0.45)]\}\,\omega_1 + \frac{1}{2}\{1+\tanh[100(\lambda-0.45)]\}\,\omega_2, \tag{2.6}$$

where

$$\omega_1 = k_1(1-\lambda)\left(\frac{p}{p_{cj}}\right)^4,\ \omega_2 = k_2(1-\lambda)^{0.5}\exp\left(-\frac{E_2}{c^2}\right).$$

The rate constants for PBX-9502 are $k_1 = 8.5$, $k_2 = 200$, $E_2 = 125$. The units here are *GPa*, *mm*, and μs. The constants in 2.6 have been determined by fitting the numerically calculated results to two experiments, one that determines the run-to-detonation distance as a function of pressure in shock ignition test, and the other that determines $D-\kappa$ dependence.

3. Analysis of the linear instability

3.1. **Steady-state one-dimensional solution.** For the analysis of the linear stability we need to find the basic state first, which is here the steady-state one-dimensional detonation. The mass, momentum, and energy equations can be directly integrated to yield algebraic relations between $p, v, e,$ and λ. To get the complete solution profiles, one integrates the reaction rate equation in which all state variables can be written as functions of λ. At the shock front, $x = 0$, the boundary conditions are those given by the Rankine-Hugoniot relations. The front speed D_s^* is determined from the Chapman-Jouguet condition at the sonic point.

3.2. **Linearized Euler equations.** Next, we rewrite the governing equations 2.1-2.4 in the shock-attached frame and linearize about the steady state (denoted by superscript (*)). The coordinate transformation from the laboratory frame (x^l, y^l, t^l) to the shock-attached frame (x, y, t) is accomplished by

$$x = x^l - D_s^* t^l - \psi(y^l, t^l),\ y = y^l,\ t = t^l, \tag{3.1}$$

where ψ is the shock front displacement from the unperturbed position. Applying this coordinate transformation and using the normal-mode decomposition of the form (prime denotes the perturbation amplitude)

$$\delta\mathbf{q}(x,y,t) = \delta\mathbf{q}'\, exp(\alpha t + iky), \tag{3.2}$$

with the transverse wavenumber k and complex growth rate α, we obtain the set of linear ordinary differential-algebraic equations with variable coefficients,

$$\mathbf{A}^*\frac{d\mathbf{f}'}{dx} + [\alpha\mathbf{B} + \mathbf{C}^*]\,\mathbf{f}' + \mathbf{b}^* = 0. \tag{3.3}$$

Here $\mathbf{f}'(x) = \begin{pmatrix} \rho'(x), & u_1'(x), & u_2'(x), & e'(x), & \lambda'(x), & p'(x) \end{pmatrix}^T$ is the state vector for perturbation amplitudes, $\mathbf{B} = diag(1,1,1,1,1,0)$, and $\mathbf{A}^*(x,\alpha)$, $\mathbf{C}^*(x,\alpha)$, and $\mathbf{b}^*(x,\alpha)$ are functions of the steady state solution.

The eigenvalues α and corresponding eigenfunctions $\mathbf{f}'$ can be determined by solving the system 3.3 subject to the Rankine-Hugoniot conditions at the front and radiation condition in the far field.

3.3. **Boundary conditions.** At the shock front the standard Rankine-Hugoniot conditions must be satisfied [9]. These conditions are linearized about the steady state and subsequently used as boundary conditions for 3.3 at $x = 0$. To determine the eigenvalues α, we need to solve the radiation condition at the end of the reaction zone. For the two-dimensional perturbations we have the following condition on the perturbation amplitudes [8]:

$$\alpha p' + \alpha \rho_b c_b u_1' + ik\rho_b c_b^2 u_2' = \rho_b c_b^2 \sigma_b \omega'. \tag{3.4}$$

The subscript b denotes the burnt state (far field) and σ and c are the thermicity and sound speed [9].

4. Conclusions

In this work we address the problem of the linear stability of high-explosive detonation waves using a recently developed equation of state that is valid for unreacted explosive, detonation products, and throughout the reaction zone. A new reaction rate law has also been developed that can reproduce experimental data on the shock ignition and front speed - curvature dependence. This law is incorporated in the present work. Another new ingredient of the current analysis is the far-field boundary condition that is required for the calculation of the stability spectrum.

The equation of state has been calibrated for two explosives, PBX-9502 and nitromethane. The structure of the steady-state Chapman-Jouguet detonation has been calculated for these explosives and its stability with respect to one- and two-dimensional perturbations is investigated.

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