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MATLAB code for highly energetic materials

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Abstract. Detonations represent high-speed chemical reactions characterized by rapid propagation, accompanied by a release of high-pressure energy. This transformative process converts unreacted explosive materials into stable product molecules, reaching a steady state known as the Chapman-Jouguet (CJ) state. This study aims to effectively describe the detonation phenomenon in energetic materials through the application of the CJ theory. Using a computational approach, we developed a MATLAB code to calculate the minimum detonation velocity (DCJ) of the explosive and analyze product expansion under constant entropy conditions.

Introduction

Detonations are high-speed chemical reactions that are characterized by their rapid propagation and high pressure accompanied by high-speed energy release. After the passage of the detonation shock wave, the reactive medium is transformed into high temperature and pressure products. Hence, detonation can be thought of as a path that transoforms the unreacted explosive into stable product molecules at the Chapman– Jouguet (CJ) state, which is a steady, chemical equilibrium shock state that conserves mass, momentum, and energy. Such characteristics make detonation a phenomenon with several potential fields of application. Nowadays, detonation seems to represent a turning point for the field of hypersonic propulsion. Several propulsion systems have been designed to exploit the detonation of energetic material to generate thrust. Among the most important ones are scramjets and pulse detonation engines (PDE), which, despite not yet being available on the international market, offer significant advantages over current architectures. The research presented aims, among its objectives, to lay the foundations for a new theory capable of reducing the uncertainty of these systems and promoting the development of such technologies in the next decade. The conservation's laws represent a fundamental tool for analyzing the properties of energetic materials. By substituting the conservation equation of mass into the conservation of momentum, removing the velocity of the products, it is possible to obtain a relationship between pressure and specific volume called the Rayleigh line :

$$p = p_0 + \rho_0^2 D^2 (v_0 - v) \tag{1}$$

where D represents the velocity of the shock wave through the explosive.

Methods

The aim of this study is to effectively describe the detonation phenomenon of energetic materials through the CJ theory. We developed a MATLAB code to compute the minimum detonation velocity (D_{CJ}) of the explosive and the expansion at constant entropy of the products once the equation of state (EOS) of the mixture is provided. The products under consideration are nine gaseous chemical species (H2, N2, O2, CO, NO, H2O, CO2, NH3, CH4) and one solid (C(s)). For

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each of these species, it is necessary to provide values for their enthalpy and entropy under standard conditions, as well as their variations as a function of temperature at standard pressure. To accomplish this, the Shomate Equation has been selected, which takes the following form for both enthalpy and entropy :

$$s^0(T) = A * ln(t) + B * t + C * \frac{t^2}{2} + D * \frac{t^3}{3} - \frac{E}{2t^2} + G \quad (2)$$

$$h^0(T) = A * t + B * \frac{t^2}{2} + C * \frac{t^3}{3} + D * \frac{t^4}{4} - \frac{E}{t} + F \quad (3)$$

where t represents temperature expressed in Kelvin divided by one thousand, and the coefficients (A, B, C, D, E, F) were obtained from the NIST database.

Another fundamental step is represented by the choice of the equation of state. For the gaseous phase, simulations were carried out using both the equation of state for ideal gases and the Becker-Kistiakowsky-Wilson equation of state (BKW) in order to evaluate the differences that the two solutions bring in terms of explosive properties. The BKW EOS has the following form :

$$p = \frac{\rho RT}{W_{mix}} \cdot Z(\rho, T, x_{i,eq}) \quad (4)$$

where the variable Z is called compressibility factor and it represents how much the mixture under consideration deviates from an ideal one :

$$Z = 1 + \chi e^{\beta\chi} \qquad \chi = \frac{\rho\kappa\sum k_i x_{i,eq}}{W_{mix}(T+\theta)^\alpha} \quad (5)$$

The parameters α, β, θ, and κ are constants computed by interpolating experimental results. Lastly, concerning the term k_i, it denotes the molar covolume of the chemical species that are being considered. For the solid phase, there are two possible paths. The first one is the simplest and less computationally demanding, it consists of introducing the hypothesis that the solid phase is incompressible. The second path, instead, takes into account compressibility effects through an equation of state. In particular, in the present case, Cowan's solid equation of state was chosen to analyze the compressibility effects of graphite at high pressures and temperatures :

$$p = P(\eta) + a(\eta)T + b(\eta)T^2 \quad (6)$$

where η represents the ratio between the density of the solid phase, for a generic temperature and pressure, and the density of the solid phase under reference conditions. P(η), a(η), and b(η) represent polynomials as a function of the density of the solid under examination.
The code is structured into three main modules :

- Explosion State
- Detonation State
- Isoentropic Expansion State

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The first module, called Explosion State, is the most computationally demanding and it is responsible for representing the Hugoniot of the products in the Clapeyron plane :

$$e(n_i, T) - e_0 = \frac{1}{2}(p(n_i, T) + p_0)(v_0 - v) \quad (7)$$

where the internal energy of the system is computed for a solid-gas double-phase mixture, and n_i represents the chemical composition in moles of the equilibrium products. The module includes an internal loop that computes the chemical equilibrium through a constrained minimization algorithm of the Helmholtz free energy. The constraints introduced in this phase are two :

- The population constraints, which require that the number of particles of each chemical element must be conserved during detonation
- The limit to the number of moles that each chemical species can have, as negative values would not be physically meaningful and therefore cannot be considered.

Concerning the second module, called Detonation State, it is responsible for interpolating the points computed to obtain a functional expression of the Hugoniot of the products. Subsequently, through the minimization algorithm, the tangent point between the Hugoniot of the products and the Rayleigh line is computed as a function of the detonation velocity (D). According to the CJ theory, the value of D that brings the two curves to be tangent is called the CJ detonation velocity and it represents a very important characteristic parameter of explosives, namely the minimum shock wave velocity that generates a detonation of the energetic material. Similarly, from the found CJ point, it is possible to compute the thermodynamic properties of the mixture, including pressure and temperature. There is another important parameter that is determined in this phase : the entropy at the CJ point, which serves as an input for the next module. Indeed, by knowing this parameter, it is possible to graphically represent the isoentropic expansion of the products starting from the CJ point in the p-v plane, assuming that the mixture is in chemical equilibrium at every point.
The third module, called Isoentropic Expansion State, takes care of this last operation through a zero-finding algorithm applied to the following equation :

$$S(v, T) = S_{CJ} \quad (8)$$

Results

One of the first results obtained from the code concerns to the possibility of highlighting the differences between an ideal gas mixture and a real one. The figure in the next page (Figure 1) shows partial results of the CJ theory obtained for the RDX explosive :

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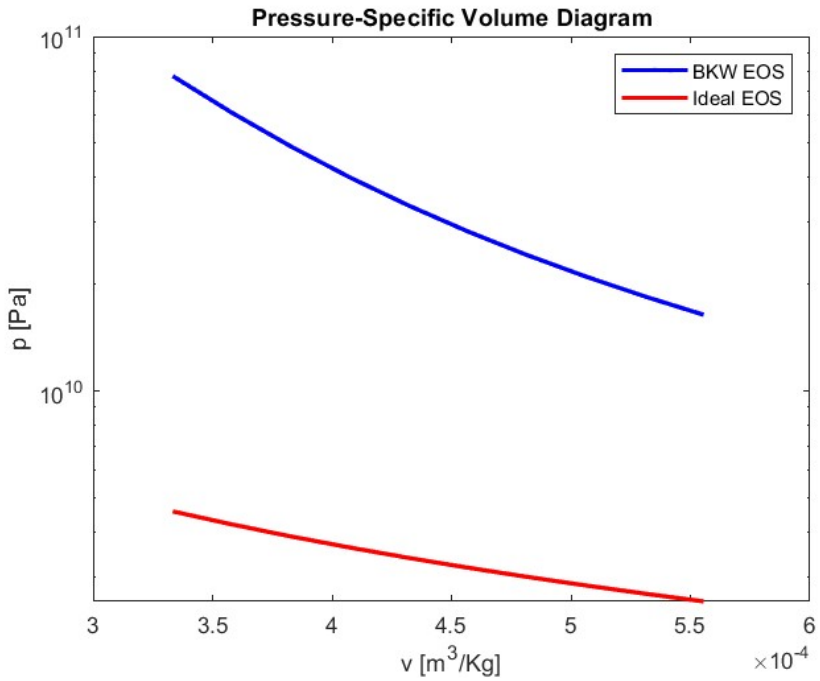

Figure 1: Comparison of the Hugoniot behaviors of RDX products using ideal and BKW equations of state

For a given specific volume, the two solutions diverge by approximately one order of magnitude, with the discrepancy increasing as the system pressure rises. The result obtained is extremely important as it suggests that the ideal gas assumption is not suitable for describing the detonation process. This outcome is in line with expectations, as detonation involves extremely high pressures and the ideal gas assumption is not an accurate representation of a mixture under such conditions.

Now, numerical results obtained for various types of energetic materials are presented and compared with experimental data taken from Mader [2] :

Table 1: Comparison between the results obtained from the numerical model and experimental data for two different types of explosives.

	Densità [Kg/m^3]	CJ Point	Experimental Results	Model Results
RDX	1,8	D [m/s]	8754	9069
		T [K]	2587	2181
		γ	2,98	3,21
	1	D [m/s]	5981	6068
		T [K]	3600	3344
		γ	2,48	2,62
HMX	1,9	D [m/s]	9100	8878
		T [K]	2364	2423
		γ	3,03	3,37

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The detonation velocity at the CJ point is the parameter that is less affected by imperfections related to the model. Moreover, it is possible to see how the detonation velocity strongly depends on the initial density of the explosive under examination, from the results obtained for RDX. In particular, for not excessively large values of density, this dependence is linear. Thus, it is possible to obtain a functional expression of the detonation velocity at the CJ point as the initial density of the energetic material changes.

Finally, it is possible to observe (figure 2) that the isoentropic expansion curve starts from the CJ point :

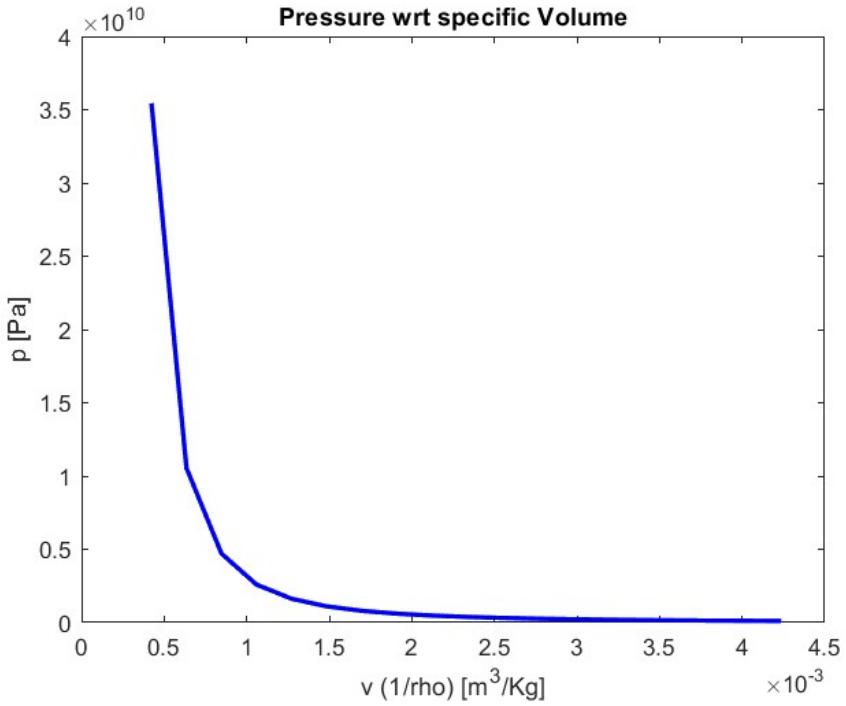

Figure 2: Expansion behavior of RDX for an isoentropic process.

It is possible to show that the three curves obtained (Rayleigh line, Hugoniot of products, and isoentropic expansion) must be tangent at the CJ point, this behavior is clearly visible in the following picture :

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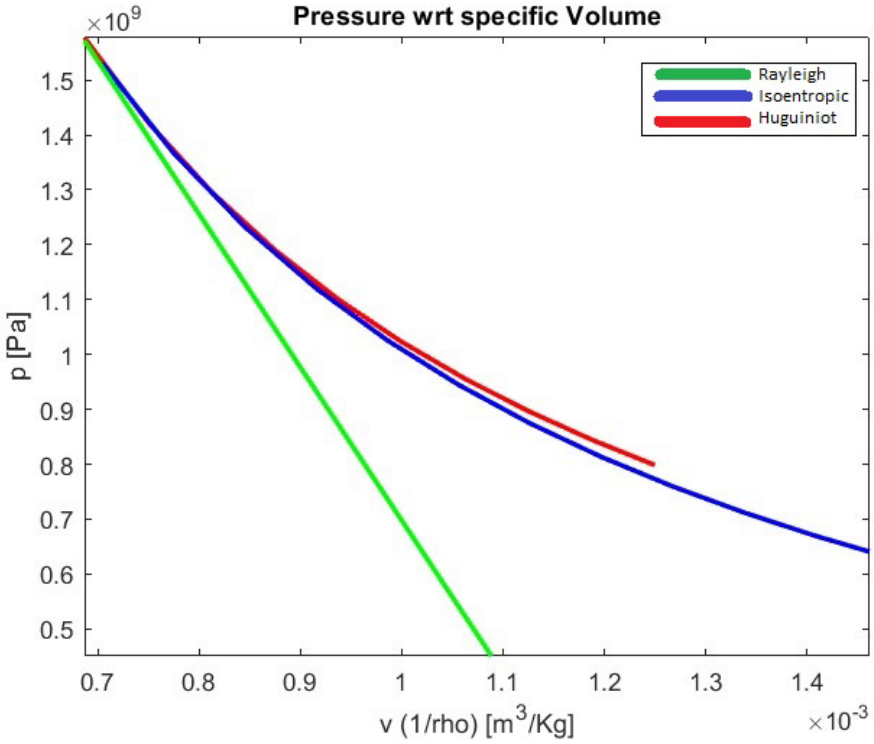

Figure 3 : Qualitative analysis between Rayleigh line, products Hugoniot and isentropic expansion in the neighborhood of the CJ point

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