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HEMSim: a new MATLAB software to simulate the behaviour of highly energetic materials upon Chapman-Jouguet hypothesis

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Abstract

In this paper, we present a comprehensive simulation framework developed in MATLAB called HEMSim (Highly Energetic Materials Simulator) for modeling ideal detonations based on the fundamental principles of the Chapman-Jouguet (CJ) theory. The code efficiently computes the properties of an ideal detonation at the CJ point under the assumption of chemical and thermodynamic equilibrium, as well as the values of an isentropic expansion, while also enabling a fit with the parameters of the well-established JWL equation of state. Our code employs advanced equations of state (IMP EXP6 or BKWC for gaseous products and Birch Murnaghan for condensed products) to accurately model the behavior of a multiphase mixture of products from an ideal detonation. To our knowledge, there are no freely available codes capable of performing these complex calculations. Our implementation hence provides a robust framework for the accurate determination of ideal detonation parameters.

Keywords: Chemical Equilibrium, Chapman-Jouguet, Ideal Detonation Code, EXP-6 Equation of State, Murnaghan equation of state.

1 Introduction

Detonation, the rapid and self-sustained chemical reaction accompanied by the release of a tremendous amount of energy, has widespread implications in various scientific and engineering disciplines [5]. From military applications to industrial safety, understanding the fundamental mechanisms underlying detonation processes is of paramount importance. The Chapman-Jouguet (CJ) theory, developed in the early 20th century, provides a simplified yet powerful framework for characterizing ideal detonations [8]. It defines the conditions under which a steady-state detonation wave can propagate without any decay or acceleration.

While analytical solutions for ideal detonation problems are limited due to their inherent complexity, numerical simulations have emerged as invaluable tools for studying and analyzing these phenomena.

There are several computational codes capable of computing the chemical equilibrium state of energetic materials and CJ conditions: for example Cheetah [12], TDS [25], Carte [7], Explo5 [23]. Unfortunately the source code and the software itself are often not available. There exist other software with available source code, mostly written in MATLAB such as SDT [2] and CT [6], but they often rely on the ideal equation of state and do not consider condensed phase products.

In this article, we present a new thermochemical code implemented in MATLAB called HEMSim (Highly Energetic Material Simulator) available as a compiled app that leverages the principles of the CJ theory to simulate ideal detonations for CHNO explosives considering a multiphase mixture for detonation products.

The simulation framework is designed to provide a user-friendly GUI for defining the initial conditions, including the explosive composition and physical properties. The code then solves the governing equations, which include the conservation laws for mass, momentum, and energy under the hypothesis of chemical equilibrium. The incorporation of the ideal detonation theory enables the code to determine the CJ state, which represents the minimum conditions required for sustaining a detonation wave.

In summary, the MATLAB code presented in this article provides a versatile and efficient tool for simulating ideal detonations based on the Chapman-Jouguet theory. By utilizing this code, researchers can delve into the intricate dynamics of detonation processes and explore new avenues for enhancing the understanding and control of explosive phenomena.

2 Description of the code

The detonation is a process of layer-by-layer, supersonic propagation of chemical reactions through an explosive. According to the generally accepted Chapman-Jouguet (CJ) model of detonation, chemical reactions occur instantaneously, under the action of a shock wave [23]. An ideal shock or detonation wave has no volume and can locally be considered a planar wave if we ignore the structure of the reaction zone. [2].

2.1 CJ Point

The Chapman-Jouguet theory allows for the computation of the Chapman-Jouguet detonation velocity, denoted by D_{CJ}). It represents the critical threshold, which is the minimum velocity required for a detonation to self-propagate through a reactive medium.
Through conservation laws [8] it is possible to compute the detonation velocity by imposing a tangency condition between two curves known as the Rayleigh line and the Hugoniot of the products as detailed in the following.
The Rayleigh line is obtained by linking the mass conservation equation to the momentum conservation equation and it can be expressed as:

$$\mathcal{R}(n,T,v): \quad p(n,T,v) - p_0 - \rho_0^2 D^2 (v_0 - v) = 0 \tag{1}$$

in which p, v represent the pressure and the specific volume ($v = \frac{1}{\rho}$, with ρ density of the material) respectively after the shock front passage in the medium, T is the temperature, n is the molar composition of the products of detonation after the shock front passage, D represents the shock front velocity. The subscript zero identifies the unshocked state of the energetic material, while quantities lacking a subscript refer to the product mixture.
In general, an equation of state of the form $p = p(v, n(v,T), T(v))$ is required to complete the equation set. The Hugoniot curve represents an energy balance between the unreacted material and the products of detonation at equilibrium:

$$\mathcal{H}(p(n,T,v),v): \quad U(p(n,T,v),v) - U_0 - \frac{1}{2}(p(n,T,v) + p_0)(v_0 - v) = 0 \tag{2}$$

where $U(p(n,T,v),v)$ represents the internal energy of the mixture and U_0 the internal energy of the unshocked material.
To find the CJ point is then necessary to compute the minimum of the 1-d function expressed in Eq.(3) [23]

$$D(v) = \sqrt{\frac{p_0 - p(n(T,v),T(v),v)}{\rho_0^2 (v - v_0)}}. \tag{3}$$

2.2 Thermodynamics

The CJ point is the equilibrium condition to which the product mixture evolves following a detonation. Carbon-rich energetic materials can result in the formation of condensed products. Therefore, it is necessary to partition the mixture properties among the different phases.
To develop a numerical code to describe the detonation phenomenon using the CJ theory, it is necessary to impose one or more Equations of State (EoS) that can represent the behavior of the mixture of products at equilibrium. The equation of state allows the computation of the following variables:

- Compressibility factor (pressure behavior) Z,
- Helmholtz free energy A,
- Internal energy U.

The complete structure of the code relies on considering the specific volume v as the independent variable: every other thermodynamic variable can be obtained by considering the Maxwell relations between A and U [20] at fixed v. For the fluid phase, the properties of the mixture split into intramolecular (ideal) and intermolecular (non-ideal) components; the latter model the non-ideal behavior of the mixture. Two different EoS can be applied.

- The first one is of experimental nature and it is called the Becker-Kistiakowsky-Wilson (BKW) EoS [16].
- The second one is based on interatomic potentials Buckingham exponential-6 representation and is referred as the EXP-6 IMP EoS [11].

For the condensed phase, properties are also split up into a reference component that models behavior at standard pressure p_0 and a portion dependant from pressure, which can be handled by the version of extended Birch-Murnaghan with thermal expansion equation of state defined in [10].

2.2.1 Ideal gas properties

To compute the ideal thermodynamic properties of the gaseous phase (internal energy $u^{id}_{gas,i}$, entropy $s^{id}_{gas,i}$ and enthalpy $h^{id}_{gas,i}$), NASA polynomial representation [18] is employed. Chemical potentials are then defined for each species i

$$\mu^{id}_{gas,i} = h^{id}_{gas,i} - T s^{id}_{gas,i} + RT \ln\left(\frac{n_{gas,i} p^{id}_{gas}}{n_{gas} p_0}\right), \quad i = 1, \dots, NG \tag{4}$$

with total gaseous pressure p^{id}_{gas} given by the ideal gas law, total moles of fluid product mixture $n_{gas} = \sum_i^{NG} n_{gas,i}$ being n_i moles of each fluid product specie, NG the number of fluid species considered among the products and R the perfect gas constant. The Helmholtz free energy of the ideal gas mixture, the internal energy are then determined by Eq.(5)

$$A^{id}_{gas} = \sum_i^{NG} n_{i,gas} \mu^{id}_{gas,i} - RT n_{gas}, \quad i = 1, \dots, NG \tag{5}$$

$$U^{id}_{gas} = \sum_i^{NG} n_{i,gas} u^{id}_{gas,i} \quad i = 1, \dots, NG \tag{6}$$

2.2.2 Standard solid properties

The properties of the solid phase have been split into a reference term that describes properties under standard pressure conditions and a term that accounts for the effects of pressure. The solid chemical species considered within the code include the two allotropic forms of carbon, graphite, and diamond.
The specific heat of each condensed specie j, $c_{p_{solid,j}}$, under standard conditions is computed by applying the Einstein two oscillator model described in [10]. It is then possible to compute the enthalpy and entropy under standard conditions for the condensed phase using numerical integration on Eq.(7)

$$h^{std}_{solid,j} = \int_{T_0}^{T} c_{p_{solid,j}}(T')\, dT', \quad s^{std}_{solid,j} = \int_{T_0}^{T} \frac{c_{p_{solid,j}}(T')}{T'}\, dT' \quad j = 1, \dots, NS \tag{7}$$

being NS the number of condensed species considered among the products. The Helmholtz free energy and the internal energy of the condensed products mixture are then determined by Eq.(8)

$$U^{std}_{cond} = \sum_j^{NS} n_{j,gas} h^{std}_{gas,j} - p v_{cond,j} \tag{8}$$

$$A^{std}_{cond} = U^{std}_{cond} - T \sum_j^{NS} n_{j,gas} s^{std}_{gas,j} \tag{9}$$

2.3 BKW EoS

The Becker-Kistiakowski-Wilson (BKW) gaseous EoS has been widely used [16]. The BKW equation of state is represented by Eq. (10):

$$p = \frac{\rho_{gas} RT}{W_{gas}} Z(\rho_{gas}, T, \chi_{gas,i}), \quad i = 1, \dots, NG, \tag{10}$$

The compressibility factor Z

$$Z = 1 + \chi e^{\beta\chi}, \qquad \chi_{gas} = \frac{\rho_{gas} \kappa \sum k_i \frac{n_{gas,i}}{n_{gas}}}{W_{gas}(T+\theta)^{\alpha}}, \tag{11}$$

in which $\rho_{gas} = 1/v_{gas}$, indicates how much the behavior of the gas mixture deviates from the ideal case. β, α, and κ are constants obtained by fitting experimental detonation velocity data for a specific energetic material and k_i represent the molar covolumes of the gaseous chemical species considered among the detonation products.

Multiple sets of adjustable parameters have been published [16],[17] with the aim of achieving better agreement with detonation velocity experimental data.

In our code, we used the BKWC set of parameters and covolumes described in [24]. One has to be careful and remember that covolumes k_i have to be multiplied by the molecular factor 10^{24} to compute Z.

The excess Helmholtz free energy A_{gas}^{ex} and the excess internal energy U_{gas}^{ex} are obtained by integration of (11) as described in [16].

2.4 EXP-6 IMP EoS

The EXP-6 IMP (Exponential 6 Inter Molecular Potential) EoS is based on intermolecular forces description among particles in the fluid mixture. It is considered theoretical and overcomes the problem of adjustable parameters used in BKW. Suceska et al. [22] in EXPLO5 code followed Brown's [1] original approach with a single interpolation domain. It is valid for a smaller range of thermodynamic states and it is designed for commercial explosives, but uses much fewer Chebyshev coefficients.

Hallstadius [13] run different Monte Carlo simulations and created a single interpolation domain valid for a wider range of state: results of running his code, EQUIC, are validated for energetic materials that are not producing condensed phase products. In our code, we follow the Fried and Howard approach, implemented in Cheetah 2.0 which developed an analytical model of the excess Helmholtz free energy. Indeed, parameters $\alpha_i, r_{m,i}, \epsilon_i$ and λ_i for EXP-6 IMP based EoS values used in our code are taken from [11] and stored in Tab. 1.

The thermodynamic properties are derived from the excess Helmholtz free energy A_{gas}^{ex}: their analytical descriptions rely on derivatives. Using the Chebyshev interpolant Φ defined in [12], these properties can be expressed by

$$Z = 1 + \Phi z + \frac{\partial \Phi}{\partial \rho} z \rho, \tag{12}$$

$$A_{gas}^{ex} = nRT\Phi z \tag{13}$$

$$U_{gas}^{ex} = -nRT^2 \left(\Phi \frac{\partial z}{\partial T} + \frac{\partial \Phi}{\partial T} z \right). \tag{14}$$

with z defined as in [11]. Due to the intricate nature of interactions among numerous chemical species, the gaseous product mixture is simplified and treated as an effective single fluid employing the van der Waals one-fluid (vdW1f) mixing rules.

The parameters for two unlike species i and j are given by the extended Lorentz-Berthelot combination rule [22] The corrective factor k_{ij}, l_{ij}, m_{ij} are expected to be close to unity, whereas in some cases [12] values up to 2 were observed. If the user want to replicate results from Cheetah 2.0, corrective parameters $r_{m,ij}, \epsilon_{ij}, \alpha_{ij}$ have to be set with the same values provided in the software.

Gaseous Product Species	k_i	α_i	$r_{m,i}$	ϵ_i	λ_i
H_2	270.0	11.51	3.424	32.11	0.0
N_2	374.0	12.68	4.201	101.1	0.0
O_2	306.0	13.65	3.832	120.0	0.0
CO	372.0	13.10	4.149	105.8	0.0
NO	394.0	12.10	5.172	123.7	0.0
H_2O	188.0	12.18	3.296	220.4	865.8
CO_2	511.0	12.78	4.293	257.8	0.0
NH_3	550.0	12.55	3.687	224.9	142.9
CH_4	420.0	13.78	4.214	152.1	0.0

Table 1: EXP-6 IMP based EoS parameters and covolumes for gaseous product species: values from [12].

2.5 Murnaghan Solid EoS

To determine the thermodynamic properties of these solid products, it is necessary to employ an equation of state that can account for the effects of high pressure and temperature.

One widely used equation of state in the field of detonation is the extended Birch - Murnaghan EoS, a modified version of the original Murnaghan by introducing a term that considers thermal expansion effects

$$v_{mol_{solid,i}} = v_{0,mol_i} \left[\frac{\eta_i}{B_{0,i}} p_{solid} + e^{-\eta_{solid,i}\alpha_{solid,i}(T-T_0)} \right]^{-1/\eta_i}, \quad i = 1, \dots, NS, \tag{15}$$

where the volume $v_{mol,solid,i}$ is expressed in $[m^3/mol]$, $v_{mol,0}$ represents the molar volume under standard conditions, $B_{0,i}$ is the bulk modulus under standard conditions, and η_i represents the derivative of the bulk modulus with respect to pressure for every solid species, $\alpha_{solid,i}$ representing the coefficient of thermal expansion of the solid specie. Here we reported the correct version of (15), while in [12] the term $\eta_{solidi,i}$ was missing.

Given the coexistence of high pressures and temperatures that characterize the detonation phenomenon, it is possible for the carbon present within the explosive to transform into diamond rather than graphite. Due to the different thermodynamic properties possessed by these two allotropic forms, it becomes necessary to define a set of parameters for carbon in the form of diamond and another set for graphite. Parameters are shown in Tab. 2. Helmholtz free energy A^{dep}_{cond} and internal energy U^{dep}_{cond} can be obtained by integration from (15) as described in [10].

Property	**Diamond**	**Graphite**
h_{0,mol_i} (kJ/mol)	1.895229	0
s_{0,mol_i} s_0 (J/mol K)	2.36	5.742
$\alpha_{solid,i}$ (K^{-1})	0.0000243	0.000232
$B_{0,i}$ (Pa)	2.295×10^9	2.317×10^8
η_i (Pa s)	4	5.52
v_{0,mol_i} (m^3/mol)	3.419	5.439

Table 2: Solid Properties for Diamond and Graphite used in Eq.(15).

2.6 Chemical equilibrium

The determination of equilibrium composition is the first step in the calculation of detonation performance [22].

Gases are assumed to be perfectly mixed so there is just one gaseous phase while each condensed has its own phase. Gaseous moles are constrained to be strictly positive since they are involved in the logarithmic therm in Eq.(4), while the condensed mole numbers and volumes only have to be non-negative, since there is the possibility to consider the absence of solid species which are included as potential constituents [9].

The reaction coming from CHNO energetic material into detonation products is defined by the general formula (16)

$$\begin{aligned} C_cH_hN_nO_o = {} & n_1H_2 + n_2N_2 + n_3O_2 + n_4CO + n_5NO \\ & + n_6H_2O + n_7CO_2 + n_8NH_3 + n_9CH_4 + \ldots + n_{10}C_{diam} + n_{11}C_{grap}, \end{aligned} \tag{16}$$

in which $n_i, i = 1, \dots, NP$ are the moles of individual chemical species per kilogram of explosive and $NP = NG + NS$ and C_{diam}, C_{grap} are respectively the number of moles of solid carbon in diamond and graphite form per Kg of explosive.

The reaction products make a reactive system in which the concentration of individual products is determined by the state of equilibrium for fixed v and T. The concentration as mole amount of products can be calculated by applying the free energy minimization technique and mass balance principle. The total Helmholtz free energy is defined as

$$A(v, T, n) = A^{id}_{gas}(v_{gas}, T, n_{gas}) + A^{ex}_{gas}(v_{gas}, T, n_{gas}) + A^{std}_{cond}(v_{cond}, T) + A^{ex}_{cond}(v_{cond}, T), \tag{17}$$

where specific volume v is related to v_{gas} and v_{solid} by the equation

$$v = \frac{\sum_i^{ngas} n_{gas,i} W_{gas,i}}{\sum_k^{NP} n_k W_k} v_{gas} + \frac{\sum_j^{nsolid} n_{solid,j} W_{solid,j} v_{solid,j}}{\sum_k^{NP} n_k W_k}, \tag{18}$$

in which $v_{solid,i} = v_{mol_{solid,i}} W_{solid,i}, \quad i = 1, \dots, NS.$

Minimizing Helmholtz free energy allows to search for thermodynamic variables in a smaller range of values defined by the specific volume v, instead of working with pressures that span a wider range of different orders of magnitude. Solving chemical equilibrium then means, for fixed v and T, finding the

$$\min_n A(n(v,T),T(v),v) \tag{19}$$

subject to linear constraints

$$b_j = \sum_{i=1}^{NP} a_{ji} n_i, \quad j = 1,\dots,NE \tag{20}$$

$$n_i \geq 0, i = 1,\dots NP, \tag{21}$$

where a_{jk} is the number of atoms of type j (in our code, considering HCNO explosives, $j = 4$) in species k and b_j is the total number (moles) of elements of type j and subject to the linear inequality (21).

The set of coefficients a_{ji} are positive integers that depend only on the elemental composition of each species in the mixture. The set of values can be represented by a $NE \times NP$ matrix A_{eq} with components $A_{eq_{ji}} = a_{ji}$ [2].

The approach we followed is to use the MATLAB optimization algorithm FMINCON to minimize the Helmholtz energy for fixed specific volume and temperature applying the linear constraints. MATLAB built-in function FMINCON implements an interior-point method [3]. We tested our algorithm by considering both the primary 9 gaseous species and the complete set of 24 gaseous species as utilized by Cheetah 2.0. The results for the concentrations of the primary species were nearly identical in both cases. Therefore, in the code, we have chosen to include only the primary 9 gaseous species to optimize performance.

2.7 Conservation law balance

For fixed specific volume v, the temperature of detonation products and the specific volume of gaseous (v_{gas}) and solid ($v_{solid,i}$) products have to be determined. Considering v as an independent (fixed) variable, we search for T that satisfies Hugoniot Eq.(2) in which the internal energy is given by Eq. (22)

$$U(v,T,n) = U^{id}_{gas}(v_{gas},T,n_{gas}) + U^{ex}_{gas}(v_{gas},T,n_{gas}) + U^{std}_{solid}(v_{solid},T) + U^{ex}_{solid}(v_{solid},T), \tag{22}$$

and for $v_{solid,i}, i = 1,\dots,NS$ that satisfy mechanical equilibrium. This leads to the solution of non-linear system

$$\begin{cases} U(v,T,n(v,T)) & = U_0 + \frac{1}{2}(p(v,T,n(v,T)) + p_0)(v_0 - v) \\ p_{gas}(v,T,n(v,T)) & = p_{solid,1}(v,T) \\ \vdots & \\ p_{gas}(v,T,n(v,T)) & = p_{solid,NS}(v,T) \end{cases}, \tag{23}$$

where U_0 is the fixed internal energy of the reactant.

Having computed each $v_{solid,i}$ for fixed v, by inversion of Eq.(18) the code computes v_{gas}. This approach is convenient because in this way solid equation of state for each phase can be written explicitly as a function of solid specific volume. Moreover, the approach of solving the whole system given by energetic balance and mechanical equilibrium as an external loop (with the internal loop given by the chemical equilibrium for fixed v,T and then $v_{solid,i}$) is found to be the best option in term of CPU time with respect to the separate equation an solving the mechanical equilibrium inside Helmholtz minimization.

The final solution to the detonation problem is obtained by a fixed point iteration between the solution of the system (23) and the chemical equilibrium described in Sect. 2.6.

The solution of the system (23) is obtained in MATLAB environment by using the built-in non-linear solver FSOLVE, which applies the trust-region method [4]. It is hence important to have some good initial estimates for the unknowns $T, v, v_{solid,i}$: in our code, we used empirical formulas provided in [14].

To find the CJ state, a 1-D minimization to find the smallest value of v that solves the problem described in Sect.2.1 is needed as the last external loop.

2.8 Isentropic expansion computation

When a highly energetic material is detonated, it undergoes a transformation into intensely hot and highly compressed gases. The density of these gases within the detonation wave front exceeds that of the original explosive material at its CJ state ($v_{CJ} > v_0$). This newly formed compressed and heated gas serves as a potent force capable of exerting pressure on its immediate surroundings. An isentropic expansion curve represents the thermodynamic behavior of detonation products during their expansion phase. This curve shows the relationship between pressure and specific volume as detonation products expand adiabatically, maintaining constant entropy.

At the CJ point, the Rayleigh line and Hugoniot curve are also tangent to the adiabatic (isentropic) expansion curve [8].

Having computed values for the CJ state, the code can calculate thermodynamic states along the isentrope passing through the post-shock states for a sequence of increasing fixed specific volumes v from v_{CJ} up to $10v_0$.

The process requires to solve Eq. (24) for temperature T foxing the entropy at the CJ point S_{CJ}

$$S(v, T, n(v, T)) = S_{CJ} \tag{24}$$

in which

$$S(v, T, n(v, T)) = S^{id}_{gas}(v, T, n_{gas}) + S^{ex}_{gas}(v, T, n_{gas}) + S^{std}_{solid}(v_{solid}, T) + S^{ex}_{solid}(v_{solid}, T) \tag{25}$$

evaluating again chemical equilibrium as described in sect.2.7 for every iteration of the algorithm for finding the temperature T.

The most frequently used EoS for explosive products expansion is the JWL EoS [26] defined by Eq.(26)

$$p = Ae^{-\frac{R_1 v}{v_0}} + Be^{-\frac{R_2 v}{v_0}} + \frac{C}{\left(\frac{v}{v_0}\right)^{\omega+1}} \tag{26}$$

where $A, B, C, R_1, R_2, \omega$ are JWL coefficients that are computed fitting isentropic pressure-specific volume data. This fit is obtained in MATLAB using the built-in function LSQNONLIN [4] that implements a trust-region reflective algorithm. These coefficients have to be compared to data experimentally derived by cylinder test.

3 Results and Discussion

A complete set of CJ data (detonation velocity, pressure, temperature and molar composition of detonation products) for PETN and TNT are provided as an example of the capability of HEMSim in Tab. 3 both for BKW EoS and EXP-6 IMP based EoS.

We validate the accuracy of our code by utilizing it to forecast the detonation velocity, pressure, and temperature across a spectrum of energetic compounds, comparing our results against experimental values and results from published codes. Tab. 4 provides the results of our code for oxygen-rich compounds, for which the condensed carbon is not present among the products, using EXP-6 IMP-based EoS. In Tab. 3 results for oxygen lean compounds, for which our code predicts the formation of condensed carbon, are provided. All HEMSim outputs are compared against experimental values and computed values published from other codes. The majority of the calculations have excellent accuracy. Discrepancies for detonation velocities are under 2%; results for detonation pressure and temperature are different among the codes considered and also experimental values span a range of 10–20% when considering different sources.

HEMSim is also capable of predicting detonation properties of a mixture of compounds. Some results are provided in Tab. 3.

In Fig.1 we plot results for detonation velocity, pressure, and predicted solid carbon (in diamond form) prediction of HEMSim for different values of initial density for PETN considering EXP-6 IMP based EoS.

The code also provides data for isentropic expansion and JWL fit. We compare our results against [21] plotting adiabatic and Gruneisen gamma as can be seen in Fig. 2. To compute adiabatic gamma γ and Gruneisen gamma Γ, a centered finite-difference numerical scheme [19] for differentiation is used.

It is important to highlight the limitation of the JWL model, which is really sensitive to fitting procedure and range of volumes considered and assumes constant Γ. This phenomenon becomes evident in the analysis of Fig.2, where a significant discontinuity is observed, emphasizing the need for more sophisticated and adaptable models to accurately represent the behavior of energetic materials during isentropic expansion. For some compounds, results for JWL fit are provided in Table 3.

Compound	**PETN**		**TNT**	
General formula	$C_5H_8N_4O_{12}$		$C_7H_5N_3O_6$	
Density [g/cm^3]	1.763		1.64	
Enthalpy of formation [kJ/mol]	-527.25		-63.2	
EoS (gaseous products)	BKWC	EXP6 IMP	BKWC	EXP6 IMP
Parameters at the CJ point				
D_{CJ} [m/s]	8495	8349	6678	6833
p_{CJ} [GPa]	30.2	29.4	17.0	17.6
T_{CJ} [K]	4335	4182	3657	3586
v_{CJ} [cm^3/g]	0.433	0.431	0.468	0.470
v_{gasCJ} [cm^3/g]	0.427	0.423	0.398	0.399
A_{CJ} [MJ/Kg]	-30.7	-30.3	-23.4	-23.4
S_{CJ} [J/Kg K]	7170	5335	6660	6801
Concentration of products at the CJ point [mol/Kg of explosive]				
H_2	-	0.01	-	0.19
N_2	6.32	6.28	6.60	6.37
O_2	-	-	0.61825	-
CO	2.82	0.81	3.80	2.79
NO	-	-	-	-
H_2O	12.64	12.51	10.95	10.05
CO_2	11.24	12.32	5.83	6.79
NH_3	-	0.09	-	0.48
CH_4	-	-	0.02	0.02
C_{grap}	-	-	-	-
C_{diam}	1.75	2.68	21.17	21.22

Table 3: Calculated detonation parameters and concentration of detonation products for PETN and TNT compared using BKWC and EXP-6 IMP based EoS. Product with concentration less than 10^{-3} are indicated by $-$.

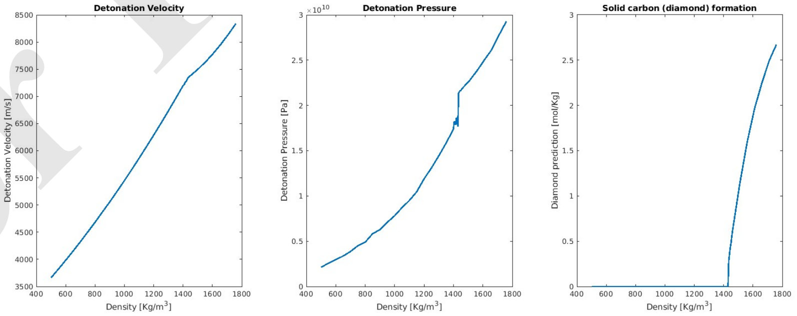

Figure 1: Prediction for PETN detonation at various initial densities. The linear correlation between initial density and predicted detonation velocity is clearly satisfied.

Compound	ρ_0 (g/cm^3)	Method	D_{CJ}(m/s)	P_{CJ}(GPa)	T_{CJ}(K)
Erythritol tetranitrate (ETN) $C_4H_6N_4O_{12}$	1.702	Experiment	7900	-	-
		EquiC	7.993	26.1	4170
		HEMSim	7920	24.8	4288
Nitroglycerin (NG) C_3H_5 N_3O_9	1.60	Experiment	7650	25.3	4300
		EquiC	7624	22.7	4356
		HEMSim	7734	22.3	4504
Liquid nitric oxide NO	1.3	Experiment	5620	10	2858
		EquiC	5578	9.63	2866
		HEMSim	5729	9.91	3106
Tetranitromethane (TNM) CN_4O_8	1.65	Experiment	6450	15.5	2231
		EquiC	6474	15.2	2246
		HEMSim	6509	15.0	2357
Hexanitroethane (HNE) $C_2N_6O_{12}$	1.86	Experiment	7580	23.8	2527
		EquiC	7570	24.1	2535
		HEMSim	7655	23.4	2688

Table 4: Experimental and calculated detonation properties by HEMSim using EXP6 IMP based EoS compared against experimental values and published results from [13].

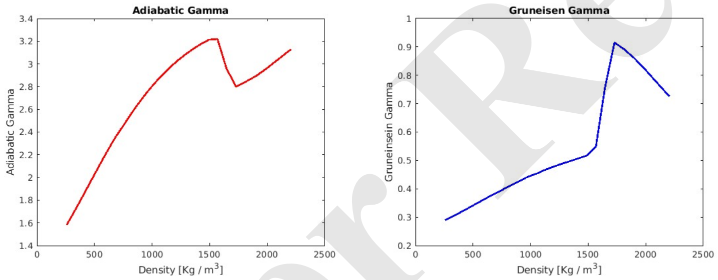

Figure 2: Isentropic derivatives: Left, adiabatic gamma $\gamma$and right, Gruneisen gamma Γ. Results are consistent with [21] calculations.

4 Conclusions

In this paper, we introduced a significant contribution to the simulation and study of ideal detonation through the development of the advanced code HEMSim. The code is able to compute the parameters of detonation of condensed energetic materials under the CJ hypothesis and the curve of expansion of detonation products in the form of JWL isentrope.

A key strength of our code lies in its implementation in MATLAB, a widely used computational environment known for its user-friendliness and widespread adoption within the scientific community. This enables researchers to quickly access the code, run simulations, and customize it to suit their specific research needs.

A distinctive feature of our code is the incorporation of realistic equations of state for both gases and condensed products of a detonation. This allows for a more accurate modeling of detonation processes and yields more reliable results. Detailed results of calculations are presented to verify the code. HEMSim has been developed with the goal of achieving performance levels comparable to the well-established available codes. This level of efficiency and accuracy enables researchers to conduct advanced simulations and obtain dependable outcomes in the field of detonation.

In summary, our code represents a significant contribution in ideal detonation simulation, facilitating research and collaboration. We believe that its freeware nature, implementation in MATLAB, and capability to integrate realistic equations of state will contribute significantly to the understanding of detonation phenomena and the development of practical applications across various scientific disciplines.

Compound	ρ_0 (g/cm^3)	**Method**	D (m/s)	P (GPa)	T (K)
Pentaerythritol-tetra-nitrate (PETN) ($C_5H_8N_4O_{12}$)	1.76	Experiment	8270	31.0	-
		Cheetah	8486	-	-
		EXPLO5	8490	30.0	4110
		HEMSim	8349	29.4	4182
Cyclotrimethylene trinitramine (RDX) ($C_3H_6N_6O_6$)	1.8	Experiment	8754	34.7	-
		EXPLO5	8770	-	-
		HEMSim	8772	32.6	3803
Cyclotetramethylene-tetranitramine (HMX) ($C_4H_8N_8O_8$)	1.89	Experiment	9115	39.3	-
		EXPLO5	9154	-	-
		HEMSim	9167	36.5	3646
Benzotrifuroxan (BTF) ($C_6N_6O_6$)	1.86	Experiment	8490	-	-
		Cheetah	8609	34.9	5259
		EXPLO5	8588	31.2	4379
		HEMSim	8536	34.3	5243
Trinitro triazido-benzen (TNTAB) ($C_6N_{12}O_6$)	1.74	Experiment	8580	-	-
		Cheetah	8739	-	-
		EXPLO5	8584	31.3	4548
		HEMSim	8451	29.5	4545
2,4,6-Trinitrophenylmethylnitramine (TETRYL) ($C_7H_5N_5O_8$)	1.73	Experiment	7720	-	-
		EXPLO5	7692	-	-
		HEMSim	7575	23.8	3996

Table 5: Detonation properties of various explosives that produce condensed carbon compared against values from [22] using EXP6 IMP based EoS.

Compound	ρ_0 (g/cm^3)	**Method**	D (m/s)	P (GPa)	T (K)
TNT/NTO (50/50) ($C_{3.8206}H_{3.0924}N_{3.6359}O_{4.0924}$)	1.71	Experiment	7370	22.6	-
		Cheetah	7418	22.5	-
		HEMSim (BKW EoS)	7346	20.4	3504
NTO/RDX/TNT (50/12/38) ($C_{3.4701}H_{3.1853}N_{3.9022}O_{4.0961}$)	1.792	Experiment	7660	26.5	-
		Cheetah	7810	25.76	-
		HEMSim (BKW Eos)	7894	24.2	3555
RDX/WAX (91/9) ($C_{3.7419}H_{7.5126}N_{4.9196}O_{4.9196}$)	1.64	Experiment	8470	-	-
		EXPLO5	7927	-	-
		HEMSim (EXP6 IMP EoS)	8123	24.3	3517

Table 6: HEMSim results for some compound mixtures. Results are compared with values in [22] and [15].

Compound	ρ_0 $[g/m^3]$	A $[GPa]$	B $[GPa]$	C $[GPa]$	R_1	R_2	ω
TETRYL	1.730	585.68	6.68	3.09	4.71	1.26	0.73
PETN	1.760	630.46	6.77	3.72	4.49	1.21	0.70
RDX	1.800	650.78	6.78	4.20	4.40	1.20	0.85
NG	1.600	593.75	6.37	3.18	4.85	1.48	0.54

Table 7: JWL fitting for isentropic expansion values for a reduced volume grid up to $10v_0$ using EXP-6 IMP based EoS.

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