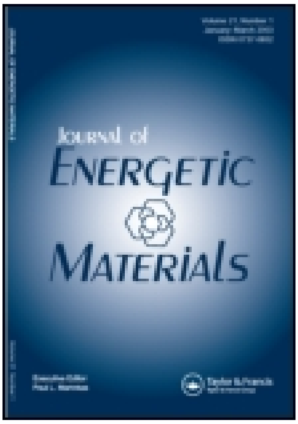

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The Optimization of Detonation Properties in Gaseous Mixtures and Mixed Explosive Materials

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The main objective of this research is to find compositions with optimum detonation properties. The detonation properties were obtained based on the Chapman-Jouguet (CJ) theory. These properties and the amount of mixture components are defined as objective functions and optimization variables, respectively. The present study was performed for both gaseous mixtures and mixed condensed explosive materials. In the former, the equivalence ratio with optimum detonation properties was found and compared with those obtained from the CEA code. It was found that, in gaseous mixtures, the optimum value for different detonation parameters occurred in different equivalence ratios. For amatol, an industrial high explosive, the best properties corresponded to a composition of 10% trinitrotoluene (TNT) and 90% ammonium nitrate (AN), while the current composition, which is widely used, consists of 20% TNT and 80% AN. It was also found that, in two-component mixed explosives, the composition for zero oxygen balance was close to the composition that yields the maximum pressure and velocity.

Keywords CJ theory; detonation properties; high explosives; optimum composition; oxygen balance

Introduction

Detonable materials are divided into two general groups, namely, gaseous mixtures and condensed high explosives. In most detonable materials, there is a composition in which the optimum performance is obtained [1]. The ability to predict the composition of new high explosives with desired (i.e., optimum) properties from first principles is very attractive to high explosive developers, because it helps to reduce the cost and danger of experimental investigations.

The study of performance of these materials by numerical methods has increased extensively in recent years [2–6]. Global detonation parameters (e.g., detonation velocity and pressure) are easily obtained using the classical equilibrium Chapman-Jouguet (CJ) theory. In this theory, it is assumed that detonation is a one-dimensional, steady supersonic shock wave supported by a negligible length reaction zone. Moreover, according to this theory, the detonation products are in thermochemical equilibrium [7].

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Several equilibrium codes have been developed in past five decades to determine the CJ parameters of gaseous mixtures as well as those of condensed explosives. Among them, Becker-Kistiakowsky-Wilson (BKW) of Mader (1956) and its next generations Stretch BKW (1961) [8–10] and Fortran-BKW (1967) [11], RUBY [12], TIGER [13], and CHEETAH [14] are more popular in energetic materials communities. On the other hand, CEA [15] and STANJAN [16] are widely utilized for gaseous mixtures. None of these codes is able to automatically find the composition that corresponds to the optimum detonation parameters [1].

In the past 20 years, numerous papers have been published regarding numerical optimization of various engineering problems. However, only a few papers are related to the optimization of explosive materials. One related paper is the work of Muthurajan et al. [1]. In this paper, it was reported that the LOTUS code can find the maximum detonation velocity based on the oxygen balance concept. However, no information was provided regarding the optimization process or optimization results.

Due to the importance of the equation of state (EOS) in the accurate prediction of detonation properties and the complexity of the determination of proper experimental coefficients of the EOS of the detonation products to cover a vast range of explosives, the optimization of the EOS parameters to reproduce detonation properties has been the subject of much research in the past three decades [17,18]. However, as stated in Muthurajan et al. [1], optimization of explosive formulations has not previously been reported in the literature.

Optimum detonation properties can be obtained by an optimization algorithm and an equilibrium code (to determine the detonation parameters). In this study, objective functions are defined as different CJ detonation parameters such as pressure, temperature, detonation velocity, detonation energy, and isentropic expansion work of the products. The optimization process is a so-called constraint optimization. The low and high limits of the percentage of the mixture components are considered as the optimization constraints.

The main objective of this study is to find the compositions of gaseous mixtures and mixed condensed explosives with optimum CJ detonation properties. In this study, a domestic equilibrium code (i.e., TMUEC-1.0)[1] was used to determine the CJ properties, and the code SolvOpt was utilized to optimize the CJ properties. SolvOpt code is an open source optimization code available in Kuntsevich and Kappel [19].

The Algorithm

The following algorithm was used to calculate the optimum detonation parameters:

1. The number and type of components in a composition are selected.
2. A guessed value for the percentage of each component for condensed explosives or the equivalence ratio for a gaseous mixture is considered.
3. The density of the composition is calculated.
4. The value of the objective function (the desired CJ detonation parameter) is calculated using TMUEC-1.0 code.
5. The objective function and constraints are analyzed by the optimization code SolvOpt.

[1] See Appendix.

6. If the constraints and the exit criterion are satisfied, the optimum composition is accepted. Otherwise, a new composition is created and the optimization process is repeated from step 3.

Oxygen Balance

The oxygen balance (OB) of an explosive is one of the most significant parameters in determining the performance of the explosive [1]. It is defined as the percentage excess/deficiency of oxygen in the explosive molecule to completely oxidize carbon and hydrogen to CO_2 and H_2O. If some oxygen molecules remain unused after the oxidizing reaction, the oxygen balance is positive. If all oxygen molecules are consumed and some fuel molecules remain unburned, the oxygen balance is negative [20]. Considering the fact that the maximum energy is released for mixtures with oxygen balance close to zero, zero oxygen balance is considered a criterion to optimize the performance of an explosive [21,22].

In this work, compositions with the general chemical formula $C_xH_yN_wO_z$ were studied. To calculate the oxygen balance, the number of oxygen molecules needed to oxidize all carbon and hydrogen molecules of the explosive was determined. For burning carbon to CO_2, the number of oxygen molecules that are needed is twice the explosive carbon content (i.e., oxygen molecules needed $= 2x$). For oxidizing hydrogen molecules to water, one oxygen is needed for two hydrogen (i.e., oxygen molecules needed $= y/2$). Hence, if there are z atoms of oxygen in the composition, the oxygen balance is defined as $(z - 2x - y/2)$. The oxygen balance is often expressed as the weight percentage of excess oxygen to explosive material; that is [5],

$$OB\% = \frac{100 \times AW(O_2) \times \left[z - 2x + \frac{y}{2}\right]}{MW(explosive)}$$

Results

Optimization of Detonation Parameters in Gaseous Mixtures

The purpose of this section is to find equivalence ratios of fuel–air mixtures corresponding to maxima in CJ properties (pressure, velocity, etc.). For this part of the study, using the CEA equilibrium code, a validation procedure is devised for validation of the optimization task. For each mixture, detonation parameters were determined for equivalence ratios between 0.5 and 3; then, the optimum properties were searched between these values.

The optimum values of CJ detonation parameters predicted in the present work were compared with the results from the CEA code for methane–air, propane–air, acetylene–air, and hydrogen–air mixtures (Tables 1–4).

An interesting point is that for acetylene–air mixtures, an increase in fuel resulted in an increase in the energy of CJ detonation products and there was no maximum value for the fuel. This behavior was also observed for energy and isentropic work in hydrogen–air mixtures.

To obtain the optimum values from the CEA code, different detonation parameters for a wide range of equivalence ratio were calculated. The results were plotted and the optimum values were obtained based on these plots. Two sets of these plots are shown in Fig. 1.

Table 1 Optimum values of CJ detonation parameters in methane–air mixtures

Detonation properties		CEA code	Present study	Percentage difference between calculated and CEA code parameters
Pressure (bar)	Optimum value	27.618	27.83	0.7653
	Equivalence ratio	1.25	1.36	
Temperature (K)	Optimum value	3,157	3,105	1.6674
	Equivalence ratio	1.18	1.16	
Energy (kJ/kg)	Optimum value	691.32	686.19	0.7407
	Equivalence ratio	0.88	0.806	
Velocity (m/s)	Optimum value	1,873.90	1,860.70	0.7017
	Equivalence ratio	1.46	1.506	
Isentropic work of detonation products (MJ/kg)	Optimum value	3.29	3.24	1.4757
	Equivalence ratio	1.66	1.69	

The results presented in Tables 1 to 4 reveal the following:

- For a given fuel–air mixture, the optimum values for different detonation properties occur at different equivalence ratios. For example, for methane–air mixtures, the maximum CJ pressure occurs at φ (equivalence ratio) $= 1.36$, and the maximum detonation velocity corresponds to $\varphi = 1.5$.
- For a specified property (e.g., detonation velocity), the optimum equivalence ratio is different in different mixtures.

The above-mentioned properties are also clearly observed in Fig. 1.

Table 2 Optimum values of CJ detonation parameters in propane–air mixtures

Detonation properties		CEA code	Present study	Percentage difference between calculated and CEA code parameters
Pressure (bar)	Optimum value	31.7	31.41075	0.91482
	Equivalence ratio	1.445	1.52	
Temperature (K)	Optimum value	3,213	3,164	1.5439
	Equivalence ratio	1.24	1.19	
Energy (kJ/kg)	Optimum value	815.81	811.47	0.53125
	Equivalence ratio	1.19	1.01	
Velocity (m/s)	Optimum value	1,888.9	1,878.45	0.5532
	Equivalence ratio	1.54	1.6	
Isentropic work of detonation products (MJ/kg)	Optimum value	3.37	3.37	0.03934
	Equivalence ratio	1.75	1.78	

Table 3 Optimum values of CJ detonation parameters in acetylene–air mixtures

Detonation properties		CEA code	Present study	Percentage difference between calculated and CEA code parameters
Pressure (bar)	Optimum value	36.865	36.3	1.5326
	Equivalence ratio	2.5	2.4513	
Temperature (K)	Optimum value	3,669.7	3,621.31	1.3186
	Equivalence ratio	1.86	1.8066	
Energy (kJ/kg)	Optimum value Equivalence ratio	With increasing fuel, energy increases and there is no maximum point		
Velocity (m/s)	Optimum value	2,112.1	2,110.39	0.8097
	Equivalence ratio	2.5	2.4993	
Isentropic work of detonation products (MJ/kg)	Optimum value	4.2401	4.2402	0.00118
	Equivalence ratio	2.5	2.4994	

Table 4 Optimum values of CJ detonation parameters in hydrogen–air mixtures

Detonation properties		CEA code	Present study	Percentage difference between calculated and CEA code parameters
Pressure (bar)	Optimum value	24.72	24.82	0.406
	Equivalence ratio	1.22	1.24	
Temperature (K)	Optimum value	3,251	3,258	0.2149
	Equivalence ratio	1.22	1.22	
Energy (kJ/kg)	Optimum value Equivalence ratio	With increasing fuel, energy increases and there is no maximum point		
Velocity (m/s)	Optimum value	2,794.4	2,789.86	0.1624
	Equivalence ratio	63	63.62	
Isentropic work of detonation products (MJ/kg)	Optimum value Equivalence ratio	With increasing fuel, energy increases and there is no maximum point		

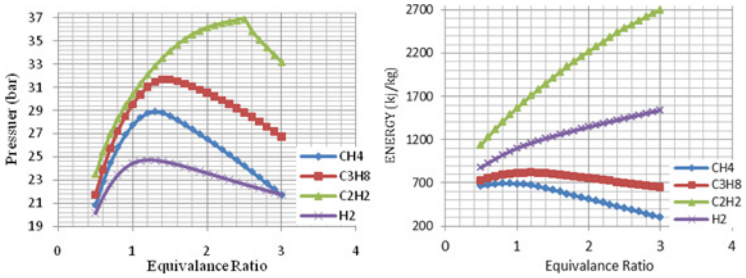

Figure 1. Detonation properties versus equivalence ratio for different fuel–air mixtures calculated using CEA code (color figure available online).

Optimization of Detonation Properties in Condensed Materials

Optimization results for condensed energetic materials are presented in this section. Before presenting the results for such high explosive materials, the equilibrium code developed in this study (i.e., TMUEC-1.0 code) is validated using some published data. The results are provided in Table 5. These results indicate the merits of the TMUEC-1.0 code for calculating CJ detonation parameters of condensed explosives. In the next step, amatol and ammonium nitrate/fuel oil (ANFO), two highly used industrial explosives, are analyzed and their proper compositions are obtained.

Optimization of Amatol

Amatol is an industrial mixed explosive that contains 20% trinitrotoluene (TNT) and 80% ammonium nitrate (AN). The percentages of AN and TNT in the composition are defined as the design variables in the optimization process. The objective function is a detonation parameter. Amatol's CJ detonation properties calculated by TMUEC-1.0 are shown in Table 6.

The optimum CJ properties for mixtures of AN and TNT are provided in Table 7 for several percentages by mass of the explosive components.

Table 5 Validation of TMUEC-1.0 code using experimental and CHEETAH data

High explosive	Detonation property	Experimental data	TMUEC-1.0	CHEETAH
PETN $\rho_{AN} = 1.76$ (g/cc)	P_{CJ} (GPa)	33.7 [5]	29.16	31.00 [14]
	D_{CJ} (km/s)	8.27 [5]	8.3	8.33 [14]
	v_{CJ} (cc/g)	0.4088 [5]	0.4329	0.423 [14]
HMX $\rho_{AN} = 1.89$ (g/cc)	P_{CJ} (GPa)	38.7 [23]	38	38.6 [23]
	D_{CJ} (km/s)	9,110 [23]	9,144	9,244 [23]
RDX $\rho_{AN} = 1.77$ (g/cc)	P_{CJ} (GPa)	33.79 [23]	32.18	33.12 [23]
	D_{CJ} (km/s)	8,639 [23]	8,676	8,807 [23]
TATB $\rho_{AN} = 1.85$ (g/cc)	P_{CJ} (GPa)	25.9 [23]	26.91	27.03 [23]
	D_{CJ} (km/s)	7,660 [23]	7,742	7,814 [23]
TNT $\rho_{AN} = 1.64$ (g/cc)	P_{CJ} (GPa)	19 [23]	18.91	19.17 [23]
	D_{CJ} (km/s)	6,950 [23]	6,764	6,843 [23]

Table 6 Detonation properties for amatol calculated by TMUEC-1.0 code

High explosive material	Density of components	Detonation properties	Result from TMUEC-1.0
Amatol (80% AN 20% TNT)	$\rho_{AN} = 1.725$	P_{CJ} (GPa)	13.96
	$\rho_{TNT} = 1.654$	v_{CJ} (cc/g)	0.517
	(g/cc)	e_{CJ} (kJ/cc)	2.709
		D_{CJ} (km/s)	6.17

The results showed that the industrial composition of amatol (i.e., 20% TNT and 80% AN) does not have optimum properties. The composition corresponding to the maximum values of pressure and velocity contained 91% AN and 9% TNT. Moreover, the composition of 85% AN and 15% TNT had the maximum value of energy. The industrial composition of amatol (i.e., 20% TNT and 80% AN) was close to the composition corresponding to the optimum value of the isentropic work of the detonation products in the CJ state. According to the present results, the best detonation properties were found when the percentage of AN in a mixture of AN +TNT was between 85 and 90%,. It is important to emphasize that the limitations usually imposed by the manufacturing process are not considered here. In fact, in addition to the current optimization suggestions, those limitations should be taken into consideration for selecting the best composition.

Table 7 also reveals that the composition with zero oxygen balance was very close to the one corresponding to the maximum pressure and velocity.

Optimization of ANFO

ANFO is another industrial mixed explosive. It consists of 94% AN and 6% fuel oil. The optimized properties of mixed explosives containing these two components (i.e., AN and fuel oil) were obtained and are shown in Table 8.

The results obtained from the optimization process were in close agreement with the industrial composition of ANFO. Only a 1% difference was observed for pressure, energy, and velocity. However, the difference was higher for isentropic

Table 7 Optimum CJ detonation parameters for AN + TNT composition

High explosive material	Density of component (g/cc)	Detonation properties	Present study: Mass percentage of (AN/TNT)	Present study: Optimum value
Amatol (AN/TNT) Zero OB: (91.3/8.7)	$\rho_{AN} = 1.725$	P_{CJ} (GPa)	(91.22/8.78)	25.22
	$\rho_{TNT} = 1.654$	v_{CJ} (cc/g)	(98.65/1.35)	0.465
		e_{CJ} (kJ/cm^3)	(85.3/14.7)	2.73
		D_{CJ} (km/s)	(91.24/8.76)	8.18
		Isentropic work of detonation products (MJ/kg)	(78.36/21.63)	64,053.5

Table 8 Optimum properties for CJ detonation for AN+Fuel oil composition

High explosive material	Density of component (g/cc)	Detonation properties	Present study Mass percentage of (AN/fuel oil)	Optimum value
ANFO (AN/fuel oil) Zero OB: (95.23/4.76)	$\rho_{AN} = 1.725$	P_{CJ} (GPa)	(95.07/4.92)	26.71
	$\rho_{Fueloil} = 1.654$	v_{CJ} (cc/g)	(0.99/99.01)	0.906
		e_{CJ} (kJ/cm^3)	(94.99/5.01)	2.836
		D_{CJ} (km/s)	(95.22/4.78)	8.43
		Isentropic work of detonation products (MJ/kg)	(77.18/22.82)	63,368.8

expansion work. The oxygen balance for pure fuel oil explosive is − 332.6 and for AN it is + 20. The zero oxygen balance of the mixed composition occurred for a mixture of 95% AN and 5% fuel oil. This composition was close to the composition that possessed the optimum pressure, velocity, and energy.

New Compositions

The optimization algorithm devised in the present study offers a powerful tool to generate new explosive materials according to an industrial requirement, without the high cost and dangers associated with experimental trials. We describe in this section how we sought the optimum composition consisting of TNT, pentaerythritol tetranitrate (PETN), and ammonium dinitramide (ADN). The mass percentages of these materials are the design variables and detonation parameters are the objective functions. The results are shown in Table 9, Fig. 2, and Fig. 3.

Table 9 Optimum properties for CJ detonation of ADN +PETN +TNT composition

Compound of high explosive materials	Density of component (g/cc)	Detonation properties	Present study Mass percentages of (ADN/PETN/TNT)	Optimum value
AND PETN TNT	$\rho_{ADN} = 1.8$	P_{CJ} (GPa)	(82.18/2.12/16.76)	30.67
	$\rho_{PETN} = 1.78$	v_{CJ} (cc/g)	(98/1/1)	0.454
	$\rho_{TNT} = 1.654$	e_{CJ} (kJ/cm^3)	(67.7/22.5/9.8)	3.436
		D_{CJ} (km/s)	(83.4/0.8/15.78)	8.7851
		Isentropic work of detonation products (MJ/Kg)	(58.01/37.33/4.65)	82,348.38

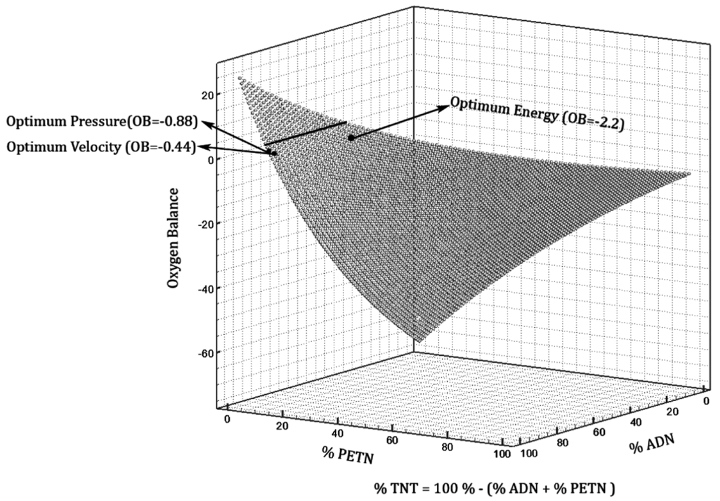

Figure 2. The hatched region shows the oxygen balance for different mass percentages of ADN and PETN in the ADN/TNT/PETN composition. The thick line shows zero oxygen balance for different percentages of the components. The locations of the optimum values of components for optimum detonation pressure, velocity, and energy are shown.

As Fig. 2 shows, when the number of components in a condensed explosive mixture exceeds two, the oxygen balance is a less reliable means of determining the optimized properties. When there are only two components, there is only one composition with zero oxygen balance. However, when the number of components

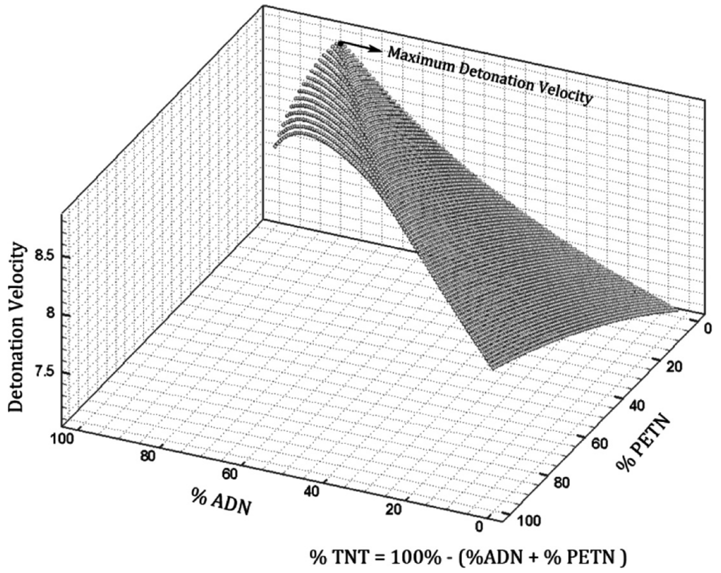

Figure 3. The hatched region shows CJ detonation velocity for different mass percentages of ADN and PETN in the ADN/TNT/PETN composition. The location of the optimum value of components for optimum detonation velocity is shown.

is more than two, there is not a unique composition with zero oxygen balance. For example, in the present three-component composition, the zero oxygen balance occurs in the range of 50 to 83 mass percent of ADN (thick line in Fig. 2). Thus, there are several compositions with zero oxygen balance.

The variation in oxygen balance with different mass percentages of ADN and PETN, as well as the location of the compositions with zero oxygen balance (i.e., the thick line), are shown in Fig. 2.

Figure 3 demonstrates the variation in detonation velocity versus different mass percentages of ADN and PETN. The location of the optimum detonation velocity is also depicted in Fig. 3.

Conclusion

Working with explosive materials is one of the highest risk tasks in laboratory and field studies. Nevertheless, motivated by technology as well as safety requirements, and despite the high cost and enormous dangers, developing new materials with desired properties has been the goal of numerous studies conducted in the field of energetic materials in the past 20 years. A highly efficient algorithm was devised in the current study to determine the optimized properties of CJ detonations in mixed explosives, with the aim of developing an inexpensive tool for designing desired explosive materials while minimizing the danger involved. The algorithm has two essential parts. The first part is an equilibrium thermochemical code to calculate the CJ (equilibrium) detonation parameters. A domestic code (i.e., TMUEC-1.0) was developed by the authors for this purpose. By comparing the detonation properties predicted by the TMUEC code with some published data (experimental data as well as the data produced by the famous equilibrium codes CHEETAH and CEA), the merits of TMUEC-1.0 code were assessed.

The equilibrium code was then used as a subroutine to determine the objective function of a standard optimization code. The open source code SolvOpt was utilized as the optimization numerical tool in this study. The equivalence ratio in gaseous mixtures and the mass percentage of components in condensed explosives were considered as the optimization variables.

The numerical tool developed may be used as a safe and friendly virtual laboratory to investigate the explosion properties of desired mixtures. Some important results obtained with this tool are summarized as follows:

- For a given fuel–air mixture, the optimum values for different detonation properties occur at different equivalence ratios.
- For a specified property (e.g., detonation velocity), the optimum equivalence ratio is different for different gaseous mixtures.
- The oxygen balance in condensed explosives is a key parameter to determine the optimized detonation properties.
- In condensed explosives, the composition for zero oxygen balance is very close to the composition corresponding to the maximum CJ pressure and velocity.
- Though the role of oxygen balance in determining the optimum properties is important in two-component materials, the composition with zero oxygen balance is not unique in mixed materials with three or more components.
- The current results indicate that the industrial composition of the mixed explosive amatol (i.e., 20% TNT and 80% AN) does not have the optimum CJ pressure and

velocity. However, this composition is very close to the composition for maximum isentropic work of detonation products in a CJ state. According to our results, when the percentage of AN in the mixture of AN +TNT is between 85 and 90%, the best performance of this mixed material is yielded.
- The results obtained from the optimization process for a mixture of the explosives TNT and AN indicate that the optimum composition is in close agreement with the industrial composition of ANFO.

The limitations usually imposed by manufacturing process were not considered. Indeed, in addition to the current optimization suggestions, those limitations should be considered in the selection of a proper composition.

Appendix

TMUEC-1.0 is an equilibrium code based on CJ detonation theory to determine the detonation properties in gaseous mixture and high explosive materials. This code was developed in the Gas Dynamics Lab at Tarbiat Modares University (TMU). In this code, the element-potential method, which has previously been used in STANJAN [16] for gaseous mixtures, is utilized to minimize the Gibbs function. The main advantage of this method is its very low computational cost and the prevention of negative mole fractions in the process of Gibbs minimization. TMUEQ-1.0 uses the BKW equation of state for high-pressure products of high explosives and the ideal gas equation of state for detonation products of gaseous reactants. The code was developed for C-H-N-O-CL-F explosives and gaseous reactants. The CJ detonation properties of high explosives determined by TMUEQ-1.0 were compared with numerous experimental data [5] as well as the published results of CHEETAH [14,23]. The agreement was very good. The results for gaseous mixtures were in excellent agreement with the results of CEA and STANJAN.

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