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Application of the Explosion Temperature for Estimation of Detonating Power of Multicomponent Explosives

MOHAMMAD HOSSEIN KESHAVARZ* and HAMID REZA POURETEDAL
Department of Chemistry, Malek-Ashtar University of Technology
Shahin-Shahr-83145/115, Islamic Republic of Iran
Fax: (98)(312)5225068; Tel: (98)(312)5225071
E-mail: mhkeshavarz@mut-es.ac.ir, mhkir@yahoo.com

A method is reported here for predicting the Chapman-Jouguet detonation pressure of multicomponent explosives at any loading density. It is assumed that the explosive reacts to form major products composed of C(s), CO, N_2, H_2O, H_2 and CO_2 as determined by the oxygen balance of the unreacted explosive. Detonation pressure can be related to the temperature of explosion, the number of moles of gaseous products and initial density of the explosive. Explosion temperature based on the assumed decomposition reaction, as a fundamental parameter, can be easily found from the condensed heat of formation of the explosive and molar heat capacity of the gaseous products. Good agreement is obtained between measured and calculated values of detonation pressure for well known mixture of explosives at any initial density defined by experiment as compared to complex computer code.

Key Words: **Explosion temperature, Detonating power, Explosives.**

INTRODUCTION

Although reliable experimental data are always preferred over values obtained by an estimation method, but in the case of detonation pressure often reliable data are not available. The Chapman-Jouguet pressure, detonation energy and detonation velocity are three important parameters that serve as figures of merit in judging the relative effectiveness of explosives. If a good correlation can be extensively used for explosives, the practical question arises as how to find the detonation properties in order that the correlation can have real predictive power.

The Chapman-Jouguet detonation pressure can be calculated by a computer code, *e.g.*, CHEETAH[1], a C version of the FORTRAN equilibrium code TIGER[2], which uses a developed database from thermodynamic characteristics of explosion products and initial composition of the high explosives. In this method, an equation of state for detonation products is usually used for determination of time-independent state of chemical equilibrium. The Becker-Kistiakosky-Wilson equation of state (BKW-EOS)[3] and the Jacobs-Cowperthwaite-Zwisler equation of state (JCZ-EOS)[4] as representative examples are two equations of state, which can be used to calculate detonation properties of explosives. The BKW-EOS has an important role in predicting detonation properties of the high explosives[5]. Kamlet and coworkers[6–9] developed semiempirical correlation to predict the Chapman-Jouguet detonation pressure and velocity of usual CHNO explosives at loading density greater than 1 g/cc on the assumption that N_2, H_2O, C(s) and CO_2 (but not CO) are the important detonation products.

It should be noted that the accuracy of estimated performance of an explosive is not necessarily enhanced by greater complexity of the method, namely as calculated by a computer code. The present procedure is remarkable because the only data used for estimating the Chapman-Jouguet detonation pressure of multicomponent explosives were the initial density and the explosion temperature. A more reliable decomposition provides a useful method for obtaining the explosion temperature from the heat capacities of gaseous products. Since the values of Chapman-Jouguet detonation pressure are hardly known for many pure and mixed explosives of interest, the present method for finding a suitable procedure, say, applying the number moles of gaseous products and explosion temperature would be needed. The present study can also be simply applied to explosives at any loading density with no difficulties.

The purpose of this work was to correlate and to predict the Chapman-Jouguet pressure of complex explosive mixtures based on the explosion temperature and the number of moles of gaseous products per unit weight of explosive, which are closely related to a more reliable decomposition procedure. An empirical feature is incorporated in the method, which enables it to describe Chapman-Jouguet pressure of explosive at all initial densities and compositions.

Explosion temperature

The composition of detonation products can be determined from experimental measurement, thermochemical equilibrium calculation or by identifying an appropriate decomposition reaction. Depending on the composition of explosive, the major components of detonation products may include N_2, CO, H_2O, CO_2 and solid carbon as well as minor amounts of H_2, NH_3, O_2, NO and other chemical species. Rice and Hare[10] studied the products concentration for 34 of CHNO explosives calculated by CHEETAH 2.0/JCZS and found that 94% of the gaseous species contain H_2O, H_2, N_2, CO_2 and CO meanwhile for 30 of these explosives, the concentration of the mentioned detonation products exceeds 97%. A more reliable decomposition reaction for CHNO explosive can be introduced so that the major products are included[11]. We can assume that all nitrogens go to N_2 while a portion of the oxygens form H_2O and carbons preferentially will be oxidized to CO rather than CO_2.

Detonation energy or heat of detonation provides information about the work capacity of the explosive, *e.g.*, secondary explosive. Explosion temperature can be defined as the maximum temperature that the gaseous products of detonation can reach if no heat is lost to the surroundings. The solid state heat of formation is the principal parameter for the calculation of explosion temperature. It can be determined by experimental[12] or some estimated methods[13–16]. The fact that heat capacities of gaseous products are functions of temperature means that a successive approximation procedure is needed to determine explosion temperature.

It was suggested that the Chapman-Jouguet detonation pressure of pure high explosives might be estimated by semiempirical equation, which presented the pressure as depending on the explosion temperature, the number of moles of detonation gaseous products per unit weight of explosive and initial density[11]. The correlation for one component explosive can be given as follows:

$$P_{CJ} = 9.5(\alpha T_{ex})^{1/2} \rho_0^2 - 9 \tag{1}$$

where P_{CJ} is the Chapman-Jouguet detonation pressure in kbar, α is the number of moles of gaseous products of detonation per gram of explosive and ρ_0 is loading density in g/cc. This correlation gives good P_{CJ} for pure explosives with different molecular structures at any loading density.

Multicomponent explosives

A mixture of some explosive compositions can be used to optimize their performance, *e.g.*, a typical mixed explosive is one which contains 60% RDX and 40% HMX. RDX has sufficient oxygen content so that it favours the oxidation of carbon into CO and CO_2 and hydrogen to H_2O, but TNT is oxygen deficient because some carbon has not been oxidized and hydrogen has remained unchanged. The deficiency in oxygen of TNT is the reason why it gives a black sooty smoke when it is detonated.

Explosion temperature and the number of moles of gaseous products of any pure explosives can be combined in an appropriate way to give the Chapman-Jouguet detonation pressure of mixed explosives at any loading density. Two equations are required which relate T_{ex} and α for mixed explosive to the pure component values and composition of mixture. The simplest way is based on the assumption that each component of mixed explosive react separately so that weight average values of T_{ex} and α for all constituents are considered. In this case, we can apply the following relations:

$$T_{ex,\,mix} = \sum_i y_i T_{ex,\,i} \tag{2}$$

$$\alpha_{mix} = \frac{\sum y_i N_i}{\sum y_i M_i} \tag{3}$$

where y_i, N_i and M_i are the mole fraction, the number of moles of gaseous products, the molecular weight of the ith component in the mixed explosive, respectively. The theoretical results from eqs. (1), (2) and (3) with experimental data for some mixed explosives are listed in Table-1. As seen, the calculated detonation pressures of six mixed explosives by the correlation as well as the experimental data of their detonation performance are compared with measured values and BKW-EOS method. Agreement with measurements has been secured in that the molecular structure of different explosives and determined explosion temperature in the expression has been made consistent with a vast number of experimental results. These results appear to hold with remarkable accuracy, as compared to a complicated computer code such as BKW-EOS, when tested with experimental data for any number of mixed explosives. It is important to stress that the present equations operate in a predictive mode. In summary, the correlation for P_{CJ} of mixed explosives requires only $T_{ex,\,mix}$ and α_{mix} at any specified loading density.

TABLE-1

CALCULATED AND MEASURED DETONATION PRESSURES (kbar) FOR SOME MULTICOMPONENT EXPLOSIVES

Explosives	ρ_0	α_{mix}	$T_{ex,\,mix}$	P_{CJ} (Exp)[a]	P_{CJ} (BKW-EOS)	P_{CJ} (Correlation)
1/0.071 moles NM ($\alpha = 0.0492, T_{ex} = 2232$)/ TNM ($\alpha = 0.0306$, $T_{ex} = 3357$)	1.197	0.0457	2306	138	153	131
1/0.25 moles NM/TNM	1.310	0.0409	2457	156	181	154
1/0.5 moles NM/TNM	1.397	0.0377	2607	168	179	175
Pentoline, 50/50 TNT ($\alpha = 0.0441$, $T_{ex} = 1909$)/ PETN ($\alpha = 0.0348$, $T_{ex} = 3542$) $C_{10.592}H_{10.7472}N_{5.8736}O_{14.6208}$	1.680	0.0394	2592	251	267	262
Composition B, 64/36 RDX ($\alpha = 0.0405$, $T_{ex} = 3176$)/ TNT ($\alpha = 0.0441$, $T_{ex} = 1909$) $C_{6.851}H_{8.750}N_{7.650}O_{9.3}$	1.713	0.0418	2726	294	284	289
Cyclotol, 77/23 RDX/TNT $C_{5.045}H_{7.461}N_{6.875}O_{7.753}$	1.743	0.0413	2890	313	305	306
Octol, 76.3/23.7 HMX ($\alpha = 0.0405$, $T_{ex} = 3164$)/ TNT ($\alpha = 0.0441$, $T_{ex} = 1909$) $C_{6.835}H_{10.025}N_{9.215}O_{10.43}$	1.809	0.0414	2803	343	333	326

[a] Experimental values are taken from Mader[5] except Pentolite which is taken from Hobbs and Baer[17].

Conclusion

The main object of this work was to investigate the likelihood of a generalized simple method for mixed explosives of somewhat more practical importance to the explosive user. We recall that knowledge concerning the Chapman-Jouguet detonation pressure and velocity are two fundamental parameters from which the detonating performance of any explosive can be determined. It can be inferred that the formation of light gaseous products and high positive heat of formation per unit weight promote a high detonation pressure. Since the former gives a greater number of moles of gaseous detonation products per unit weight of explosive, the next leads to greater release of energy upon detonation and a higher explosion temperature. The central idea is to use explosion temperature to determine P_{CJ} that is related to solid state heat of formation of explosive and heat capacities of gaseous detonation products at or near explosion temperature. By using data of the pure constituents, it is simply possible to estimate the Chapman-Jouguet detonation pressure of a mixture.

A convenient estimate of reliable decomposition of the mixed explosive is obtained if it is assumed that each component reacts to form major products composed of C(s), CO, N_2, H_2O, H_2 and CO_2 as determined by the oxygen balance of the unreacted explosive. As seen in Table-1, good agreement is obtained between measured and calculated values of the detonation pressure at initial density of explosive defined by experiment with respect to complicated BKW-EOS computer code.

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