Estimation of Detonation Velocity and Detonation Pressure for CHNO Explosive Mixtures

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An empirical method recently reported for estimating detonation velocity (D) and detonation pressure (P) of pure CHNO explosives is extended to CHNO explosive mixtures. Two computation schemes are derived for the parameter G:adding their corresponding weighted G values of pure constituents (G_I) and deriving from the hypothetical chemical composition of the explosive mixture (G_{II}). The calculated D and P values from the G_I scheme, the G_{II} scheme and BKW are extensively compared to the experimental values. It is shown that the G_I scheme is able to estimate simply and accurately the D values (within an average deviation of ±1.32%) or P values (within an average deviation of ±4.77%) for a wide range of explosive types.

1. INTRODUCTION

In a recent paper[1], we have introduced an empirical method to estimate detonation velocities and detonation pressures of pure CHNO explosives in a simple manner. The method requires only the initial density and a parameter obtained from the chemical nature of the explosive. It is shown to estimate simply and accurately detonation velocities and detonation pressures of a wide range of pure CHNO explosives.

Because explosives are frequently used in mixtures, it is practical to discuss the estimation of detonation performances for explosive mixtures. Although numerous equations of state (e.g. BKW[2], LJD[2], and KHT[3]) have been used in the estimation of explosive mixtures, empirical methods are attractive because they are simple, do not require a computer or sophisticated programs, and effectively reproduce the results of the equation−of−state methods. These empirical methods include a method originally developed by Urizar[4], a method of Kamlet[5], and a method proposed by Wu Xiong[6]. The present paper will describe the predictive capability of the previous method[1] for CHNO explosive mixtures.

2. CALCULATION SCHEME

The equations used in Reference 1 for estimating detonation velocities and detonation pressures of CHNO explosives are as follows (herein the equations have been rearranged according to the units):

$$D=(0.99G+2.63)\ \rho_o+2.33G+0.65 \quad (1)$$

$$P=(1.60G+1.945)\ ^2\rho_o^2 \quad (2)$$

where D and P are detonation velocity (km/s) and detonation pressure (GPa) respectively at the initial density ρ_o(g/cm³). G is the gas coefficient of the explosive, which is defined from the chemical nature, i.e., chemical elemental composition and structural type, of the explosive by the H_2O–CO_2 decomposition assumption of the detonation gas products.

It is often possible to use data on the pure constituents to estimate properties of an explosive mixture. The detonation velocity of an explosive mixture can be estimated as the sum of the detonation velocities of the constituents weighted by their corresponding volume fractions in Urizar method[4]. Kamlet ϕ[5] of an explosive mixture can be computed by using weighted−average N, M, and Q (see the definition of ϕ in Reference 5) values of pure constituents, using the hypothetical values of chemical elemental composition and heat of formation (i.e., the explosive mixture is assumed as a pure explosive with the same composition) and adding the weighted ϕ values of pure

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constituents. It is shown that the third computation method of ϕ has the advantages of simplicity and high accuracy[7].

There are two schemes for the computation of gas coefficient G values for explosive mixtures. One scheme is that adding their corresponding weighted G values of pure constituents (defined as G_I in this paper) and the other scheme is that deriving from the hypothetical chemical composition of the explosive mixture (defined as G_{II}). For an explosive mixture with the hypothetical chemical composition of $C_aH_bN_cO_d$ ($b/2 \leqq d \leqq 2a+b/2$), the G_{II} value may be computed from the following equation[1],

$$G_{II}=b+2(c+d)/4a+2(b+c) \tag{3}$$

Two computation examples of G_I will be presented for clarification. Consider an explosive mixture of two pure explosives, Cyclotol−77/23 (RDX/TNT). The G values of RDX and TNT are 0.833 and 0.523 respectively[1]. Thus the G_I value of Cyclotol−77/23 is given by

$$G_I=0.77\times0.833+0.23\times0.523=0.761 \tag{4}$$

Consider an explosive mixture which contains one or more pure explosives and one or more inert materials, e.g., EDC−11 (HMX/RDX/TNT/Wax /Trylene−64/4/30/1/1). The G values of pure explosives, HMX, RDX and TNT are 0.833, 0.833 and 0.523 respectively[1]. We can expect that there are small contributions to the G_I value from inert materials and the contributions can be ignored in the computation of G_I for an explosive mixture. Thus the G_I value of EDC−11 is given by

$$G_I=0.64\times0.833+0.04\times0.833+0.30\times0.523+0 \\ =0.723 \tag{5}$$

3. RESULTS AND DISCUSSION

Table 1 lists the experimental values of detonation velocity and detonation pressure of 46 explosive mixtures taken from the recent reference books[2),4),8)], together with the calculated values from G_I and G_{II} values by Equations (1) and (2) and by BKW. The calculated values by BKW are taken from Reference 2. The formulations and chemical elemental compositions of these explosive mixtures can be seen in the original references[2),4),8)]. In addition to mixtures of CHNO type, Table 1 also includes explosive mixtures containing F, Cl and P (not to be confused with the P in Equation (2)). These explosive mixtures cover a broad range of explosive types and are considered to be representative of CHNO explosive mixtures. The G values of pure CHNO explosives are taken from Reference 1. Equation (3) is not applicable to NM/TNM−1/0.50 in which $d>2a+b/2$, but we arbitrarily take the G_{II} value of this explosive mixture as 1.000.

The equations generated by a linear least−squares fit of the detonation velocity data in Table 1 are given by Equations (6)−(8), respectively.

G_I scheme,

$$D_{exp}=0.897D_{cal}+0.866 \\ (n=73, r=0.976, MD=\pm1.32\%) \tag{6}$$

G_{II} scheme,

$$D_{exp}=0.835D_{cal}+1.325 \\ (n=73, r=0.858, MD=\pm2.97\%) \tag{7}$$

BKW,

$$D_{exp}=1.017D_{cal}-0.228 \\ (n=33, r=0.992, MD=\pm1.27\%) \tag{8}$$

where n is the number of data points used, r is the correlation coefficient, and MD is the average percent deviation between the calculated and experimental values. A relatively good correlation between the calculated and experimental values of detonation velocity is observed for the G_I scheme. The correlation obtained for the G_{II} scheme (Equation (7)) appears poorer than for the G_I scheme. However the result obtained from BKW (Equation (8)) is similar to that of the G_I scheme.

It can also be seen that the data points which deviated by $>\pm5\%$ are Comp A−3 and NM−TNM mixtures for the G_I scheme. Why then is Comp A−3 (RDX/Wax−91/9) with greater deviation? We find no satisfactory explanations on this problem. Reference 4 gives an experimental detonation velocity−initial density equation ($D(\rho_o)$) for RDX as follows,

$$D=3.47\rho_o+2.56 \tag{9}$$

Reference 8 gives a similar equation. The calculated D values by Equation (9) at $\rho_o=1.61$ and 1.64g/cm³ are 8.15 and 8.25km/s respectively, which are smaller

Table1 Calculated and Experimental Detonation properties for CHNO Explosive Mixtures

Explosive	G_I	G_{II}	ρ_0 (g/cc)	experimental			calculated					
				D	P		D(km/s)			P(GPa)		
				(km/s)	(GPa)	Ref.	from G_I	from G_{II}	BKW	from G_I	from G_{II}	BKW
Comp A-3	0.758	0.683	1.61	8.27		a	7.858	7.556				
			1.64	8.47		a	7.959	7.656				
Comp B	0.721	0.695	1.56	7.48		a	7.546	7.445				
			1.61	7.67		a	7.713	7.611				
			1.72	7.92		a	8.081	7.976				
Comp B-A	0.713	0.695	1.700	7.915		b	7.982	7.910				
			1.715	7.911		b	8.032	7.959				
			1.717		29.5	a				28.1	27.6	
			1.72	7.99		a	8.049	7.976				
Comp B-3	0.709	0.693	1.62	7.70		a	7.70	7.571				
			1.715		28.7	a				27.9	27.4	
			1.72	7.89		a	8.033	7.969				
Comp B-64/36	0.721	0.708	1.713	8.018	29.22	b	8.058	8.006	8.084	28.2	27.8	28.4
			1.713	8.03	29.4	c	8.058	8.006	8.084	28.2	27.8	28.4
Comp C-3	0.740	0.708	1.60	7.63		a	7.754	7.629				
Comp C-4	0.758	0.699	1.59	8.04		a	7.791	7.447				
			1.601	8.19		a	7.828	7.484				
			1.66	8.37		a	8.028	7.680				
Cyclotol-60/40	0.709	0.678	1.72	7.90		a	8.033	7.908				
Cyclotol-75/25	0.756	0.746	1.74	8.20		a	8.290	8.250				
			1.76	8.30		a	8.357	8.317				
Cyclotol-77/23	0.761	0.752	1.743	8.252	31.25	b	8.319	8.284	8.311	30.4	30.1	30.5
			1.743	8.250	31.3	c	8.319	8.284	8.311	30.4	30.1	30.5
			1.752		31.6	a				30.7	30.4	
EDC-11	0.723	0.707	1.782	8.213	31.5	c	8.297	8.228	8.384	30.6	30.1	31.5
EDC-24	0.791	0.742	1.776	8.713	34.2	c	8.555	8.354	8.636	32.5	31.0	33.4
HMX/Exon[d,e]	0.754	0.787	1.833	8.665	34.3	c	8.595	8.733	8.625	33.4	34.5	34.0
LX-04[d]	0.708	0.738	1.86	8.46		a	8.496	8.621				
			1.865	8.53		c	8.512	8.638	8.698			
			1.865		35.0	a				33.0	34.0	34.8
			1.87	8.54		a	8.529	8.655				
LX-07[d]	0.750	0.731	1.87	8.64		c	8.700	8.624	8.805			
LX-09[d]	0.805	0.808	1.838	8.84		c	8.825	8.837	8.823			
LX-09-0[d]	0.804	0.808	1.837		37.7	a				35.2	35.4	
LX-09-1[d]	0.805	0.808	1.84	8.81		a	8.821	8.844				
LX-10[d]	0.791	0.799	1.86	8.82		c	8.841	8.875	8.89			
			1.86		37.5	a				35.7	35.9	36.4
LX-10-1[d]	0.787	0.799	1.87	8.85		a	8.859	8.909				
LX-11[d]	0.666	0.706	1.87	8.32		a	8.354	8.520				
LX-14	0.796	0.785	1.81	8.76		c	8.692	8.641	8.749			
			1.833		37.0	a				34.8	34.7	
LX-14-0	0.796	0.785	1.835	8.83		a	8.777	8.791				
LX-15[d]	0.499	0.460	1.584	6.84		a	6.761	6.601				
LX-17-0[d]	0.463	0.605	1.900		30.0	a				26.0	30.6	
			1.908	7.63		a	7.622	8.221				
NM/TB-85.5/14.5[f]	0.641	0.581	1.088	5.840	10.0	c	5.696	5.491	5.945	10.4	9.8	10.6

(Table1 Continued)

Explosive	G_I	G_{II}	ρ_o (g/cc)	experimental			calculated					
				D	P		D(km/s)			P(GPa)		
				(km/s)	(GPa)	Ref.	from G_I	from G_{II}	BKW	from G_I	from G_{II}	BKW
NM/TNM−1/0.071[g]	0.682	0.833	1.197	6.570	13.8	c	6.195	6.726	6.798	13.2	15.4	15.3
NM/TNM−1/0.25[g]	0.581	1.000	1.31	6.88	15.6	c	6.217	7.722	7.094	14.2	21.6	18.1
NM/TNM−1/0.50[g]	0.522	1.000	1.397	6.780	16.8	c	6.262	8.037	6.908	15.1	24.5	17.9
Octol−76.3/23.7	0.760	0.749	1.809	8.452	33.8	b	8.540	8.494	8.555	32.7	32.3	33.3
			1.809	8.476	34.3	c	8.540	8.494	8.555	32.7	32.3	33.3
Octol−75/25	0.756	0.746	1.81	8.48		a	8.526	8.485				
PBX−9007[d]	0.750	0.676	1.60		26.5	a				25.3	23.5	
			1.64	8.09		a	7.929	7.636				
PBX−9010[d]	0.750	0.636	1.78	8.37		a	8.401	7.935				
			1.781	8.363	31.9	c	8.406	7.938	8.371	31.4	27.8	27.9
			1.783		32.8	a				31.5	27.9	
PBX−9011	0.750	0.732	1.767	8.5	29.8	b	8.358	8.284	8.496	30.9	30.3	31.9
			1.767		32.4	a				30.9	30.3	31.9
			1.77	8.50		a	8.368	8.294				
			1.777	8.50		b	8.392	8.318				
PBX−9205	0.766	0.707	1.67	8.17		a	8.094	7.858				
PBX−9404[d]	0.802	0.816	0.969	5.905	9.2	c	5.837	5.549	5.976	9.8	9.9	9.9
			1.84	8.80	37.5	a	8.819	8.877		35.3	35.8	
			1.844	8.802	36.8	b	8.832	8.892	8.879	35.4	35.9	36.3
			1.844	8.80	36.5	c	8.832	8.892	8.879	35.4	35.9	36.3
			1.846	8.781		b	8.840	8.900				
PBX−9407[d]	0.783	0.801	1.60	7.91	28.7	a	7.922	7.933		26.2	26.7	
			1.61	7.91		c	7.956	8.027	7.886			
PBX−9408[d]	0.790	0.810	1.842	8.787		c	8.776	8.859	8.865			
PBX−9501	0.800	0.801	1.834	8.792		b	8.790	8.794				
			1.84	8.83		b	8.810	8.814				
			1.841	8.826		c	8.814	8.818	8.886			
PBX−9502[d]	0.475	0.611	1.894	7.589		b	7.629	8.201	7.707			
			1.894	7.71		c	7.629	8.201	7.707			
			1.90	7.71		a	7.647	8.221				
PBX−9503[d]	0.525	0.639	1.90	7.72		a	7.857	8.338				
Pentolite−50/50	0.625	0.684	1.65	7.465		a	7.466	7.701	7.740			
			1.68	7.52		a	7.564	7.800				
			1.70	7.53		a	7.629	7.866				
RDX/Exon[d,e]	0.751	0.780	1.786	8.404	32.0	c	8.425	8.543	8.403	31.6	32.5	31.7
TATB/HMX/KelF[d,e]	0.60	0.681	1.898	8.167		c	8.167	8.508	8.553			
X0204[d]	0.691	0.759	1.909	8.44		c	8.588	8.873	8.791			
X0219[d]	0.450	0.596	1.914	7.63		c	7.587	8.202	7.638			

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than the experimental values of Comp A−3 at corresponding densities and are very close to the calculated values (8.15 and 8.26km/s) from Equation (1). If the experimental D values of Comp A−3 were true, it

would be an interesting fact for explosive engineers.

Considering the lower accuracy in experimental measurement of detonation pressure (P), the agreements between the calculated and experimental values of P in Table 1 are very good for the G_I scheme (Equation (10)) and BKW (Equation (12)). The result obtained from the G_{II} scheme (Equation (11)) is poorer than that from the G_I scheme and BKW.

G_I scheme,

$$P_{exp}=1.042P_{cal}+0.04 \quad (n=32, r=0.993, MD=\pm 4.77\%) \tag{10}$$

G_{II} scheme,

$$P_{exp}=1.115P_{cal}-2.54 \quad (n=32, r=0.955, MD=\pm 6.91\%) \tag{11}$$

BKW,

$$P_{exp}=1.074P_{cal}-1.90 \quad (n=22, r=0.991, MD=\pm 4.10\%) \tag{12}$$

It is also seen that the calculated values of P from the G_I scheme are lower than the experimental values in most cases.

At this stage, we can see that the G_I scheme compares favorably to the G_{II} scheme and BKW which depends upon the particular equations of state and requires the sophisticated computer program for estimating D and P values of CHNO explosive mixtures. The real advantage of the G_I scheme lies in its simplicity and its reasonable accuracy.

A possible reason for greater deviations of NM−TNM mixtures is that the computation of G_I or G_{II} assumes no interactions or complete interactions between the detonation products of the two explosive compounds. From the results in Table 1, it seems that there are some interactions in detonation products of NM−TNM mixtures. The discussion on this detonation chemistry problem is beyond the scope of this paper.

4. CONCLUSION

The empirical method recently reported in Reference 1 for estimating D and P values of pure CHNO explosives is extended to CHNO explosive mixtures and other type explosive mixtures. Two computation schemes are derived for the parameter G: adding their corresponding weighted G values of pure constituents (G_I) and deriving from the hypothetical chemical composition of the explosive mixture (G_{II}). The calculated D and P values from the G_I scheme, G_{II} scheme and BKW are extensively compared to the experimental values. It is shown that the G_I scheme is able to estimate simply and accurately the D and P values of explosive mixtures. The success of this empirical method encourages us to work on estimating other detonation performances of explosives. We shall report on additional work in this area in due course.

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CHNO系混合爆薬の爆速および爆圧の推算

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著者らはすでに，ＣＨＮＯ系化合爆薬の爆速（D）と爆圧（P）を推定する経験的な方法を提案したが，今回はＣＨＮＯ系混合爆薬についてその応用を試みた。Gパラメーターは各成分の加重平均値（G_I）と混合爆薬を単一化合物と仮定した計算値（G_{II}）とを用い，それぞれのＤとＰの計算を行い，ＢＫＷ値あるいは実験値との比較を行った。その結果，G_Iを用いた場合は，G_{II}の場合よりも広い範囲の爆薬類について正確（D値のバラツキは±1.32%以内，Ｐ値のバラツキは±4.77%以内）であり，しかも簡単に求めることができた。

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