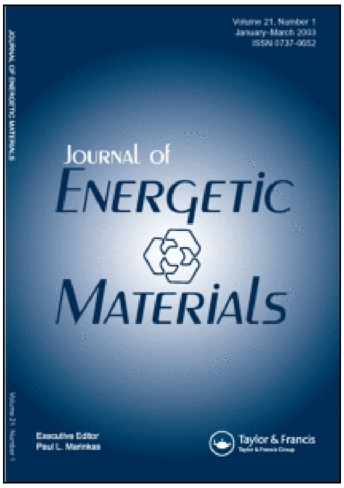

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A Simple Method For Calculating Detonation Parameters of Explosives

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Detonation velocity of explosives including single compounds and mixtures may be calculated by means of a simple empirical equation $D = aQ^{1/2} + bw\rho_0$, $a = 67.6$, $b = 243.2$; adiabat exponent by a equation $\Gamma = r + \Gamma_0(1 - e^{-0.546\rho_0})$. Thus, the detonation pressure can be estimated from the theoretical equation $P = \rho_0 D^2/(1 + \Gamma)$. Q is the heat of detonation, w is the potential energy. Γ is the adiabat exponent, and ρ_0 is the initial density. The agreements between the calculated results and the experimental data are reasonably satisfactory.

INTRODUCTION

Detonation parameters of explosives are required in engineering applications.

The most widely used equation of state is the semiempirical BKW EOS calibrated by Mader.[1] With it and its FORTRAN BKW code, the detonation properties of hundreds of explosives have been calculated.[1] Recently, the author proposed a new equation of state called VLW EOS for detonation products based on the virial theory and the thermodynamic functions whih is of higher accuracy.[2,3] By using VLW EOS and its FORTRAN VLW code, the detonation properties of explosives composed of CHNO, CNO, HNO, NO, HN, CHNOF, and CHNF have been calculated. And good agreements between the calculated results and the experimental data were

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obtained.[3] But these calculations are rather complex, and a simple but high accuracy way is proposed for engineering applications in this paper.

FORMULAE

1. Detonation velocity

The detonation velocity can be calculated by an empirical equation

$$D = aQ^{1/2} + bw\rho \qquad (1\text{-}1)$$

where D is the detonation velocity(m/sec); ρ, the initial density (g/cc); Q, the heat of detonation(cal/g); w, the potential energy; the constants a = 67.6, b = 243.2.

From Eq.(1-1), we can see that the detonation velocity D depends on two parties, one is the heat energy $aQ^{1/2}$, the other is the potential energy $bw\rho$.

When $\rho \to 0$, and let r = 1.244, then

$$D \to 67.6Q^{1/2} \approx 64.6(2(r^2 - 1)Q)^{1/2} \text{ (m/sec)}$$
$$\approx (2(r^2 - 1)Q)^{1/2} \text{ (cal/g)}$$

In this case, Eq.(1-1) is in agreement with that of the detonation velocity of idea gases in theory.

The heat of detonation Q can be obtained from

$$Q = -(\Sigma N_i \Delta H_i - \Delta H_f)/M$$

where H_i is the heat of formation of species i; H_f, the heat of formation of explosives; N_i, the molar species i; M, the formula weight of explosive.

Table 1. The heat of formation of species

N2	H2O	CO2	CO	CH4	O2	H2	C(s)
0	-57.8	-94.05	-26.4	-17.8	0	0	10

The potential energy w can be obtained from

$$w = \Sigma N_i K_i / M$$

where K_i is the covolume of species i; N_i, the number of moles of species i.

Table 2. The covolume of species

H20	CO2	CO	N2	H2	O2	CH4	C(s)
250	600	390	380	214	350	528	(46)

2. Adiabat exponent

In 1961, Apin assumed that the adiabat exponent only depends on the species of detonation products. He proposed[6]

$$1/\Gamma = \Sigma(X_i/\Gamma_i) \qquad (1\text{-}2)$$

where X_i is the molal fraction of species i; Γ_i is the adiabat exponent of species i.

On the other hand, in 1973, Defourneaux assumed that the adiabat exponent Γ only depends on the initial density. So he proposed[8]

$$\Gamma = 1.9 + 0.6\rho_0 \qquad (1\text{-}3)$$

It is evident that Eq.(1-2) and Eq.(1-3) are in contradiction with each other.

In this paper, we propose that the adiabat exponent should be considered as both the species of detonation products and the initial density.

$$\Gamma = r + \Gamma_0(1 - e^{-0.546\rho_0}) \qquad (1\text{-}4)$$

$$\Gamma_0 = \Sigma N_i / \Sigma(N_i/\Gamma_{0i})$$

where $r = C_p/C_v$, C_p is the specific heat at constant pressure; C_v, the specific heat at constant volume. And let r = 1.25.

The values of Γ_i have been fitted from the experimental results avaiable by P vs ρ_0, and listed in table 3.

From Eq.(1-4), when $\rho_0 \rightarrow 0$, $\Gamma \rightarrow r = 1.25$;

$\rho_0 \rightarrow \infty$, $\Gamma \rightarrow r + \Gamma_0$

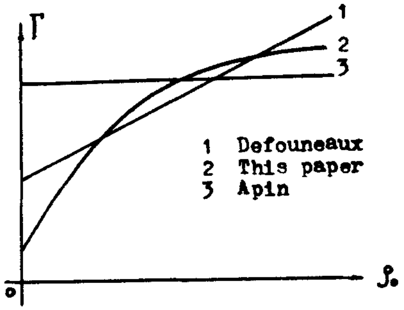

Table 3. The values of Γ_i of detonation products

N2	H20	CO2	CO	CH4	O2	H2	C(s)
3.8	1.68	3.1	2.67	2.93	3.35	3.4	3.5

3. Detonation pressure

According to the detonation theory, we have

$$P = \frac{\rho_0 D^2 . 10^{-5}}{\Gamma + 1} \qquad (1-5)$$

where P is the C-J pressure (Kbar); D and Γ are estimated from Eq.(1-1) and Eq.(1-4)

4. Detonation products

It is vitally important to determine the detonation compositions when the detonation parameters are going to be calculated.

As far as we know, in BKW EOS and VLW EOS, the calculations of equilibrium composition are used to adopt the way of modified minimization of free energy technique. However, they are only to be carried out by sophisticated multiiterative processes involving several subroutines of the total system. This is inconvenient for engineering calculations. So we prefer to use a simple empirical method. After we having analysed the results from both the experiments and theoretical calculations, CHNO explosives and plastic material may be decomposed under detonation as described in table 4.

Table 4. Detonation equations of CHNO explosives and plastic material under detonation

Oxygen Balance	Type	Decomposing Equations
1. Rich or zero	$d-\frac{b}{2}-2a\geq 0$	$C_aH_bN_cO_d=\frac{c}{2}N_2+\frac{b}{2}H_2O+aCO_2+\frac{1}{2}(d-\frac{b}{2}-2a)O_2$
2. Slightly deficient	$d-\frac{b}{2}-2a<0$	$C_aH_bN_cO_d=\frac{c}{2}N_2+0.43bH_2O+(\frac{d}{2}-\frac{b}{4})CO_2+0.07bCO$ $+0.035bCH_4+(a-\frac{d}{2}+0.145b)C$
3. Deficient	$d-\frac{b}{2}-a\leq 0$	$C_aH_bN_cO_d=\frac{c}{2}N_2+0.35bH_2O+(\frac{d}{2}-\frac{b}{4})CO_2+0.15bCO$ $+0.075bCH_4+(a-\frac{d}{2}+b/40)C$
4. Seriously deficient	$d-\frac{b}{2}\leq 0, a>d$	$C_aH_bN_cO_d=\frac{c}{2}N_2+0.54dH_2O+0.46dCO+0.23dCH_4$ $+(a-0.69d)C+(\frac{b}{2}-d)H_2$
5. Seriously deficient	$d-\frac{b}{2}\leq 0, a<d$	$C_aH_bN_cO_d=\frac{c}{2}N_2+aCO+(d-a)H_2O+(\frac{b}{2}-d+a)H_2$

After substituting the heat of formation of table 1, whose signs should be changed, the covolume of table 2, and the adiabat exponent of table 3 into table 4 respectively, this lead us to obtain as follows in table 5.

Table 5. The formulae of Q, w, and Γ_0 of explosive compounds and components of explosive mixtures

Oxygen Balance	Type	w.M	Q.M/1000	Γ_0
1. Rich or zero	$d-\frac{b}{2}-2a \geq 0$	$250a+37.5b+190c+175d$	$28.9b+94a+\Delta H_f$	$\frac{0.25b+0.5c+0.5d}{0.0241a+0.223b+0.1316c+0.149d}$
2. Slightly deficient	$d-\frac{b}{2}-2a < 0$	$46a+9.95b+190c+277d$	$2.365b+52d-10a+\Delta H_f$	$\frac{a+0.43b+0.5c}{0.2857a+0.2549b+0.1316c+0.018d}$
3. Deficient	$d-\frac{b}{2}-a \leq 0$	$46a+36.75b+190c+277d$	$1.772b+52d-10a+\Delta H_f$	$\frac{a+0.35b+0.5c}{0.2857a+0.2166b+0.1316c+0.018d}$
4. Seriously deficient	$d-\frac{b}{2} \leq 0$, $a \geq d$	$46a+107b+190(c+d)$	$54.37d-10a+\Delta H_f$	$\frac{a+0.5b+0.5c-0.46d}{0.2857a+0.147b+0.1316c+0.081d}$
5. Seriously deficient	$d-\frac{b}{2} \leq 0$, $a < d$	$354a+107b+190c+36d$	$57.8d-31.4a+\Delta H_f$	$\frac{a+0.5b+0.5c}{0.0734a+0.147b+0.1316c+0.3d}$

Generally speaking, table 5 is valid for $C_aH_bN_cO_d$ whose $a \neq 0$, $b \neq 0$, $c \neq 0$, and $d \neq 0$. If any of them equals zero, it should be modified as follows:

1. when $a = 0$, $w' = 1.25w$, and $\Gamma_0' = 1.25\,\Gamma_0$
2. when $b = 0$, $w' = 1.06w$, and $\Gamma_0' = 0.7\Gamma_0$ (except Type 1)
3. when $c = 0$, and $d = 0$, $w' = 1.06w$, if it belongs to Type4.
4. when $c = 0$, and $d = 0$, $w' = 1.04w$, if it belongs to Type 5.

CALCULATION

1. Explosive compounds

In order to calculate the detonation velocity, detonation pressure and adiabat exponent conveniently, we list the values of Q, w and Γ_∞ of both the commonly used explosives and components of explosive mixtures in table 6. Here we take RDX(ρ_0 = 1.8g/cc) for example.

First of all, find the values Q = 1384, w = 14.23 and Γ_∞ = 2.65 from table 6., and then substitute them in Eq.(1-1), Eq.(1-4) and Eq.(1-5) i.e.

$$D = 67.6*(1384)^{1/2} + 243.2*14.23*1.80$$

$$= 8744 (m/sec) \quad (D^{exp} = 8754)$$

$$\Gamma = 1.25 + 2.65*(1 - e^{-0.546*1.80})$$

$$= 2.91 \quad (\Gamma^{exp} = 2.98)$$

$$P = \frac{1.8*(8744)^2*10^{-5}}{1 + 2.91}$$

$$= 352.1 \text{ (Kbar)} \quad (P^{exp} = 347)$$

For some compounds or components or new material whose Q, w, and have not been listed yet in table 6, in this case, they have to be calculated with table 5. We take HNB (ρ_0= 1.973 g/cc, ΔH_f = 35 cal/mole) for example

$$Q = (94*6 + 35)*1000/348 = 1722 \text{ (cal/g)}$$

$$w = (250*6 + 190*6 + 175*12)/348 = 13.62$$

$$\Gamma = (0.5*6 + 0.5*12)/(0.024*6 + 0.1316*6 + 0.149*12)$$

$$= 3.3$$

Substitute them in Eq.(1-1), Eq.(1-4), Eq.(1-5), we obtain

$$D = 9340 \text{ (m/sec)} \quad (D^{exp} = 9300)$$

$$= 3.43$$

$$P = 389 \text{ (Kbar)} \quad (P^{exp} = 420)$$

2. Explosive mixtures

Suppose that Q, w, and Γ satisfy following combined rules

$$Q = \sum X_i Q_i \tag{2-1}$$

$$w = \sum X_i w_i \tag{2-2}$$

$$\Gamma = \frac{\sum N_i}{\sum N_i/\Gamma_i} = \frac{\sum X_i/M_i}{\sum X_i/\Gamma_i M_i} \tag{2-3}$$

where w is the total potential energy; Γ, the total adiabat exponent; X_i, the weight per cent of component i. And Q is the total heat of detonation. If any component in mixture is of rich oxygen balance, its Q, in consideration of chemical reaction to be occured, should be modified as follows

$$Q' = Q + 35{,}000n/M \ (\text{cal/g})$$

here n is the number of oxygen atom, except those of which have been formed to water or oxides.

Thus, Eq.(1-1), Eq.(1-4), and Eq.(1-5) can be used for calculations of explosive mixtures.

Table 7. Comparison the calculations by Eq.(1-1), Eq.(1-4) and Eq.(1-5) to the experimental data

	Explosive	C–J Param	Expt'l	Ref.	This paper
	RDX	D	8754	1	8744
	$\rho_0 = 1.8$	P	347		352
		Γ	2.98		2.91
	TNT	D	6950	1	6972
CHNO	$\rho_0 = 1.64$	P	190		202
		Γ	3.16		2.94
	HMX	D	9100	1	9086
	$\rho_0 = 1.90$	P	393		394
		Γ	3.0		2.96

(continued)

	Explosive	C-J Param	Expt'l	Ref.	This paper
	PETN	D	8300	1	8541
	$\rho_0 = 1.77$	P	335		340
		Γ	2.64		2.79
	DATB	D	7500	1	7684
	$\rho_0 = 1.788$	P	259		261
		Γ	2.9		3.04
	TATB	D	7860	1	7889
	$\rho_0 = 1.895$	P	315		290
		Γ	2.72		3.07
	Expl. D	D	6850	1	6904
	$\rho_0 = 1.55$	P			197
		Γ			2.75
CHNO	EDNA	D	8235	5	8179
	$\rho_0 = 1.663$	P			299
		Γ			2.72
	TNB	D	7200	5	7307
	$\rho_0 = 1.64$	P			218
		Γ			3.01
	TNA	D	7300	5	7373
	$\rho_0 = 1.72$	P			232
		Γ			3.03
	R-salf	D	7800	5	7777
	$\rho_0 = 1.57$	P			248
		Γ			2.83
	NM	D	6320	4	6412
	$\rho_0 = 1.135$	P	144		141
		Γ			2.32

(continued)

	Explosive	C-J Param	Expt'l	Ref.	This paper
CHNO	RDX 78	D	8306	5	8348
	TNT 22	P	317		312
	ρ= 1.755	Γ			2.915
	COMP B	D(ρ= 1.720)	7920	4	8079
	RDX 63	P(ρ= 1.717)	295		282
	TNT 36	Γ(ρ= 1.717)			2.96
	PBX 9011	D(ρ= 1.770)	8500	4	8527
	HMX 90	P(ρ= 1.767)	324		325
	Estane 10	Γ(ρ= 1.767)			2.94
	PBX 9407	D	7910	4	7915
	RDX 94	P	287		265
	EXON 6	Γ			2.78
	ρ= 1.6				
	PBXN 3	D	8195	*	8165
	HMX 86	P			287
	Nylon 14	Γ			2.87
	ρ= 1.667				
	HMX 90.54	D	8665	1	8616
	EXON 9.46	P	343		349
	ρ= 1.833	Γ	3.01		2.92
	PBX 9205	D	8170	4	8248
	RDX 92	P			292
	PST 6	Γ			2.89
	DOP 2				
	ρ= 1.67				
	BTNEN 56	D	8701	*	8765
	RDX 44	P			410
	ρ= 1.845	Γ			2.94
	BTNEN 32	D	8884	*	8946
	HMX 68	P			425
	ρ= 1.882	Γ			2.96
	HMX 78.72	D	8771	*	8764
	AN 21.28	P			372
	ρ= 1.825	Γ			2.77

(continued)

	Explosive	C-J Param	Expt'l	Ref.	This paper
CHNO	BTNEN	D(ρ= 1.925)	8657	*	8609
		P(ρ= 1.927)	357.6		345
		Γ(ρ= 1.927)	2.99		3.14
	ANFO	D	4900	7	4738
	AN 94	P	60		55
	Oil 6	Γ			2.27
	ρ_0 = 0.8				
	NM 1mole	D	6570	1	6571
	TNM 0.071mole	P	138		153
	ρ_0 = 1.197	Γ	2.74		2.38
	NM 1mole	D	6880	1	6855
	TNM 0.25mole	P	156		175
	ρ_0 = 1.309	Γ	2.89		2.52
CNO	HNB	D	9300	1	9340
	ρ_0 = 1.973	P	420	9	389
		Γ			3.3
	BTF	D	8485	1	8531
	ρ_0 = 1.859	P	360	4	358
		Γ			2.78
	TNM	D	6360	1	6446
	ρ_0 = 1.64	P	159		159
		Γ	3.17		3.28
HNO	NH_4NO_3	D	4500	1	4639
	ρ_0 = 1.05	P			65.8
		Γ			2.43
	HN	D	8691	1	8685
	ρ_0 = 1.626	P			319
		Γ			2.84
	HN 30	D	8025	1	8006
	HY 70	P			185
	ρ_0 = 1.14	Γ			2.94
	HN 79	D	8600	1	8612
	HY 21	P			261
	ρ_0 = 1.4418	Γ			3.1

(continued)

	Explosive	C-J Param	Expt'l	Ref.	This paper
	FEFO	D(ρ_0 = 1.607)	7500	4	7498
		P(ρ_0 = 1.59)	250		246
		Γ(ρ_0 = 1.59)			2.58
	LX 04	D(ρ_0 = 1.86)	8500	4	8512
	HMX 85	P(ρ_0 = 1.865)	350		345
	Viton A 15	Γ(ρ_0 = 1.865)			2.93
CHNOF	LX 17	D	7630	4	7731
	TATB 92.5	P			280
	Kel-F 7.5	Γ			3.07
	ρ_0 = 1.908				
	PBX 9010	D	8363	1	8327
	RDX 90	P	319		317
	Kel-F 10	Γ	2.91		2.89
	ρ_0 = 1.781				
	RDX 37.4	D	7300	1	7124
	TNT 27.8	P	215		208
	Al 30.8	Γ	3.64		3.59
	Wax 4.0				
	ρ_0 = 1.88				
CHNOAl	TNT 74.766	D	6665	7	6661
	Al 18.691	P	175		168
	Wax 4.672	Γ	3.24		3.4
	G 1.869				
	ρ_0 = 1.68				
	BTNEN 88	D	8441	•	8404
	Al 12	P			304
	ρ_0 = 1.957	Γ			3.54
	NH_4NO_3 90	D	5600	1	5602
HNOAl	Al 10	P			98.4
	ρ_0 = 1.05	Γ			2.35
	PBX 9404	D	8800	1	8816
	HMX 94	P	365		365
	NC 3	Γ	2.91		2.92
	CEF 3				
	ρ_0 = 1.844				

• This work

Table 6. The values of Q, w, and Γ_0 of explosive compounds and components of mixtures

Material	M.W.	Q(Cal/g)	w	Γ_0	C	H	N	O	
TNT, Trinitrotoluene	227.1	1027	12.05	2.856	7	5	3	6	
RDX, Cyclotrimethylene trinitramine	222.1	1384	14.23	2.65	3	6	6	6	
HMX, Cyclotetramethylene-tetranitramine	296.2	1379	14.23	2.65	4	8	8	8	
EDNA, Ethylene dinitramine	150.1	1160	14.53	2.469	2	6	4	4	
PA, Picric acid	229.1	1100	12.63	2.961	6	3	3	7	
DATB, 1,3-Diamino-2,4,6-trinitrobenzene	243.1	1048	12.636	2.875	6	5	5	6	
TATB, 1,3,5-Triamino-2,4,6-trinitrobenzene	258.2	874.5	12.78	2.836	6	6	6	6	
Tetryl, N-Methyl-N,2,4,6-tetranitroaniline	278.0	1253	12.78	2.89	7	5	5	8	
PETN, Pentaerythritol Tetranitrate	316.1	1480	13.80	2.48	5	8	4	12	
Expl. D, Ammonium picrate	246.0	884.3	13.0	2.75	6	6	4	7	
DINA, Di(2-nitroxyethyl)-nitramine	240.1	1300	14.3	2.48	4	8	4	8	
TNB, 1,3,5-Trinitrobenzene	213.1	1266	12.29	2.98	6	3	3	6	
R-salt, Cyclotrimethylene trinitrosamine	174.1	1148	14.37	2.748	3	6	6	3	
TNA, 2,4,6-Trinitroaniline	228.1	1018	12.47	2.92	6	4	4	6	
DNPN, Bis(2,2-dinitropropyl) nitramine	326.2	1265	13.9	2.75	6	10	6	10	
NG, Nitroglycerine	227.1	1488	13.57	2.48	3	5	3	9	
NQ, Nitroguanidine	104.1	636.1	15.42	2.80	1	4	4	2	
NM, Nitromethane	61.0	1208	14.72	2.31	1	3	1	2	
TNTAB, 1,3,5-Triazido-2,4,6-trinitrobenzene	336.1	1554	13.3	3.02	6	0	12	6	
BTF, Benzotris(1,2,5-oxadiazole-1-oxide)	252.1	1573	12.94	2.41	6	0	6	6	
HY, Hydrazine	32.0	710	24.0	3.8	0	4	2	0	
Al, Aluminium	26.98	3710	-1.0	4.0	0	0	0	0	Al
G, Graphyte	12.0	0	3.83	4.0	1	0	0	0	
FEFO, Bis(2-fluoro-2,2-dinitroethyl) formal	320.1	1450	12.6	2.3	5	6	4	10	F2

(continued)

Material	M.W.	Q(Cal/g)	w	Γ_o	C	H	N	O		
TNM, Tetranitromethane	190.1	single 522	12.29	3.43	1	0	4	8		
		mixed 1593	12.29	3.43						
AN, Ammonium Nitrate	80.0	single 355	13.18	2.75	0	4	2	3		
		mixed 793	14.8	2.75						
BTNEN, Bis(2,2,2-trinitro-ethyl)nitramine	388.1	single 1297	13.19	2.9	4	4	8	14		
		mixed 1640	13.19	2.7						
HN, Hydrazine Nitrate	95.0	single 891	16.87	2.71	0	5	3	3		
		mixed 1075	17.0	2.71						
DOP, Di-2-ethylexyl phthate	390.6	-57	15.2	3.22	24	38	0	4		
SA, Stearic acid	248.5	-602	17.79	3.3	18	36	0	2		
NC, Nitrocellulose	(262.6)n	975	13.4	2.52	(6	7	2.25	9.5)n		
PVAC, Polyvinyl acetate	(86.1)n	-363	14.0	2.78	(4	6	0	2)n		
Nylon, 6/66	(339.4)n	-315	16.2	3.26	(18	33	3	3)n		
Wax	(14.0)n	-713	18.6	3.45	(1	2	0	0)n		
PMMA, Polymethy mathacrytale	(100.0)n	-412	14.64	2.92	(5	8	0	2)n		
Oil	(14.0)n	-400	18.5	3.45	(1	2	0	0)n		
PIB, Polyisobutylene	(56.1)n	-713	18.5	3.45	(4	8	0	0)n		
PST, Polystyrene	(104.1)n	-276	16.93	3.45	(8	8	0	0)n		
Viton A, Vinylidine fluoride	(187.1)n	800	9.0	2.6	(5	3.5	0	0	F6.5)n	
Kel-F,	(413.5)n	500	8.0	2.5	(8	2	0	0	F11	Cl3)n
CEF, Tris- -chloroethyl-phosphate	(285.5)n	-450	14.0	2.8	(6	12	0	4	P1	Cl3)n
EXON, Vinichloride/Tri-fluorochloroethylene Copolymer 1.5:1	(179.1)n	700	10.0	2.4	(4	3	0	0	F3	Cl2)n
PVN, Polyvinyl Nitrate	(89.0)n	1250	13.72	2.52	(2	3	1	3)n		
Estane	(100.0)n	367	13.9	2.99	(5.14	7.5	0.19	1.76)n		
PVB, Polyvinyl Butyral	(159.2)n	-166	15.53		(9	19	0	2)n		

CONCLUSION

1. Formulae

$$D = 67.6\, Q^{1/2} + 243.2\, w$$

$$\Gamma = 1.25 + \Gamma_0 (1 - e^{-0.546\rho})$$

$$P = \rho D^2 \times 10^{-5} / (1 + \Gamma)$$

are valid for both CHNO explosive compounds and CHNO explosive mixtures, but they can be popularized for other explosives containing F, Cl, P, Al etc., if the parameters Q, w, and Γ are calibrated by a set of given D and P in advance.

2. If the Q, w, and Γ of the explosives or components of mixtures are listed in table 6, we can calculated their D, Γ and P conveniently. If not, we may calculate them by means of table 5.

3. The results calculated by this simple way are in good agreement with those of experiments. They are good enough for engineering applications.

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