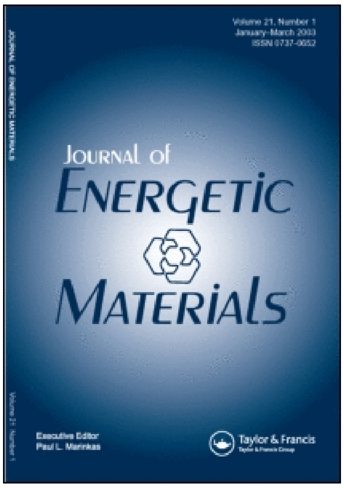

Journal of Energetic Materials
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713770432

Comments on "a simple method for calculating detonation parameters of explosives"

Hel Karel[a]
[a] Research Institute for Industrial Chemistry, Czechoslovakia

To cite this Article Karel, Hel(1992) 'Comments on "a simple method for calculating detonation parameters of explosives"', Journal of Energetic Materials, 10: 4, 287 — 298

To link to this Article: DOI: 10.1080/07370659208018927

URL: http://dx.doi.org/10.1080/07370659208018927

Comments on "A Simple Method for Calculating Detonation Parameters of Explosives"

Hel Karel

Research Institute for Industrial Chemistry,
VCHZ Synthesia, Pardubice - Semtín,
Czechoslovakia

The present contribution deals with a modified method of estimating the detonation parameters starting with a general formulation of the adiabat for explosives as expressed using the adiabatic exponent $\gamma_J = f(\rho_0)$ according to Wu Xiong[1]. The author uses also the works of Russian authors.[2,7,8]

INTRODUCTION

A great number of authors have devoted their efforts to developing simple methods of determining the detonation parameters. The present contribution starts with the results published by Wu Xiong[1] and A.L. Krivchenko.[2]

Journal of Energetic Materials Vol. 10, 287-298 (1992)
Published in 1992 by Dowden, Brodman & Devine, Inc.

THEORY

Urbanski and Galas studied the effects of inert liquids on the detonation velocity of PETN and RDX mixed with such liquids and published their results in 1939.[4] They conclude that the detonation velocity of such mixtures depends on the velocity of sound in the liquid used. They relate this assumption to the Chapman - - Jouguet condition $D = c_J + u_J$. Owing to the fact that the ZND /Zeldovich, von Neuman and Doering/ detonation model was reported after 1939, Urbanski and Galas could not give a quantitative support for the relation c_J - velocity of sound c_o in the explosive mixture.

In the hydrodynamic theory of detonation based on the polytropic equation of state, the form of which was found by means of statistical physics, there appear effects of the elastic and thermal components of pressure. The former component may be related to repulsive forces, the latter one to heat motion of molecules.[5]

In the wave - theory interpretation the detonation front propagation taking place in the nonreacted explosive is described by the condition

$$D = c_N + u_N , \qquad /1/$$

wherein the subscript N indicates that the conditions relate to the von Neuman point. The elastic forces may be represented by a material constant such as the velocity of sound c_o, and the energy release taking place in the zone of chemical reaction under the conditions of detonation is characterized by the mass velocity u_J.

In determining the von Neuman pressure spike p_N, the ZND model of detonation results in the approximative value equal to a double of pressure p_J.[6]

If we want to determine the shape of the generalized adiabat of explosive, we are to consider different conditions and adiabatic exponents in the detonation wave front and in the Chapman - Jouguet plane.

For the parameters at the detonation front and at the Chapman - Jouguet plane the following relations are valid:

$$u_N/D = 2/(\gamma_N + 1), \qquad /2/$$

$$u_J/D = 1/(\gamma_J + 1). \qquad /3/$$

From the relations /2/ and /3/ using the relation defining the adiabatic-coefficient value at the detonation front and at the Chapman - Jouguet plane

$$\gamma_N = \gamma_J \, \rho_J/\rho_N = \gamma_J - 1 \qquad /4/$$

gives a relation

$$u_N/u_J = 2(\gamma_J + 1)/\gamma_J . \qquad /5/$$

The sound velocity at the Chapman - Jouguet plane satisfies the relation

$$c_J/c_o = \rho_J/\rho_o = (\gamma_J + 1)/\gamma_J \qquad /6/$$

The $c_J \rightarrow c_N$ change corresponds to the change $\gamma_J \rightarrow \gamma_N = \gamma_J + 1$, and thus

$$c_N/c_o = (\gamma_J + 2)/(\gamma_J + 1), \qquad /7/$$

Using the condition /1/ and also the relation /5/ and /7/ gives the generalized adiabat as expressed by the bulk sound velocity c_o and by the adiabatic exponent γ_J.

$$D = (\gamma_J + 2)c_o/(\gamma_J + 1) + 2(\gamma_J + 1)u_J/\gamma_J =$$

$$= A + B\,u_J \qquad /8/$$

The mass velocity as encountered in the formula /8/ can by expressed by a well-known relation

$$u_J = \left[2(\gamma_J - 1)\,Q/(\gamma_J + 1)\right]^{1/2}, \qquad /9/$$

wherein Q is the heat of explosion.

Further steps of the procedure for determining the detonation parameters can be taken, e.g., on the basis empirical dependences of type $\gamma_J = f(\rho_o)$ and $Q = f(\alpha, \rho_o)$, wherein α is the oxygen factor of $C_aH_bN_cO_d$ - type explosive expressed as $\alpha = 2d/(4a + b)$.

According to Pepekin[7] only a proportion of the heat of explosion Q is contributory to the detonation due to the fact that not all the heat released quickly enough, the releasing factor η_r depending on the oxygen and on the initial density[2,7]

$$\eta_r = Q_\rho / Q = (\alpha + 1{,}65)\rho_o / 5{,}5 \qquad /10/$$

The detonation velocity is given as

$$D = A + B\left[2(\gamma_J - 1)\eta_r Q / (\gamma_J + 1)\right]^{1/2} \qquad /11/$$

The bulk sound velocity may be estimated from the Rao formula[9]

$$c_o = (\rho_o z_i \beta_i / M)^3, \qquad /12/$$

wherein M is the molecular weight, z_i is the number of chemical bonds and β_i are the contributions of individual bonds[8].

The velocity of sound propagating in a multicomponent explosive is given by a relation reading as

$$c_{om} = (\rho_{om} \Sigma X_i / \rho_{oi} c_{oi})^{-1}, \qquad /13/$$

wherein ρ_{om} is the density of multicomponent explosive, c_{oi} is the velocity of sound for the i-th component, and X_i is the mass fraction of the i-th component.

For the ρ_{om} there is valid

$$\rho_{om} = (\Sigma X_i / \rho_{oi})^{-1}. \qquad /14/$$

The adiabatic exponent is determined from the Wu Xiong relation[1]

$$\gamma_J = 1{,}25 + \gamma_o (1 - e^{-0{,}546\rho_o}), \qquad /15/$$

wherein

$$\rho_o = (\Sigma X_i/M_i)/(\Sigma X_i/ M_i \gamma_{oi})$$

The results of estimated for the detonation parameters are given in Table 1.

EXAMPLES OF CALCULATIONS

1. RDX $C_3H_6N_6O_6$

Data reported by Wu Xiong[1]

Heat of explosion $Q = 5792\ J.g^{-1}$

Initial density $\rho_o = 1{,}8\ g.cm^{-3}$

Adiabatic exponent $\gamma_J = 2{,}912$

Molecular weight $M = 222{,}1$

Results of calculation

a/ determining the sound velocity - eq. /12/

$$z_i\beta_i = 6\beta_{C-H} + 6\beta_{C-N} + 3\beta_{N-NO_2} =$$

$$6.95{,}2 + 6.20{,}7 + 3.330 = 1685{,}4$$

$$c_o = (1{,}8.1685{,}4/222{,}1)^3 = 2547{,}9\ m.s^{-1}$$

b/ oxygen factor and energy release factor η_r - eq. /10/

$$\alpha = 2.6/(4.3 + 6) = 0{,}6667$$

$$\eta_r = (0{,}6667 + 1{,}65)\,1{,}8/5{,}5 = 0{,}7582$$

c/ particle velocity - eq. /9/

$$u_J = [2(2{,}912 - 1)\,0{,}7582.5792.10^3/(2{,}912 + $$
$$+ 1)]^{1/2} = 2084 \ \mathrm{m.s^{-1}}$$

d/ detonation velocity - eq. /8/

$$D = (2{,}912 + 2)2547{,}9/(2{,}912 + 1) +$$
$$+ \ 2(2{,}912 + 1)\ 2084/(2{,}912) = 8797 \ \mathrm{m.s^{-1}}$$

e/ detonation pressure

$$p_J = \rho_o D^2.\ 10^{-6}/(\gamma_J + 1) = 1{,}8.8\ 797^2.10^{-6}/$$
$$/(2{,}912 + 1) = 35{,}6 \ \mathrm{GPa}$$

2. RDX/TNT 50/50 $C_{4,9775}H_{5,4705}N_{4,4818}O_{5,9549}$

Heat of explosion	$Q = 5062 \ \mathrm{J.g^{-1}}$
Initial density	$\rho_o = 1{,}67 \ \mathrm{g.cm^{-3}}$
Adiabatic exponent	$\gamma_J = 2{,}9$
Molecular weight	$M = 223{,}4$

Results of calculation

a/ mixture density - eq. /14/ and velocity of sound eq. /13/

$$\rho_{om} = (0{,}5/1{,}67 + 0{,}5/1{,}8)^{-1} = 1{,}7227 \ \mathrm{g.cm^{-3}}$$

$$c_{om} = 1{,}65.2162.1{,}8.2548/(1{,}65.2162.0{,}5 +$$
$$+ 1{,}8.2548.0{,}5)\,1{,}7227 = 2331 \ \mathrm{m.s^{-1}},$$

where $\rho_{oTNT} = 1{,}65 \ \mathrm{g.cm^{-3}}$, $\rho_{oRDX} = 1{,}8 \ \mathrm{g.cm^{-3}}$,

$X_{TNT,RDX} = 0,5.$

b/ oxygen factor and release factor - eq. /10/

$$\alpha = 2.5,9649/(4.4,9775 + 5,4705) = 0,47$$

$$\eta_r = (0,47 + 1,65)\,1,67/5,5 = 0,6433$$

c/ particle velocity - eq. /9/

$$u_J = [2(2,9 - 1)0,6433.5062.10^3/(2,9 + 1)]^{1/2} = 1782 \text{ m.s}^{-1}$$

d/ detonation velocity - eq. /8/

$$D = (2,9 + 2)2331.1,67/(2,9 + 1)1,7727 + 2(2,9 + 1)1782/2,9 = 7628 \text{ m.s}^{-1}$$

e/ detonation pressure

$$p_J = 1,67.7628^2.10^{-6}/(2,9 + 1) = 24,8 \text{ GPa}$$

CONCLUSIONS

Equation /8/ as derived in the present work can be used for determining the adiabat on the basis of three measurable quantities c_o, γ_J and Q. The generalized adiabat can be applied to predicting the detonation parameters, provided the c_o, Q, $\eta_r = f(\alpha, \rho_o)$ and γ_J values are known.

The reliability of the detonation velocity predictions depends on the correctness of the above-mentioned values serving as inputs to the calculation formula.

Table 1. Material and explosion parameters of explosives and explosive components calculated by the present procedure

Explosive	ρ_o ($g.cm^{-1}$)	c_o ($km.s^{-1}$)	γ_J	Q ($J.g^{-1}$)	D_{calc} ($km.s^{-1}$)	D_{exp}[11] ($km.s^{-1}$)	D^3 ($km.s^{-1}$)	P_{Jcalc} (GPa)	P_{Jexp}[11] (GPa)	P_J^3 (GPa)
TNT liquid	1,45	1.90	2,81	4300	6,39	6,59[10]	6,41	15,5	18,2[10]	15,9
TNT cast	1,64	2,16	2,94	4300	6,97	6,95	6,99	20,2	20,2	20,5
RDX	1,8	2,55	2,91	5970	8,8	8,75	8,79	35,6	34,3	34,2
HMX	1,9	2,70	2,96	5770	9,1	9,10	9,12	39,8	39,3	38,1
TATB	1,93	2,98	3,1	3660	8,06	7,86	7,95	30,7	31,5	29,2
HCO	1,875	2,37	2,99	6228	8,91	$8,8^+$	9,06	37,9	-	37,3
EDNA	1,663	2,66	2,72	4855	8,13	8,24	8,13	29,5	27,3	27,8
TNB	1,64	1,96	3,01	5300	7,3	7,27	7,29	21,8	21,9	22,6
NM	1,135	1,3	2,32	5060	5,6	6,29	6,39	10,6	12	13,3
NQ	1,78	3,75	2,99	2660	8,19	8,20	7,87	29,9	-	27,3
HNB	1,973	1,99	3,23	7350	9,57	9,50	9,35	42,7	42	40,7
NTO	1,93	2,99	3,18	4950	9,02	-	8,3	37,5	-	32
OCNC	2,098[13]	1,39	2,83	7515	9,01	-	9,83	44,5	-	46,7

Table 1. (continued)

PAPNBC	1,987[13]	2,836	3,03	5843	9,50	-	10,89[11]	44,52	-	55,76
AN	1,05	1,97	2,45	1486	4,97	3,95[12]	5,26	7,5	-	-
AP	1,0	1,46	2,87	1400	4,47	-	-	5.17	-	-
RDX/TNT										
50/50	1,67	2,33	2,9	5062	7,63	7,55	7,70	24,8	24	25,1
RDX/TNT/AP										
40/40/20	1.764	2,41	2,94	4035	7,43	7,34	-	24,7	21,5	-
RDX/TNT/AP/Al										
40/40/10/10										
	1,76	2,53	3,3	4035	7,59	7,54	-	23,6	19,6	-
RDX/TNT/Al										
40/40/20	1,83	2,25	3,46	4050	7,38	7,42	-	22,4	21	-
AN/Al 90/10	1,05	2,25	1,74	1708	5,6	5,6	-	9,84	-	-
Tamchynit	1,24	$1,51^{++}$	3,1	2850	5,86	$5,27^{++}$	-	9,9	-	-
Al	2,7	5,29	4[1]							

+ ρ_o = 1,845 $g.cm^{-1}$, ++ exp. value · ∅ 75 mm

TNT - Trinitrotoluene

RDX - Cyclotrimethylenetrinitramine

HMX - Cyclotetramethylenetetranitramine

TATB - 1,3,5-triamino-2,4,6-trinitrobenzene

HCO - 1,3,3,5,7,7-hexanitro-1,5-diazacyclooctane

EDNA - Ethylene dinitramine

TNB - 1,3,5-trinitrobenzene

NM - Nitromethane

NQ - Nitroguanidine

HNB - Hexanitrobenzene

NTO - 3-nitro-1,2,4-triazol-5-on

OCNC - Octanitrocubane

PAPNBC - 2,4,6,8,10-pentanitro-2,4,6,8,10-pentaazabicyclo/5,3,0/decane

AN - Ammonium nitrate

AP - Ammonium perchlorate

Tamchynit - slurry AN/$NaNO_3$/H_2O/Fuel/NaOH/Microballoons
63/13/12/5,6/2,4/4

Al - Aluminium

REFERENCES

1. Wu Xiong, Journal of Energetic Materials 3, 263 /1985/
2. A.L. Krivchenko, Fizika Goreniya i Vzryva 3, 83 /1984/
3. M.J. Kamlet and S.J. Jacobs, J. Chem. Phys. 48, 23 /1968/
4. T. Urbański and T. Galas, Compt. Rendus 209, 558 /1939/
5. J.B. Zeldovich and A.S. Kompaneets, "Theory of Detonation", Academic Press, New York - London, 1960
6. J.B. Zeldovich, Zh. Exper. Theor. Fiz. 19, 542 /1940/
7. V.I. Pepekin, Polish J. Chem. 55, 1405 /1981/
8. I.M. Voskoboinikov et al., Fizika Goreniya i Vzryva 4, 285 /1967/
9. M.R. Rao, Chem. Phys. 9, 9 /1941/
10. W.C. Davis et al., Phys Fluids 8, 12, 2169 /1965/
11. C.L. Mader, "Numerical Modeling of Detonation", Univ. of Calif. Press, Berkeley, 1979
12. A. Miake, Kogyo Kayaku 52, 2, 131 /1991/
13. Wu Xiong et al., " Ninth Symp./International/ on Detonation," Vol. I , p. 435, Red Lion 1989