# THEORETICAL EVALUATION OF HEAT OF EXPLOSION OF ALUMINISED AND NON ALUMINISED EXPLOSIVES

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## ABSTRACT

New rules for the evaluation of heat of explosion of aluminised and non-aluminised explosives are proposed. It is shown that the energy calculated by the new rules agree fairly well with the actual energy, where as that obtained by old rules has deviation of about 20% for the case of non aluminised explosives. For the case of aluminised explosives, present rule gives results which agree fairly with the experiments. Energy evolved in later reaction is also discussed.

## INTRODUCTION

Kamlet and Jacob (1968) have given a relation for finding the explosion products in the case of CHON explosives. Their rule is based on the exact numerical calculations of Mader (1979), with the help of computer. Heat of explosion (HOE) of CHON explosives calculated by their rule agree fairly with the actual H.O.E., where as that calculated by Springall Roberts rules (c.f.Tomar and Murty 1979), deviates by 20% Mader has not given explosion products for aluminised explosives in his book.

Based on the Kamlet-Jacobs rules, we, in the present paper have formulated rules for decomposition products in the case of aluminised explosives. Heat of explosion is calculated by the present rules for various aluminised explosives and results are compared with those obtained by S-R Rules, as well as by experimental method (Madan et.al 1983). It is found that the present rules give good estimation of Heat of Explosion as compared to that obtained by S-R rules. In case of aluminised explosives, energy evolved in later reaction is also calculated. This energy is directly responsible for the increase in shock impulse.

## FORMULATION OF THE RULES

Chemical reaction at C-J plane is quite complex and it is not possible to know experimentally, what is happening at that time. S-R rules are based on the final products of detonation, obtained by calorimetry method.

Kamlet and Jacob (1968) have formulated rules for the explosion products of CHON explosives. These rules are based on the calculation done by Mader (1979), by computer. If a CHON explosive has x,y,z,w as carbon, hydrogen, oxygen and nitrogen atoms respectively in one molecule of the the explosive, then the explosion products will be given as

$$C_xH_yO_zN_w \longrightarrow y/2\ H_2O + \tfrac{1}{2}(z-y/2)\ CO_2 + w/2\ N_2 + (x-z/2+y/4)C_{amp} \quad (1)$$

where $C_{amp}$ is the carbon left in amorpous form.

Energy of TNT is calculated first by S-R rules and then by the above rule, given by equation (1) are tabulated in table I.

Table I

| Method | H.O.E Kcal/Kg | Actual HOE Lcal/Kg | Deviation from actual energy |
|---|---|---|---|
| S-R rules | 976.10 | 1210.0 | 19.33 |
| K-J rules | 1272.42 | 1210.0 | 5 approx |

It is seen from table I that the Kamlet-Jacob (K-J) rules give better value of energy of explosion for TNT. This fact can easily be verified for other known CHON explosives. In table II, we have compared the products of explosion of some CHON explosives by different rules.

To formulate the rules for the products of detonatio of aluminised explosives, we assume that first product is $H_2O$. That is, whole of the hydrogen present in the explosive first reacts with the oxygen and forms water. This reaction will hold if $y/2 < z$. If $y/2 > z$, then remaining hydrogen will be liberated as free hydrogen. Such explosives are cal oxygen deficient explosives. For the explosive which has sufficient oxygen, remaining oxygen will combine with the aluminium present to form AlO and $Al_2O$. Third product form will be $CO_2$. Nitrogen will be liberated as free nitrogen a remaining carbon as carbon amorpous.

Based on the above assumptions. products of explos of aluminised explosives are given as

$$C_xH_yO_zN_vAl_t \longrightarrow \frac{Y}{2} H_2O + \frac{t}{2} AlO + \frac{t}{4} Al_2O + \frac{1}{2}\left(Z - \frac{Y}{2} - \frac{3t}{4}\right) CO_2 + \frac{V}{2} N_2 + \left(x - \frac{Z}{2} + \frac{Y}{4} + \frac{3t}{8}\right) Camp \quad \ldots\ldots(2)$$

where $Z > \frac{Y}{2} + \frac{3t}{4}$. If z is less than or equal to $\frac{Y}{2} + \frac{3t}{4}$ we define the explosive to be oxygen deficient or sufficient respectively. Equation (2) gives rule for the explosion products at C-J plane for the aluminised explosives. The energy which is librated at this stage is responsible for the formation of the shock wave. In later reaction AlO and $Al_2O$ formed in the above reaction will again react with the $CO_2$ to form $Al_2O_3$ as

$$AlO + \frac{1}{2} CO_2 \longrightarrow \frac{1}{2} Al_2O_3 + \frac{1}{2} CO \quad ..(3)$$

$$Al_2O + 2\,CO_2 \longrightarrow Al_2O_3 + 2\,CO \quad ..(4)$$

since this reaction is highly exhothermic, again a large quantity of heat will be liberated. Time of liberation of energy depends on the rate of reaction of the above reactions. This later energy released is responsible for the increase, of shock impulse.

In table III we have compared the energy released at C-J plane with that obtained experimentally by Streak photogra (Madan et.al 1983). Energy evolved in later reaction is also given . Total energy evolved is the sum of the energies released in first reaction and second reaction. This total energy is compared with that obtained by S-R rules. It is seen from the table III that energy released by aluminised explosives in first reaction agrees nicely with that obtained by experimental technique.

## RESULTS AND DISCUSSIONS

Heat of explosion for various aluminised compositions are calculated by the present rules and also by the S-R rules. The special feature of the present rule is that the energy is released in two phases. In first phase it is assumed that equal amounts of aluminium reacts to form AlO and $Al_2O$ (Cook 1957). In the first phase approximately half of the total energy evolved is librated. This energy is called the energy librated at C-J plane and it agrees fairly well with that obtained by experimental techniques. These results are tabulated in table III.

| | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| TNT | $C_7H_5O_6N_3$ | 1.0 | 2.5 | 2.5 | 1.0 | 1.66 | 1.75 | 3.0 | 0.188 | 0.0 | 1.5 | 0 | 0 | 3.0 | 5.15 | 5. |
| RDX | $C_3H_6O_6N_6$ | 3.0 | 3.0 | 3.0 | 0.5 | 1.49 | 1.50 | 2.0 | 0.022 | 0.0 | 0.0 | 0.111 | 0.0 | 0.5 | 1.49 | 1. |
| PETN | $C_5H_8O\ N_4$ | 4.0 | 4.0 | 4.0 | 1.5 | 3.89 | 4.0 | 5.0 | 0.223 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.89 | 1. |
| HMX | $C_4H_8O_8N_8$ | 2.0 | 4.0 | 4.0 | 0.67 | 2.0 | 2.0 | 2.67 | 0.018 | 0.0 | 2.0 | 0.0 | 0.0 | 0.67 | 2.0 | 2. |
| DATB | C H O N | 1.0 | 2.5 | 2.5 | 1.0 | 1.73 | 1.75 | 3.0 | 0.055 | 0.0 | 1.5 | 0.0 | 0.0 | 2.0 | 4.22 | 4.2 |
| TATB | C H O N | 1.0 | 3.0 | 3.0 | 1.0 | 1.5 | 1.5 | 3.0 | 0.006 | 0.0 | 2.0 | 0.0 | 0.0 | 2.0 | 4.5 | 4.5 |

TABLE-III

| Charge Details | Experimental data: Density g/cc | VOD Km/s | Detonation pressure K.Bars | Energy of explosion Cal/g | Theory: Energy of explosion | Energy of explosion II reaction | Total Energy of exp. by the present method | Energy of explosion by S.R rules | % deviation of energy Ist reaction from experimental energy |
|---|---|---|---|---|---|---|---|---|---|
| RDX/TNT/Wax/Al 20/50/25/5 | 1.70 | 6.8943 | 185.53 | 3.3536 | 553.9608 | 607.9834 | ..... | 607.9834 | 2008.8803 | 9 |
| RDX/TNT/Al 0/50/50 | 1.9334 | 6.1239 | 124.87 | 4.8066 | 202.6212 | 130.2577 | ..... | 130.2577 | 1690.5631 | 35.7 |
| RDX/TNT/Al 5/50/45 | 1.901 | 6.375 | 135.92 | 4.6841 | 232.0906 | 161.9778 | ..... | 161.9778 | 1873.2859 | 30.21 |
| RDX/TNT/Al 10/50/40 | 1.870 | 6.5814 | 150.18 | 4.3934 | 282.6355 | 227.1562 | ..... | 227.1562 | 2056.6101 | 19.6 |
| RDX/TNT/Al 15/50/35 | 1.84 | 6.792 | 163.92 | 4.1782 | 337.1627 | 296.3531 | 122.6601 | 419.0132 | 2238.7184 | +2 |
| RDX/TNT/Al 20/50/30 | 1.8058 | 7.081 | 190.64 | 3.7495 | 458.5380 | 471.3598 | 261.9078 | 733.2676 | 2178.7682 | -2 |
| RDX/TNT/Al 25/50/25 | 1.779 | 7.173 | 204.96 | 3.4659 | 557.9625 | 609.4829 | 581.7117 | 1191.1946 | 1975.3048 | +9 |
| RDX/TNT/Al 30/50/20 | 1.789 | 7.5095 | 253.13 | 2.9855 | 851.0540 | 766.9147 | 807.7403 | 1574.655 | 1731.2465 | 10 |
| RDX/TNT/Al 30/50/15 | 1.7723 | 7.620 | 257.685 | 2.9935 | 870.9931 | 911.5735 | 855.3636 | 1766.9371 | 1487.1176 | 10 |
| RDX/TNT/Al 35/50/10 | 1.751 | 7.760 | 261.370 | 3.0342 | 876.3148 | 1064.0541 | 573.2479 | 1637.3320 | 1243.0010 | 21 |
| RDX/TNT/Al | 1.734 | 7.880 | 264.929 | 3.0642 | 883.9392 | 1187.917 | 421.3090 | 1608.2260 | 1077.0318 | -34 |

It is concluded that aluminised explosives do not releases energy instantanecusly but release in two phase. The energy released in first phase is only responsible for the shock formation. The energy released in later reaction is responsible for sustaining the shock and increasing its impulse. It is seen experimentally that for some explosives, this later energy released also depend on the grain size of aluminium Finer is the aluminium, larger is the later energy released. Thisis perhaps due to the fact that aluminium oxides, formed at the surface of larger grains, do not allow the further reaction. More studies in this direction are required to be undertaken.

ACKNOWLEDGEMENT

Thanks are due to Col. Harindar Singh, Deputy Director and Sh. D.S.Murty, Assistant Director for interest and Director TBRL for giving permission to publish the present work.

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