

The simplest method for calculating energy output and Gurney velocity of explosives

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Abstract

Two correlations are introduced for calculating Gurney velocity as a useful parameter for thermochemical estimation of explosive energy output. For $C_aH_bN_cO_d$ explosives, only the chemical composition of high explosive as well as its condensed or estimated gas phase heat of formation, which later is calculated by group additivity rules, is needed for calculating Gurney velocity. The introduced simple correlations in the present work may be applied to any explosive that contains the elements of carbon, hydrogen, nitrogen and oxygen with no difficulties at any loading density. There is no need to use any assumed decomposition reaction in present work. Gurney velocity are calculated for different pure and explosive formulations and compared with measured Gurney velocity at specified loading density. The results show that the agreement is good for present method as compared to previous correlations.

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1. Introduction

Reliable experimental data are always preferred over values obtained by computer codes or estimation procedures but all too often reliable data are not available in the field of energetic materials. Detonation parameters can be determined theoretically either by the use of computer codes, e.g. TIGER [1], or estimates based on the chemical composition and/or structure via different correlations. Complicated computer code can be used when the heat of formation and the density of explosive substance are known and the equation of state is assumed. Many of equations of state such as Becker–Kistiakosky–Wilson (BKW) [2], the Jacobs–Cowperthwaite–Zwisler (JCZ) [3,4] and Kihara–Hikita–Tanaka (KHT) [5] have been developed to describe shock and detonation performance of condensed matter. Some empirical correlations were also recently introduced for reliable detonation parameters of ideal and non-ideal pure or mixed explosives of different classes [6–15].

It can be supposed that a specific energy value is more appropriate than detonation properties for the ballistic characterization of an explosive. The calculated velocities and impulse imparted to driven materials can be obtained by a specific energy descriptor. Application of the simplified energy balance first suggested by Gurney [16] many years ago, can be used to correlate only elemental composition and estimated condensed or gas phase heat of formation of explosive. The purpose of this work is to present two correlations for obtaining thermochemical estimation of explosive energy output in driven metal. The introduced correlations in this work can be used for calculating the velocity of explosively driven metal over a range of geometries and loading factors. However, our main intent was to investigate the likelihood of obtaining a generalized formulation for Gurney energy as one of explosive parameters of somewhat more practical importance to explosive user. The purpose of this work was to correlate detonation Gurney velocity with explosive's elemental composition, loading density and condensed or gas phase heat of formation which later can be determined by the additivity rules of a group estimation method related to the molecular structure, e.g., the methods of Benson et al. [17], Yoneda [18], Joback [19], etc. The correlations can be applied to pure explosives as well as to solid explosive mixtures. The method has

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been tested on some well-known mixtures of explosives, where experimental data are available, and compared with two methods of Hardesty–Kennedy [20] and Kamlet–Finger [21]. It should be noted that the results predicted by the new simple method are comparable with outputs of complex computer codes, e.g. TIGER thermochemical code with JCZ3 equation of state [22] corresponding to the conversion of kinetic energy by threefold expansion of the products, and that accuracy is not necessarily enhanced by greater complexity. The present method for estimating detonation Gurney velocity at any loading density, without using experimental data, can be used where only an estimate gas phase of formation is needed. The most important aspect of the present work is that easily calculated gas phase heat of formation of a new explosive can be used to determine its Gurney velocity because there is no need to use the experimental values of solid or liquid heat of formation which is usually necessary in previous methods.

2. Explosive energy output and Gurney velocity

A suitable framework for considering the transfer of chemical energy to the kinetic energy of expanding product mixture and driven solid material can be suggested by the Gurney model through the difference between the internal energy (E_s) of the isentropically expanded products and that of the unreacted explosive (E_0) in the content of the Gurney model. Then, energy output from this difference can be assumed as a measure of energy available for driving metal in which this approach ignores the wave dynamics in the flow of the product gases. Gurney's model assumes that all fragments move out at the same initial velocity, and that the velocity of gaseous explosion products increases from zero at the center of mass of explosive out to a maximum that is also the velocity of casing fragments at moment of break-up. It is felt that the Gurney energy (E) or velocity ($\sqrt{2E}$) provides a more relevant absolute indicator of the ability of an explosive to accelerate metal under a wide variety of loading conditions and geometries of interest. Since the Gurney model permits quantitative estimation of the velocity or impulse imparted to metal by detonating explosives rather than simply rank-ordering explosives, this is special merit of it. The velocity profile in the product gases is also linear in material coordinates for this model. One can write an energy balance, which is sufficient to determine for any the metal velocity of symmetric geometries, the results indicate that the terminal metal velocity (U) is a function of the ratio of metal mass to explosive charge mass. For simple asymmetric configuration, a momentum balance is also required and must be solved simultaneously. The metal velocity for some simple geometries filled with explosives are expressed as below:

$$\text{Cylindrical tube : } \frac{U}{\sqrt{2E}} = \left(\frac{m}{c} + \frac{1}{2} \right)^{-1/2} \quad (1)$$

$$\text{Sphere : } \frac{U}{\sqrt{2E}} = \left(\frac{m}{c} + \frac{3}{5} \right)^{-1/2} \quad (2)$$

$$\text{Symmetrical sandwich : } \frac{U}{\sqrt{2E}} = \left(\frac{m}{c} + \frac{1}{3} \right)^{-1/2} \quad (3)$$

where m and c are the mass per unit length of the metal and explosive, respectively. The measured values of U with known geometry and m/c can be used to correlate $\sqrt{2E}$. It should be mentioned that dimensionless ratio $U/\sqrt{2E}$ in each case is a function of the ratio m/c .

Hardesty and Kennedy [20] have shown that Gurney velocities are reasonable well approximated by TIGER computer code and JCZ3 [22] equation of state computations of energy to threefold expansion along the detonation isentrope:

$$\sqrt{2E} = \left(\sqrt{2(E_0 - E_s)} \right)_{V/V_0=3} \quad (4)$$

The JCZ3 equation of state was formulated to allow a general treatment for any explosive formulation of thermodynamic state properties of a mixture of product species for densities ranging from atmospheric to the C–J state as well as to permit reliable estimation of internal energy states during expansion. Eq. (4) confirms that energy transfer between the detonation products and the driven metal is limited in many cases by rupturing the metal rather than by side losses. Hardesty and Kennedy [20] have also related the Gurney velocity to the characteristic φ quantity used by Kamlet and Jacobs [23] to determine detonation pressures and velocities. The characteristic φ quantity has the following form:

$$\varphi = NM^{1/2}Q^{1/2} \quad (5)$$

where N is the number of moles of gaseous detonation products per gram of explosive, M is the average molecular weight of these gases and Q is the heat of detonation in calories per gram. The correlation of Hardesty and Kennedy based on φ is given as follows:

$$\sqrt{2E} = 0.6 + 0.54\sqrt{1.44\varphi\rho_0} \quad (6)$$

Kamlet and Finger [21] followed the somewhat different path to arrive at a method for calculating Gurney velocities:

$$\sqrt{2E} = 0.887\varphi^{0.5}\rho_0^{0.5} \quad (7)$$

3. Development new correlations

Theoretical calculations are more convenient and useful in comparing the relative detonation parameters of one explosive with another. It can be inferred from experimental data that Gurney velocity depends on three principal parameters for any $C_aH_bN_cO_d$ explosive namely the composition, the heat of formation and loading density of explosive.

It was found that it is possible to express Gurney velocity of an explosive, the same as recently developed some detonation parameters [10–13], only from explosive's elemental composition without using any assumed detonation products. This concept was also formed the basis of an approach proposed earlier by the other authors, e.g. by Stine [24] and Rothstein and Petersen [25,26], for defining and evaluating in a fairly simple and straightforward manner detonation velocity.

The effectiveness of an explosive upon detonation depends on the amount of energy available in it and the rate of release of available energy. The heat of formation can be used for showing the heat content of explosive because the heat of detonation depends on the heat of formation of explosive per unit weight and greater energy content leads to greater release of energy upon detonation. Heat of formation is also an important property to evaluate instabilities and performances of energetic materials, which can be determined experimentally or estimated for some classes of explosives [27–30].

Loading density is also an important property for calculating the performance of explosives. Experimental measurements of Gurney velocity reveal that their values depend on loading density of explosives. As seen in Eqs. (6) and (7), previous methods of Hardesty and Kennedy [20] as well as Kamlet and Finger [21] also showed this dependency.

We have found that the following equation with some adjustable parameters is suitable for finding Gurney velocity correlation as function of the above-mentioned basic parameters:

$$\sqrt{2E} \text{ (km s}^{-1}\text{)} = X_1 + \left(\frac{X_2a + X_3b + X_4c + X_5d + X_6\Delta H_f^\circ}{\text{MW}} \right) \rho_0^{X_7} \quad (8)$$

where a , b , c and d are stoichiometric coefficients for an explosive of general formula $C_aH_bN_cO_d$, MW and ΔH_f° are the molecular weight and the heat of formation of explosive, respectively, and X_1 – X_7 are adjustable coefficients which can be obtained from the best fit of experimental data. This equation provides the basis for a simple procedure for estimation of Gurney velocity, which requires as input information only the elemental composition, loading density, and heat of formation of explosive. Since previous studies have been shown that some of detonation parameters can be found from gas phase heat of formation without using experimental condensed heat of formation, we have also used condensed as well as gas phase heat of formation of explosive so that later can be calculated from an additivity method such as Benson [17], Yoneda [18] and Joback [19], etc. Some pure and mixed $C_aH_bN_cO_d$ explosives, which are listed in Table 1, have been chosen as database for finding adjustable parameters. To find the adjustable parameters of Eq. (2), we have used the method of Kamlet and Hurwitz [31]. The results show that two optimized correlations (9) and (10) can be used for reliable calculating Gurney velocity by using condensed and gas phase heat of formation of explosive respectively:

$$\sqrt{2E} \text{ (km s}^{-1}\text{)} = 0.227 + \left(\frac{7.543a + 2.676b + 31.97c + 35.91d - 0.196\Delta H_f^\circ(\text{s})}{\text{MW}} \right) \rho_0^{0.5} \quad (9)$$

$$\sqrt{2E} \text{ (km s}^{-1}\text{)} = 0.220 + \left(\frac{6.620a + 4.427b + 29.03c + 37.61d - 0.051\Delta H_f^\circ(\text{g})}{\text{MW}} \right) \rho_0^{0.5} \quad (10)$$

The condensed and gas phase heats of formation as well as chemical formula of some pure and mixed explosives are shown in Table 1. Eqs. (9) and (10) confirm previous foundations [20,21] that energy delivered strongly depends on density. The calculated Gurney velocities are insensitive, especially in Eq. (10), to large variation in the heat of formation of unreacted explosive that are also consistent with the results of previous

Table 1
Parameters used in calculations

| Explosive ^a | Chemical formula | Condensed phase ^b ΔH_f° (kcal/mol) | Gas phase ^c ΔH_f° (kcal/mol) |
|------------------------|---|--|--|
| COMP A-3 | C _{1.87} H _{3.74} N _{2.46} O _{2.46} | 2.84 | 34 |
| COMP B | C _{2.03} H _{2.64} N _{2.18} O _{2.67} | 1.28 | 10 |
| COMP C-3 | C _{1.90} H _{2.83} N _{2.34} O _{2.60} | 3.21 | 29 |
| CYCLOTOL-77/23 | C _{1.75} H _{2.59} N _{2.38} O _{2.69} | 3.58 | 13 |
| CYCLOTOL-75/25 | C _{1.78} H _{2.58} N _{2.36} O _{2.69} | 3.21 | 12 |
| HMX | C ₄ H ₈ N ₈ O ₈ | 17.93 | 45 |
| LX-14 | C _{1.52} H _{2.92} N _{2.59} O _{2.66} | 1.50 | 45 |
| NM | CH ₃ NO ₂ | –27.03 | –18 |
| OCTOL-78/22 | C _{1.74} H _{2.59} N _{2.40} O _{2.69} | 3.05 | 11 |
| OCTOL-75/25 | C _{1.78} H _{2.58} N _{2.36} O _{2.69} | 2.78 | 11 |
| PETN | C ₅ H ₈ N ₄ O ₁₂ | –128.7 | –174 |
| RDX | C ₃ H ₆ N ₆ O ₆ | 14.71 | 38 |
| TACOT | C ₁₂ H ₄ N ₈ O ₈ | 110.5 | 129 |
| TETRYL | C ₇ H ₅ N ₅ O ₈ | 4.67 | 9 |
| TNT | C ₇ H ₅ N ₃ O ₆ | –15.0 | –4 |

^a See Appendix A for glossary of compound names.

^b Heat of formation of pure explosives were obtained from [32].

^c Heat of formation calculated by Joback additive group procedure [19].

works [20,21]. The physical implication for $C_aH_bN_cO_d$ explosives is that the contribution of the four elements present in the unreacted explosive is far more important, in terms of influencing Gurney velocity, than details of the bonding arrangements within the molecular structure. This is significant in view of the large uncertainty that may be associated with the heats of formation of new explosives. Gurney velocities estimated by this method for pure and mixed explosives are given in Table 2 and compared with measured values and calculated from the methods of Kamlet and Finger as well as Hardesty and Kennedy. As indicated in Table 2, the newly calculated Gurney velocities of two Eqs. (9) and (10) show surprisingly good agreement with experimental values at specified loading densities. Comparison of calculated results with experimental data listed in Table 2 may be taken as appropriate validation of the new simple method for use with $C_aH_bN_cO_d$ explosives. It should be noted that the present method is the simplest method and at the same time gives reliable results. It is seen that the present method approximates the measured results most closely because predicted Gurney velocities for 15 explosives by using both of Eqs. (9) and (10) have a root mean square (rms) of deviations for experiment 0.04 km/s. Meanwhile, rms deviation for Hardesty and Kennedy

is 0.08 km/s and for Kamlet and Finger is 0.05 km/s. Considering different experimental values for some of explosives, e.g. TNT, the agreement between calculated and measured Gurney velocities is very good. It is possible to use data of heat of formation on the pure constituents to estimate Gurney velocities of mixture. Heat of formation of an explo-

Table 2
Comparison of Gurney velocity of the new correlations, using solid and gas phase heat of formation, and Hardesty and Kennedy (H–K) [20] as well as Kamlet and Finger (K–F) [21] methods with measured values

| Name | ρ_0 (g/cc) | Gurney velocity (km/s) | | | | | | | | |
|----------------------|-----------------|------------------------|------|--------------------|------|--------------------|---------|------------------------|----------|-------------------------|
| | | Measured ^a | H–K | Dev _{H–K} | K–F | Dev _{K–F} | Eq. (9) | Dev _{Eq. (9)} | Eq. (10) | Dev _{Eq. (10)} |
| COMP A-3 | 1.59 | 2.63 | 2.63 | 0.00 | 2.65 | 0.02 | 2.63 | 0.00 | 2.63 | 0.00 |
| COMP B | 1.71 | 2.70 | 2.68 | –0.02 | 2.70 | 0.00 | 2.68 | –0.02 | 2.68 | –0.02 |
| | 1.717 | 2.756–2.821 | 2.68 | – | 2.70 | – | 2.68 | – | 2.68 | – |
| | 1.717 | 2.71 | 2.68 | –0.03 | 2.70 | –0.01 | 2.68 | –0.03 | 2.68 | –0.03 |
| COMP C-3 | 1.60 | 2.68 | 2.63 | –0.05 | 2.65 | –0.03 | 2.62 | –0.06 | 2.62 | –0.06 |
| CYCLOTOL 77/23 | 1.754 | 2.79 [20] | 2.76 | –0.03 | 2.79 | 0.00 | 2.77 | –0.02 | 2.77 | –0.02 |
| CYCLOTOL 75/25 | 1.754 | 2.79 | 2.75 | –0.05 | 2.78 | –0.02 | 2.77 | –0.03 | 2.76 | –0.04 |
| HMX | 1.89 | 2.97 | 2.92 | –0.05 | 2.98 | 0.01 | 2.97 | 0.00 | 2.97 | 0.00 |
| LX-14 | 1.68 | 2.80 | 2.74 | –0.06 | 2.79 | –0.01 | 2.79 | –0.01 | 2.76 | –0.04 |
| NM | 1.14 | 2.41 | 2.37 | –0.04 | 2.39 | –0.02 | 2.41 | 0.00 | 2.41 | 0.00 |
| OCTOL 78/22 | 1.821 | 2.83 [20] | 2.80 | –0.03 | 2.84 | 0.01 | 2.83 | 0.00 | 2.82 | –0.01 |
| OCTOL 75/25 | 1.81 | 2.80 | 2.78 | –0.02 | 2.82 | 0.02 | 2.81 | 0.01 | 2.81 | 0.01 |
| | 1.821 | 2.83 | 2.79 | –0.04 | 2.82 | –0.01 | 2.81 | –0.02 | 2.81 | –0.02 |
| | 1.821 | 2.83 | 2.79 | –0.04 | 2.82 | –0.01 | 2.81 | –0.02 | 2.81 | –0.02 |
| PETN | 1.76 | 2.93 | 2.84 | –0.09 | 2.90 | –0.03 | 2.93 | 0.00 | 2.93 | 0.00 |
| RDX | 1.77 | 2.88 | 2.85 | –0.03 | 2.90 | 0.02 | 2.88 | 0.00 | 2.88 | 0.00 |
| TACOT | 1.61 | 2.12 | 2.38 | 0.26 | 2.32 | 0.20 | 2.26 | 0.14 | 2.26 | 0.14 |
| TETRYL | 1.62 | 2.50 | 2.55 | 0.05 | 2.55 | 0.05 | 2.50 | 0.00 | 2.50 | 0.00 |
| TNT | 1.63 | 2.37 | 2.43 | 0.06 | 2.38 | 0.01 | 2.37 | 0.00 | 2.37 | 0.00 |
| | 1.63 | 2.419–2.505 | 2.43 | – | 2.38 | – | 2.37 | – | 2.37 | – |
| rms Deviation (km/s) | | | | 0.08 | | 0.05 | | 0.04 | | 0.04 |

^a All measured values of Gurney velocity are reported in Ref. [32] except where noted.

sive mixture can be calculated from the heat of formation of individual components and their percent concentrations in the mixture.

Undoubtedly there are the other pure and mixed explosives whose Gurney velocities have been measured but the explosive compounds in Table 2 represent those $C_aH_bN_cO_d$ explosives obtained during a fairly extensive review in open literature [32]. As seen in Table 2, there are individual compounds such as TNT, RDX and PETN, which have C–NO₂, N–NO₂ and O–NO₂ bonds, respectively. This suggests that the new method can be applied for some classes of explosives, e.g. Plastic-bonded compositions (PBXs), sheet explosives, melt castable explosive formulations and pressed compositions. PBXs are representative of today's state-of-the-art military explosives, which formed from energetic solids and binder ingredient. PBX-9404 (with chemical formula $C_{1.40}H_{2.75}N_{2.57}O_{2.69}Cl_{0.03}P_{0.01}$, $\Delta H_f(s) = 0.08$ kcal/mol [32] and $\Delta H_f(g) = 42$ kcal/mol) is one of the PBX explosives for which experimental Gurney velocity is 2.90 km/s [32]. Although it does not follow the general formula $C_aH_bN_cO_d$, its calculated Gurney velocity by Eqs. (9) and (10) are 2.93 and 2.90, respectively. 2,4,6-Trinitro-1,3,5-triazine ($C_3N_6O_6$) is one of the high energy-density explosives which is a representative of novel class $C_nN_{2n}O_{2n}$ free hydrogen explosives [33]. There is no information about its synthesis is available in literature [34]. Its estimated solid heat of formation and density are 46 kcal/mol and 2.1 g/cm³ [34]. Calculated Gurney velocity by Eqs. (9) and (10), using estimated $\Delta H_f(g) = 42$ kcal/mol in later, are 2.90 and 2.87 km/s, respectively, which are consistent with values obtained by Hardesty and Kennedy (2.87 km/s) [20] as well as Kamlet and Finger (2.91 km/s) [21].

4. Conclusions

It is proposed here that the ballistic performance of a high explosive can be easily calculated only from elemental composition of explosive. In this paper, two correlations have been introduced for estimating the Gurney energy or Gurney velocity for $C_aH_bN_cO_d$ explosives at any bulk of interest. Two reliable correlations Eqs. (9) and (10) are especially useful if that specific energy can be used with the Gurney model. We feel that the introduced correlations represent a significant advance in a priori estimation of explosive energy output. One can estimate the Gurney velocity of a real or hypothetical $C_aH_bN_cO_d$ explosive only from elemental composition as a function of the initial loading density. This is possible to use the new correlations even for $C_aH_bN_cO_d$ explosives where the condensed or gas phase heat of formation of explosive is relatively uncertain. Moreover, the introduced correlations can be used to reliable estimate of a mixture of explosives.

The principal conclusion of this work is that it is possible on the basis of elemental and heat of formation to estimate quite well the performance of many organic explosives in metal driving applications. The results of this work are remarkable for explosive user because the energy output of an explosive is readily calculated by a desk calculator of about the same reliability as one could expect from a more complex computer code and equation of state, e.g. TIGER and JCZ3. There is also no need to assume specified detonation products, as with the previous methods of Hardesty and Kennedy as well as Kamlet and Finger. It is important to emphasize that Eq. (10) is suitable for determination of Gurney velocity of new explosives or their mixture with common explosives at any loading den-

sity and does not require knowledge of solid or liquid heat of formation.

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Appendix A. Glossary of compound names

1. COMP A-3: 91/9 RDX/Wax
2. COMP B: 63/36/1 RDX/TNT/Wax
3. COMP C-3: 77/4/10/5/1/3 RDX/TNT/DNT/MNT/NC/TETRYL
4. CYCLOTOL-77/23: 77/23 RDX/TNT
5. CYCLOTOL-75/25: 75/25 RDX/TNT
6. HMX: cyclotetramethylene tetranitramine
7. LX-14: 95.5/4.5 HMX/Estane
8. NM: nitromethane
9. OCTOL-78/22: 77.6/22.4 HMX/TNT
10. OCTOL-75/25: 75/25 HMX/TNT
11. PETN: pentaerythritol tetranitrate
12. RDX: cyclotrimethylene trinitramine
13. TACOT: tetranitrodibenzo-1,3a,4,6a-tetrazapentalenene
14. TETRYL: *N*-methyl-*N*-nitro-2,4,6-trinitroaniline
15. TNT: 2,4,6-trinitrotoluene

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