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## An Alternative Method for Estimation of Gurney Velocity Based on Assumed Detonation Products

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**Abstract:** A new method for prediction of Gurney velocity of explosives is introduced in which energy output is correlated with the heat of detonation, the number of moles of gaseous products of detonation per gram of explosive and the average molecular weight of gaseous products. It is assumed that the CHNO explosive reacts to form products composed of  $N_2$ , CO,  $H_2O$ ,  $CO_2$ ,  $H_2$ ,  $O_2$  and C(s) as determined by the oxygen balance of the unreacted compound. Good agreement is obtained between measured and calculated values of Gurney velocity as compared to previous correlations which assumed the reaction products to consist of  $N_2$ ,  $H_2O$ ,  $CO_2$  and either C(s) or  $O_2$ .

**Key words:** explosion mechanics; detonation products; gurney velocity; correlation; explosive; metal acceleration

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### 1 Introduction

The detonation products are largely gases, which in high temperature and high pressure regime, are highly non-ideal. Detonation parameters such as pressure and velocity can be calculated by a computer code, e. g. TIGER<sup>[1]</sup>, which uses a database of thermodynamic characteristics of explosion products and initial composition of high explosives. Moreover, empirical correlations can also be used to determine important properties of energetic compounds<sup>[2]</sup>. Some new methods have also been introduced to determine detonation parameters of ideal and non-ideal pure or mixed explosives as well as the other important properties of energetic compounds<sup>[3-24]</sup>.

Since specific energy value can permit calculation of velocities and impulse imparted to driven materials, it is more appropriate than detonation properties for the ballistic characterization of an explosive. The purpose of this work is to present a new method for estimation of Gurney velocity<sup>[25]</sup> in conjunction with a simple energy partitioning model to solve a wide range of problems involving the acceleration of metal by detonating explosives of arbitrary density. In this paper the effect of choosing new suggested decomposition procedures<sup>[7]</sup> will be studied to estimate the reliable energy output for  $C_aH_bN_cO_d$  explo-

sives at any bulk density of interest with respect to previous methods<sup>[26,27]</sup> which use the assumed detonation products of Kamlet<sup>[28]</sup>. The new method can be applied to pure explosives as well as to solid explosive mixtures somewhat more practical importance to explosive user so that it calculate the velocity of explosively-driven metal over a range of geometries and loading factors. However, the results will be compared with experimental data of well-known pure mixtures of explosives, where measured data are available, and Hardesty and Kennedy (H&K)<sup>[26]</sup> as well as Kamlet and Finger (K&F)<sup>[27]</sup> methods.

### 2 Gurney Velocity Based on Kamlet Procedure

Detonation products are formed by the possibility of the existence of more than one phase as detonation wave propagates through the explosive medium. The equilibrium composition of gaseous products can be determined from experimental measurement, thermochemical equilibrium calculation, or by identifying an appropriate decomposition reaction. Kamlet and Jacobs<sup>[28]</sup> suggested detonation pressures and velocities correlations for CHNO explosives at initial densities above  $1 \text{ g} \cdot \text{cm}^{-3}$  on assumption that  $N_2$ ,  $H_2O$ , C(s) and  $CO_2$  (but not CO) are the important detonation products. They used the parameter  $\varphi$  to obtain the following correlations for calculation of detonation velocities and pressures at loading densities,  $\rho_0$ , greater than  $1 \text{ g} \cdot \text{cm}^{-3}$ :

$$P = K\varphi\rho_0^2 \quad (1)$$

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$$D = A\varphi^{1/2}(1 + B\rho_0) \quad (2)$$

where

$$\varphi = NM^{1/2}Q_{\text{det}}^{1/2} \quad (3)$$

and  $K$ ,  $A$  and  $B$  are constant. In Eq. (3)  $M$  is the average molecular weight of gaseous products,  $N$  is the number of moles of gaseous detonation products per gram of explosive and  $Q_{\text{det}}$  is the heat of detonation in calories per gram. The heat of detonation can be determined from the heats of formation of reactants and decomposition products of the explosive through the relation<sup>[28]</sup>:

$$Q_{\text{det}} \cong - \frac{\Delta H_f(\text{detonation products}) - \Delta H_f(\text{explosive})}{\text{formula weight of explosive}} \quad (4)$$

Gurney<sup>[25]</sup> suggested a simple model in which a given explosive liberates a fixed amount of specific energy ( $E$ ) on detonation that is converted to kinetic energy partitioned between the driven metal and gaseous products. Since the process of metal acceleration might be accounted by limiting the degree of expansion of products gases to that which is considered to occur within the effective interval, it has limited duration. The measured Gurney energy is significantly less than chemical energy of unreacted explosive because any internal energy remaining in the gaseous products does not contribute to its value. The Gurney velocity or energy can provide a more relevant absolute indicator of the ability of an explosive to accelerate under a wide variety of initial densities and geometries of

interest. Hardesty and Kennedy (H&K)<sup>[26]</sup> correlated Gurney velocities ( $\sqrt{2E}$ ) with  $\varphi$  and  $\rho_0$  as follows:

$$\sqrt{2E} = 0.6 + 0.54(1.44\varphi\rho_0)^{1/2} \quad (5)$$

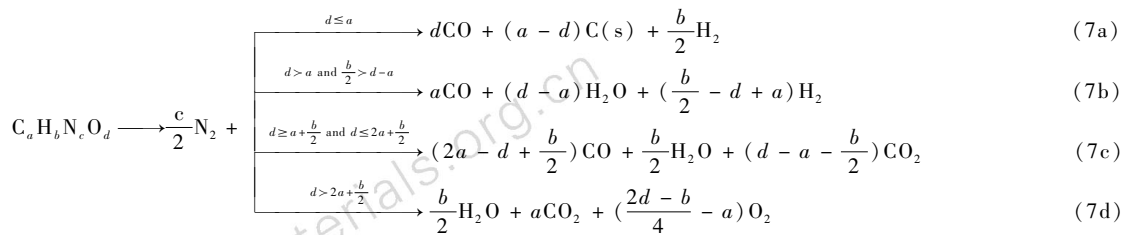
Later Kamlet and Finger (K&F)<sup>[27]</sup> introduced the following correlation with the same variables:

$$\sqrt{2E} = 0.887\varphi^{0.5}\rho_0^{0.4} \quad (6)$$

K&F correlation predicts better results than H&K correlation with respect to the measured Gurney velocities.

### 3 New Method for Predicting Gurney Velocities

The major components of detonation products of CHNO explosives may include  $N_2$ ,  $CO$ ,  $H_2O$ ,  $CO_2$  and solid carbon as well as minor amounts of  $H_2$ ,  $NH_3$ ,  $O_2$ ,  $NO$  and other chemical species. CHEETAH<sup>[29]</sup> is a C version of the FORTRAN equilibrium code TIGER, which can be used to estimate detonation products of explosives. The products concentrations for CHNO explosives calculated by Cheetah 2.0/JCZS indicate that the gaseous species  $H_2O$ ,  $H_2$ ,  $N_2$ ,  $CO_2$  and  $CO$  are predominant detonation products<sup>[30]</sup>. To obtain a good approximation of major detonation products, it can be assumed that all nitrogens go to  $N_2$  while a portion of the oxygens form  $H_2O$  and carbons preferentially will be oxidized to  $CO$  rather than  $CO_2$  so that the following pathways are satisfied:



It is found that predicted detonation pressures and velocities of explosives are close to experimental values over a wide range of loading densities greater than  $1 \text{ g} \cdot \text{cm}^{-3}$  as well as less than  $1 \text{ g} \cdot \text{cm}^{-3}$ <sup>[7,31]</sup>. Moreover predicted heats of detonation by using above decomposition products are much better than those obtained based on Kamlet's method<sup>[7,17]</sup>. It was found that predicted heats of detonation for  $H_2O$  (g) using the new decomposition procedure and Kamlet's method have root mean square (rms) deviations of 0.954 and  $1.006 \text{ kJ} \cdot \text{g}^{-1}$  from experiment, respectively. Moreover, Kamlet's method shows larger deviation from experiment (rms deviation =  $1.365 \text{ kJ} \cdot \text{g}^{-1}$ ) as compared to the new method (rms deviation =  $1.048 \text{ kJ} \cdot \text{g}^{-1}$ )<sup>[7]</sup> for

$H_2O(1)$ . However, the results have indicated that Eq. (7) can give reliable prediction of  $Q_{\text{det}}$ , and therefore  $\varphi$ , as compared to decomposition products of Kamlet's method<sup>[7]</sup>.

The study on Gurney velocity for various  $C_aH_bN_cO_d$  explosives has shown that it is possible to obtain new correlation based on four different mentioned decomposition paths. It is found that the following equation with some adjustable parameters are suitable for finding Gurney velocity correlation of  $C_aH_bN_cO_d$  explosive as function of the above mentioned basic parameters:

$$\sqrt{2E} = Z_1 + Z_2\rho_0^{Z_3} + Z_4\varphi_{\text{mod}}^{Z_5} \quad (8)$$

where,  $\varphi_{\text{mod}}$  is modification of Eq. (3) based on decomposi-

tion paths (7a) to (7d) for an explosive of general formula  $C_a H_b N_c O_d$  and  $Z_1$ - $Z_5$  are adjustable coefficients which can be obtained from the best fit of experimental data. The reported experimental values of the Gurney velocity have been listed for some  $C_a H_b N_c O_d$  explosives in Table 1 where their measured data are available in open literature. However, experimental data of Table 1 have been chosen as database for finding adjustable parameters so that R-squared value or the coefficient of determination of this correlation

is 0.991<sup>[32]</sup>. The optimized correlation can be given as:

$$\sqrt{2E} = -8.341 + 3.045\rho_0^{0.3} + 4.268\varphi_{\text{mod}}^{0.3} \quad (9)$$

Comparison of the new correlation with measured values and estimated values from the methods of H&K<sup>[26]</sup> and K&F<sup>[27]</sup> methods are given in Table 1. The calculated Gurney velocities by new method show surprisingly good agreement with experimental values as compared to H&K<sup>[26]</sup> and K&F<sup>[27]</sup> methods. Average deviations are 0.02 km · s<sup>-1</sup> for Eq. (9), 0.05 km · s<sup>-1</sup> for Eq. (5) and 0.03 km · s<sup>-1</sup> for Eq. (6).

**Table 1** Comparison of calculated Gurney velocities by the new correlation, H&K<sup>[26]</sup> and K&F<sup>[27]</sup> with measured values

compound <sup>a)</sup>	$\rho_0/\text{g} \cdot \text{cm}^{-3}$	Gurney velocity / km · s <sup>-1</sup>						
		measured <sup>b)</sup>	new	Dev <sub>new</sub>	H-K	Dev <sub>H-K</sub>	K-F	Dev <sub>K-F</sub>
COMP A-3	1.59	2.63	2.66	0.03	2.63	0.00	2.65	0.02
COMP B	1.71	2.70	2.67	0.03	2.68	0.02	2.70	0.00
	1.717	2.756 – 2.821	2.67	–	2.68	–	2.70	–
	1.717	2.71	2.68	0.03	2.68	0.03	2.70	0.01
CYCLOTOL-77/23	1.754	2.79 <sup>[26]</sup>	2.80	0.01	2.76	0.03	2.79	0.00
CYCLOTOL-75/25	1.754	2.79	2.79	0.00	2.75	0.04	2.78	0.01
HMX	1.89	2.97	2.98	0.01	2.92	0.05	2.98	0.01
LX-14	1.68	2.80	2.80	0.00	2.74	0.06	2.79	0.01
NM	1.14	2.41	2.41	0.00	2.37	0.04	2.39	0.02
OCTOL-78/22	1.821	2.83 <sup>[26]</sup>	2.83	0.00	2.80	0.03	2.84	0.01
OCTOL-75/25	1.81	2.80	2.81	0.01	2.78	0.02	2.82	0.02
	1.821	2.83	2.82	0.01	2.79	0.04	2.82	0.01
PETN	1.76	2.93	2.90	0.03	2.84	0.09	2.90	0.03
RDX	1.77	2.88	2.92	0.04	2.85	0.03	2.90	0.02
TACOT	1.61	2.12	2.14	0.02	2.38	0.26	2.32	0.20
TETRYL	1.62	2.50	2.48	0.02	2.55	0.05	2.55	0.05
TNT	1.63	2.419 – 2.505	2.49	–	2.43	–	2.38	–
average deviation/km · s <sup>-1</sup>				0.02		0.05		0.03

Note: a) See Appendix for glossary of compound names; b) All measured values of Gurney velocity are reported in Ref [33] except where noted.

## 4 Conclusions

An empirical new correlation is used to calculate Gurney velocity as an important parameter for thermochemical estimation of explosive energy output by assuming four paths for determining detonation products. The introduced correlation represents a significant advance in a priori estimation of explosive energy output by H&K<sup>[26]</sup> and K&F<sup>[27]</sup> methods. It is found that new decomposition procedure can give us a new correlation for more reliable predicting energy output with respect to previous correlation which use Kamlet decomposition products. Comparison of calculated results with experimental data listed in Table 1 may be taken as appropriate validation of Eq. (9) as compared to previous Eqs. (5) and (6). The

new correlation may be applied to any  $C_a H_b N_c O_d$  explosives at any loading density.

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### Appendix: Glossary of compound names

1. HMX: Cyclotetramethylenetetranitramine ( $C_4 H_8 N_8 O_8$ )
2. NM: Nitromethane ( $CH_3 NO_2$ )
3. PETN: Pentaerythritol tetranitrate ( $C_5 H_8 N_4 O_{12}$ )
4. RDX: Cyclomethylene trinitramine ( $C_3 H_6 N_6 O_6$ )
5. TACOT: 2, 4, 8, 10-Tetranitro-5H-benzotriazolo [ 2, 1, a ]-benzotriazol-6-ium, hydroxide, inner salt ( $C_{12} H_4 N_8 O_8$ )
6. TETRYL: N-Methyl-N-nitro-2,4,6-trinitroaniline ( $C_7 H_5 N_5 O_8$ )
7. TNT: 2,4,6-Trinitrotoluene ( $C_7 H_5 N_3 O_6$ )

8. COMP A-3; 91/9 RDX/wax ( $C_{1.87}H_{3.74}N_{2.46}O_{2.46}$ )
9. COMP B; 63/36/1 RDX/TNT/wax ( $C_{2.03}H_{2.64}N_{2.18}O_{2.67}$ )
10. CYCLOTOL-77/23; 77/23 RDX/TNT ( $C_{1.75}H_{2.59}N_{2.38}O_{2.69}$ )
11. CYCLOTOL-75/25; 75/25 RDX/TNT ( $C_{1.78}H_{2.58}N_{2.36}O_{2.69}$ )
12. LX-14; 95.5/4.5 HMX/Estane 5702-F1 ( $C_{1.52}H_{2.92}N_{2.59}O_{2.66}$ )
13. OCTOL-78/22; 77.6/22.4 HMX/TNT ( $C_{1.74}H_{2.59}N_{2.39}O_{2.69}$ )
14. OCTOL-75/25; 75/25 HMX/TNT ( $C_{1.78}H_{2.58}N_{2.36}O_{2.69}$ )

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