



## **The Applicability of Kamlet's Method for the Prediction of the Velocity of Detonation (VOD) of Polyurethane (PU) Based Binary Explosive Compositions**

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**Abstract:** The velocity of detonation (VOD) of polyurethane (PU) based binary explosive compositions is assessed by Kamlet's method and compared with experimental results for a few compositions. These compositions are used as booster compositions for the initiation of main charges and the velocity of detonation is determined empirically for compositions with explosives like RDX, HMX, TATB, FOX-7, CL-20. For some of the compositions, the VOD was determined experimentally and found to match the predicted values. For RDX/PU (95/5) explosive composition, the experimental and estimated VODs at 1.66g/cm<sup>3</sup> bulk charge density, are 8211 and 8224 m/s respectively. For CL-20/PU (95/5) composition, at a charge density of 1.82 g/cm<sup>3</sup>, the calculated VOD was 8775 m/s against the experimental value of 8943 m/s. The applicability of Kamlet's method for the prediction of the VOD for 95/5 Explosive/PU compositions was also established. These findings contradict an earlier hypothesis concerning the weight average estimation of Kamlet's parameter  $\phi$  and establish closer estimates of the VOD using the weight average assessment of the parameters 'N', 'M' and 'Q'.

**Keywords:** explosives, booster, velocity of detonation, polyurethane (PU), Kamlet's method

### **Introduction**

Binary explosive compositions containing an explosive and a binder are used in explosive trains for the initiation of main charges. They are used as boosters to transfer shock from the detonator to the main charge, leading to initiation of the main charge. The quantity of the explosive component in these

boosters is greater than 90% and they are made by pressing [1]. The explosive ingredient in the booster composition may be RDX, HMX, CL-20, FOX-7, PETN, TATB, NTO, *etc.*, and the binder component may be hydrocarbons like wax, polyurethane (PU) [2, 3], hydroxyl terminated polybutadiene (HTPB) [4], Viton [5], poly-ethylene vinyl acetate (EVA) [6, 7] *etc.* Earlier wax based compositions (which were cheap and easy to process) were used for this purpose, but now PU based explosive compositions have been used for better consistency, higher performance and good shelf life. In the present article, the velocity of detonation (VOD) of different PU based explosive compositions are assessed by the popular Kamlet method [8-11] which is validated for the prediction of the VOD with less than 5% deviation. In fact, for explosive compositions, Kamlet's method may be applied in various ways and one of the objectives of the present paper is to ascertain the suitability and the appropriate application method for PU based explosive compositions. The validation of the derived results by comparison with experimental measurements of the VOD by the Pin Oscillographic Technique (POT) [12] for a few booster compositions was also carried out.

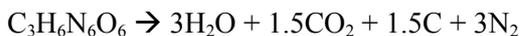
### Velocity of Detonation (VOD) predictions

For the prediction of the VOD of an explosive composition, the input parameters for the empirical method proposed by Kamlet are molecular formula, density and heat of formation. For a given explosive composition, an arbitrary estimate of the products of explosion is obtained by assuming that oxidation of hydrogen precedes that of carbon; hydrogen forms water followed by carbon forming carbon dioxide, if enough oxygen is present. Using the heat of formation of the composition and of the products of the explosion, the chemical energy ( $Q$  in cal/g) released in the detonation is estimated. From the products of the explosion, the number of moles of gaseous molecules ( $N$ ) produced per unit weight of explosive and the average molecular weight ( $M$ ) of the products of explosion is calculated. From these parameters, using Equations 1 and 2, the velocity of detonation of the composition is obtained.

$$\text{Kamlet parameter, } \phi = N\sqrt{MQ} \quad \text{Eq. 1}$$

$$\text{Velocity of detonation, VOD (m/s)} = 1010 \times (1+1.3\rho) \times \sqrt{\phi} \quad \text{Eq. 2}$$

For example, for a single ingredient RDX, the molecular formula is  $C_3H_6N_6O_6$ , the density is  $1.805 \text{ g/cm}^3$ , and the heat of formation is  $14.71 \text{ kcal/mol}$ . The molecular weight of RDX is  $222.174 \text{ g/mol}$ . An arbitrary chemical reaction leading to the products of explosion is given below.

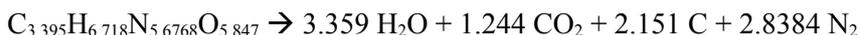


Since the molecule is oxygen deficient (which most explosives are), unburnt carbon is obtained in the products of explosion. The heat of formation of water and carbon dioxide are - 93.98 kcal/mol and - 57.79 kcal/mol, respectively. Various parameters for the estimation of the VOD are calculated :  $Q = 1481.06$  cal/g,  $N = (3+1.5+3)/222.174 = 0.033757$ ,  $M = 27.2212$ . With these parameters, and using Equation 1,  $\phi = N\sqrt{MQ} = 6.77807$ . The VOD of RDX is estimated using Equation 2 as 8799.6 m/s, which is close to the variously reported experimental value of 8750 m/s [13].

For explosive compositions, the molecular formula of the equivalent composition, the actual density and the heat of formation calculated from the weight sum of the heats of formation of the ingredients, are used to calculate the VOD. In this paper, the molecular formula, density and heat of formation of PU is taken as  $\text{C}_{10}\text{H}_{18.717}\text{N}_{0.273}\text{O}_{3.294}$ ,  $1$  g/cm<sup>3</sup> and -162.3 kcal/mol, respectively. These values are laboratory measured values, using an elemental analyzer-mass spectrometer (MS), Buoyancy Method, and thermogravimetric analysis (TGA), respectively. The values of the density and the heat of formation of the explosive ingredients were taken from an explosive database.

## Analysis and Discussion

To illustrate the analysis of various binary booster compositions, the RDX/PU based explosive composition is considered. For a 95/5 explosive composition containing 95% RDX and 5% PU by weight, the VOD was obtained by the POT technique as 8211 m/s at a formulation density of 1.66 g/cm<sup>3</sup>. The equivalent molecular formula for an explosive mixture was obtained using the procedure described in Ref. 8. For the calculation of the theoretical maximum density (TMD), the equality of volume is considered and the formula for the calculation is written as  $\{1/\text{TMD}\} = \{0.95/\rho_{\text{RDX}} + \{0.05/\rho_{\text{PU}}\}$ ]. The equivalent molecular formula, theoretical maximum density (TMD) and molecular weight for the explosive composition are  $\text{C}_{3.395}\text{H}_{6.718}\text{N}_{5.6768}\text{O}_{5.847}$ ,  $1.735$  g/cm<sup>3</sup> and  $220.668$  g/mol respectively. The density achieved in the practical composition was around 95% of TMD. The arbitrary chemical reaction leading to the products of explosion is shown below.



From this equation, various intermediate parameters are calculated:  $Q = 1436.086$  cal/g,  $N = 0.033722$ ,  $M = 29.654$ . With these parameters, using Equation 1,  $\phi = N\sqrt{MQ} = 6.959038$ . The VOD of the composition is estimated using Equation 2 as 8414 m/s, which is close to the reported experimental value but is on the high side.

Another approach for the estimation of the VOD of explosive compositions, using the Kamlet method is by taking the weight average values of 'N', 'M' and 'Q' for the composition and then estimating  $\phi$  and the VOD. For the RDX/PU (95/5) composition, the values of 'N', 'M' and 'Q' are 0.034498, 26.2572 and 1414.17 cal/g, respectively. This gives a value of  $\phi = N\sqrt{MQ} = 6.647638$  from Equation 1 and  $VOD = 8224$  m/s from Equation 2.

In fact, Zhou Xing Xi et al [14] have analyzed the following three methods for the estimation of the VOD using Kamlet's method for explosive compositions: (i) using the equivalent composition approach as discussed above, (ii) using the weight average values of 'N', 'M' and 'Q' for the explosive composition and using Equations 1 and 2 above, the VOD can be estimated after calculating  $\phi$ , (iii) using the weight average value of  $\phi$ . After analysis for various explosive compositions, it was concluded in their paper that, the third method is suitable, which is fortunate since it is also less calculation intensive. Method (iii) was used for different explosive compositions in the generation of Table 1. For PU, the value of the Kamlet parameter  $\phi$  was calculated as 1.63968. The Kamlet Parameter of the RDX/PU 95/5 composition was calculated as  $(0.95 \times 6.77807 + 0.05 \times 1.63968 =) 6.52115$ . Using Equation 2, the VOD was calculated as  $(1010 \times \{1 + 1.3 \times 1.66\} \times 6.52115 =) 8145$  m/s. The values of the Kamlet parameter  $\phi$  for the different explosive ingredients were calculated and the VODs of the binary 95/5 (explosive/PU) compositions are compiled in Table 1 for a bulk density of 95% of TMD.

In Table 1, the Kamlet parameter  $\phi$  was calculated from the weight average value of the individual components and is given by  $[0.95 \times \phi_{\text{explosive}} + 0.05 \times 1.63968]$ . The theoretical maximum density (TMD =  $\rho$ ) was calculated from the densities of the individual components by the expression  $[\rho_{\text{explosive}} / (0.95 + 0.05 \times \rho_{\text{explosive}})]$ . The VOD was estimated at 95% of TMD and Equation 2 was used for the calculation. It is clear from the Table 1 that higher values of the Kamlet parameter  $\phi$  give higher values of VOD. However, the role of the density of the explosives cannot be ruled out. The DATB/PU (95/5) composition shows a higher value of  $\phi$  than the TATB/PU (95/5) composition, but the estimated VOD of the TATB/PU composition is on the high side. This is due to the higher value of the TMD of the TATB/PU composition. CL-20, RDX, HMX and PETN based 95/5 binary explosive compositions (with PU) have closely similar values of  $\phi$  but

CL-20 has the highest density amongst them and thus has a higher value of the estimated VOD. PETN/PU (95/5) has the lowest VOD in this group (of four) due to the low value of its TMD.

**Table 1.** VOD estimated by the Kamlet's method at 95% of TMD for binary explosive/PU (95/5) compositions

Composition (95/5 by wt.)	Kamlet parameter $\phi$	TMD of the composition	VOD at 95% TMD
RDX/PU	6.77807	1.735	8106
HMX/PU	6.76505	1.827	8390
PETN/PU	6.78794	1.713	8040
Tetryl/PU	5.61177	1.669	7194
HNS/PU	4.87626	1.678	6737
DATB/PU	5.07279	1.763	7105
TATB/PU	4.99893	1.850	7293
CL-20/PU	6.75573	1.879	8550
FOX-7/PU	6.09808	1.805	7906
NTO/PU	5.43031	1.844	7578
DNAN/PU	4.24847	1.505	5859

For some of the explosive compositions, the experimental value of the VOD was measured by the POT technique and the results are compiled in Table 2. The table also contains the values of the VOD estimated by all three methods derived from Kamlet's approach for the same explosive compositions. The value of the density is the bulk density of the explosive charge and is generally around 95% of TMD, which can be obtained from Table 1.

**Table 2.** Estimation of VOD by Kamlet's method for binary explosive compositions

Explosive composition (95/5 by wt.)	Density (g/cm <sup>3</sup> )	Velocity of detonation (m/s)			
		Measured experimentally	Method i	Method ii	Method iii
RDX/PU	1.66	8211	8414	8224	8145
FOX-7/PU	1.70	7972	8095	7931	7858
HMX/PU	1.75	8543	8732	8520	8439
CL-20/PU	1.82	8943	8907	8775	8667

In the earlier paper [6], method iii was proposed to be the more accurate method, but from the experimentally measured values of the VOD for the four different binary explosive compositions, method ii seems to be more accurate. So, for the binary explosive/PU (95/5) compositions, method ii proposed for the Kamlet approach is suitable for estimation of the VOD. Rather than using the weight average of  $\phi$ , the calculation of  $\phi$  from the weight average values of 'N', 'M' and 'Q' gives VOD values close to the experimentally measured values.

## Conclusion

Various binary compositions containing explosive/PU (95/5 by weight) were studied using the Kamlet approach for the estimation of the velocity of detonation (VOD). The VOD was estimated using the weight average value of the Kamlet parameter  $\phi$  at 95% of the theoretical maximum density (TMD) for RDX, HMX, PETN, Tetryl, HNS, DATB, TATB, CL-20, FOX-7, NTO and DNAN. The dependence of the VOD on the density as well as on the Kamlet parameter  $\phi$  was investigated. The VOD for some of the explosive compositions, containing RDX, HMX, CL-20 and FOX-7, were experimentally determined, and contrary to an earlier reported hypothesis, that the weight average of the Kamlet parameter  $\phi$  gives an estimated VOD close to the experimental VOD, the weight average of 'N', 'M' and 'Q' gave better estimates of VOD for PU based, binary explosive compositions.

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