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Daniel J. Whelan[a]; Gunter Bocksteiner[a]
[a] Aeronautical and Maritime Research Laboratory, Defence Science and Technology Organisation, Melbourne, Victoria, Australia

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VELOCITY OF DETONATION, CHARGE DIAMETER AND CRITICAL DIAMETER IN UNCONFINED RDX-DRIVEN HETEROGENEOUS EXPLOSIVES

Daniel J Whelan and Gunter Bocksteiner

Aeronautical and Maritime Research Laboratory, Defence Science and Technology Organisation, PO Box 4331, Melbourne, Victoria 3001, Australia.

ABSTRACT

The relationship between the experimentally-determined velocity of detonation of unconfined, cylindrical charges of RDX-driven PBXs and composite explosives, V(d), and charge diameter, d, has been examined critically. It has been found that, for many formulations, the data can be fitted more satisfactorily to an elliptical relationship between V(d) and (1/d) than to a linear relationship but this depends, at least in part, on the particle size distribution and shape of the RDX used in the formulation. It has also been observed that the experimentally-determined critical diameter of the formulation, d_c, can be directly related to the linear coefficient in the elliptical V(d) / d relationship, **a***, by the equation, $d_c = 2.208\ \mathbf{a}^*$. This leads to a practical outcome, namely:- that the critical diameter of an explosive formulation may be estimated without the need to prepare a large number of charges, very close to or less than the expected d_c.

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INTRODUCTION

The measured steady-state velocity of detonation (V of D) of a cylindrical charge of an explosive formulation depends on the diameter of the charge, d, and its degree of confinement and the mathematical relationship between V of D and d, has been an area of continuing interest for over forty years [1-15]. In addition, it has become commonplace to determine experimentally the V of D at different charge diameters and to use the data to calculate its value at infinite diameter, D. Seldom, however, do the compilations of such data [16,17] record data in its entirety even though there is practical information which can be gleaned from a knowledge of the way that the V of D depends on d. In some cases, one finds quoted values for D and the experimentally-determined critical diameter, d_c; in others, only V of D at a particular charge diameter and density is quoted.

From the early work summarised by Eyring et al.[2] in 1949 it became apparent that, for many unconfined monomolecular explosives, there was an experimentally validated linear relationship between V of D and the reciprocal of the diameter of the charge, 1/d, which took the form

$$V(d) = \mathbf{D}\,(1 - [\mathbf{a} / d]) \qquad [\text{Eq. } 1]$$

where V(d) is the V of D of a detonating unconfined cylindrical charge of diameter d, and **D** and **a**, curve-fitting constants. Logically enough, **D** is the limiting value of the V of D for a charge of infinite diameter and **a** can be considered a constant characteristic of the explosive formulation.

While Eyring et al. related **a** specifically to the reaction zone length of the detonating system [2], the term, reaction zone length, is usually associated with the

advancing reaction front with the vectors describing the direction of the detonation velocity and the reaction zone being normal to the wave front at every point along this front. However, this particular description of **a**, as defined by Eq. 1, has been recognised as inadequate and subsequent approaches have revealed that there is a connection between V(d), the radius of curvature *at the central axis of the detonation front* and the critical diameter of the charge [7-15].

For many heterogeneous or composite explosives and for those, in particular, at high densities (> 95 % TMD), Eq. 1 was seen to be inadequate, especially when the charge diameter approached the experimentally determined critical diameter, d_c. For this reason, Campbell and Engelke [9,10] introduced an additional term into the Eyring equation, which took the overall form

$$V(d) = \mathbf{D}\ (\ 1 - [\mathbf{a} / d] - [\mathbf{a}\ d_c'/ d\ (\ d - d_c'\ )]\ ) \qquad [\text{Eq. } 2]$$

where **D**, **a** and d_c' are again curve fitting constants, with d_c' being referred to as a calculated critical diameter to distinguish it from the experimentally determined d_c. This relationship enabled a large amount of V(d) data to be rationalised mathematically. However, its main shortcomings are that one needs a considerable bank of experimental data to determine and to confirm the calculated values of **D**, **a** and d_c' and that simple iterative curve-fitting techniques sometimes give lines of best fit with values of **a** and d_c' which are either inappropriate (negative values for d_c') or follow no simple trend [18].

In this paper, the experimental V(d) / d data for several RDX-driven explosive formulations, including those reported by Campbell and Engelke, have been reexamined and it has been found that there is a better set of relationships between V(d) and (1/d) and d_c than that described in Eq. 2.

FORMULATIONS

The experimental data from the following formulations were examined in detail:-

PBXW-115 (Aust.) [19,20]

Formulation: RDX (Bimodal, Fine [160 μm] Type I equivalence [HMX-free], 60 %, Very fine [20 μm] Type II equivalence [containing 6 - 6.5 % coprecipitated or occluded HMX], 40 %) 20 %, AP 43 %, Al 25 %, HTPB/IPDI Polyurethane Binder 12%. Cast-cured.

RDX Particle Size: est. 105 μm; Charge density 1.79 Mg m^{-3}.

PBXW-115 (USA) [20-23]

Formulation: RDX (Bimodal, Fine, Type II, 60 %, Very fine [20 μm] Type II, 40 %) 20 %, AP 43 %, Al 25 %, HTPB/IPDI Polyurethane Binder 12%. Cast-cured.

RDX Particle Size: est. 60 μm [23]; Charge density 1.79 Mg m^{-3}.

Composition A, modified *(James)* [4]

Formulation: RDX 91.8 %, Wax 8.2 %. Charge density, 1.69 Mg m^{-3}.

RDX Particle Size: 30 %, <35 μm; 45 %, 35-150 μm; 25 % >150 μm.

Mean particle size: 85 μm.

Composition B *(Malin et al.)* [5]

Formulation: RDX 63 %, TNT 37 %. Slow solidification process.

RDX Particle Size: 80 % < 400 μm; Charge density, 1.70 Mg m^{-3}.

Composition B *(Gibbs and Popolato)* [10]

Formulation: RDX 63 %, TNT 36 %, Wax 1 %; Charge density, 97.6 % TMD. RDX Particle Size [15] : 99 % of RDX > 75 μm.

Cyclotol 77/23 *(Gibbs and Popolato)* [10]

Formulation: RDX 77 %, TNT 23 %; Charge density, 99.1 % TMD.

Amatex 20 *(Gibbs and Popolato)* [10]

Formulation: RDX 40 %, TNT 40 %, Ammonium Nitrate 20 %; Charge density 94.3% TMD.

PBX-L#3 *(de Longueville et al.)* [24]

Formulation: RDX 82.4 %, Polyether-based PU Binder 17.6 %. Cast-cured. RDX Particle Size: unspecified; Charge density 1.58 Mg m^{-3}.

Original Authors' Designation: Sample 3

PBX-L#5 *(de Longueville et al.)* [24]

Formulation: RDX 82.4 %, Silicone Binder 17.6 %. Cast-cured.

RDX Particle Size: unspecified; Charge density 1.58 Mg m^{-3}.

Original Authors' Designation: Sample 5

PBX-M#C (Moulard et al.) [25-27]

Formulation: RDX 70 %, HTPB / IPDI PU Binder 30 %. Cast-cured.

RDX Particle Size: Monomodal, 134 μm ; Charge density 1.45 Mg m^{-3}.

Original Authors' Designation: C (coarse)

PBX-M#VF (Moulard et al.) [25-27]

Formulation: RDX 70 %, HTPB / IPDI PU Binder 30 %. Cast-cured.

RDX Particle Size: Monomodal, 6 μm ; Charge density 1.45 Mg m^{-3}.

Original Authors' Designation: VF (very fine).

PBXN-107A (Nanut and Parker) [28]

Formulation: RDX (Trimodal Blend: Coarse 850 μm, 50 %, Fine 160 μm, 31.%, Very Fine 20 μm, 19 %) 86 %, Acrylate Binder 14 %. Cast-cured.

PBXC-117A (Nanut and Parker) [28]

Formulation: RDX (Trimodal Blend: as for PBXN-107A) 71 %, Acrylate Binder 12 %, Aluminium powder 17 % . Cast-cured.

Composition C-4 (Pandow et al.) [7]

Formulation: RDX [either Class 1 (50 %), Class 5 (50 %) or Class 1 (75%), Class 5 (25 %)], 91 %; Plasticised PIB, 9 %.

This composition appears very similar to the Composition A : modified, described earlier in this compilation [4].

RESULTS AND DISCUSSION

When the present authors [19] looked critically at various sets of experimental V(d) / d data from unconfined RDX-driven PBXs and composite explosives, including those cited by Campbell and Engelke [9,10], they found that the experimental results (Table 1) usually fitted an elliptical relationship between V(d) and 1/d of the form

$$V(d)^2 = D^2 (1- [a^* / d]^2) \qquad [Eq. 3],$$

considerably better than the simple linear relationship, Eq. 1; this conclusion was arrived at by comparing the linear least squares plots following Eq. 1 and Eq. 3 and examining the data at higher d values; it can be illustrated by reference to the

published experimental data for PBXW-115 (USA) [21]. In Eq. 3, once again, **D** and **a*** are curve fitting constants, whose values are most easily obtained from a linear plot of $V(d)^2$ vs $(1/d)^2$.

In Table 1, the results of the analysis of the experimental V(d) data reported for the various RDX-driven formulations listed above are summarised.

In at least ten of the fourteen cases examined, analysis of the data in Table 2, based not only on considerations of the linear least squares (LLSQ) coefficients of determination but also on the values of V(d) for the larger diameter charges, indicates that these data follow Eq. 3 rather more closely than Eq. 1.

TABLE 1

An Analytical Description of the Relationship between the Observed Velocity of Detonation and Charge Diameter for Unconfined Charges of the Various RDX-driven Heterogeneous Explosives, described in the Formulations Section.

PBXW-115 (Aust.) [19,20] **:** Charge Diameters: 80 mm to 200 mm.

Critical diameter: 80 mm (1 x Go, 1 x No Go).

$$[V, \text{meter s}^{-1}] = 5913.37\{1 - (11.048 \times 10^{-3} / [d, \text{meter}])\}$$

Linear Least Squares (LLSQ) Coefficient of Determination = 0.9680

$$[V, \text{meter s}^{-1}]^2 = (5641.77)^2 \{1 - (35.254 \times 10^{-3} / [d, \text{meter}])^2\}$$

LLSQ Coefficient of Determination = 0.9833

TABLE 1 (cont.)

PBXW-115 (USA) [20-23] : Charge Diameters: 36 mm to 69 mm.

Critical diameter: 37.6 ± 1.6 mm.

$[V, \text{meter s}^{-1}] = 6193.4\{1 - (6.849 \times 10^{-3} / [d, \text{meter}])\}$

LLSQ Coefficient of Determination = 0.9076

$[V, \text{meter s}^{-1}]^2 = (5760.0)^2 \{1 - (18.325 \times 10^{-3} / [d, \text{meter}])^2\}$

LLSQ Coefficient of Determination = 0.9364

Composition A [4] : Charge Diameters: 4.2 mm to 25.4 mm.

Critical diameter: < 4.2 mm.

$[V, \text{meter s}^{-1}] = 8299.8\{1 - (0.757 \times 10^{-4} / [d, \text{meter}])\}$

LLSQ Coefficient of Determination = 0.9511

$[V, \text{meter s}^{-1}]^2 = (8266.8)^2 \{1 - (0.741 \times 10^{-3} / [d, \text{meter}])^2\}$

LLSQ Coefficient of Determination = 0.9938

Composition B [5] : Charge Diameters: 5.71 mm to 20 mm.

Critical diameter: 2.0 mm [4], 1.94 mm [13].

Original Authors' Designation: (Malin) Type 1.

$[V, \text{meter s}^{-1}] = 7964.9\{1 - (2.5989 \times 10^{-4} / [d, \text{meter}])\}$

LLSQ Coefficient of Determination = 0.9627

$[V, \text{meter s}^{-1}]^2 = (7864.9)^2 \{1 - (1.5173 \times 10^{-3} / [d, \text{meter}])^2\}$

LLSQ Coefficient of Determination = 0.9970

TABLE 1 (cont.)

Composition B [10] : Charge diameters: 25.5 mm to 4 mm.

Critical diameter: 4.3 mm.

$$[V, \text{meter } s^{-1}] = 8023.3 \{1 - (3.3885 \times 10^{-4} / [d, \text{meter}])\}$$

LLSQ Coefficient of Determination = 0.9004

$$[V, \text{meter } s^{-1}]^2 = (7894.3)^2 \{1 - (1.6609 \times 10^{-3} / [d, \text{meter}])^2\}$$

LLSQ Coefficient of Determination = 0.9815

Cyclotol 77/23 [10] : Charge diameters: 102 mm to 5.6 mm.

Critical diameter: 6.0 mm.

$$[V, \text{meter } s^{-1}] = 8259.7 \{1 - (2.998 \times 10^{-4} / [d, \text{meter}])\}$$

LLSQ Coefficient of Determination = 0.9072

$$[V, \text{meter } s^{-1}]^2 = (8202.3)^2 \{1 - (2.004 \times 10^{-3} / [d, \text{meter}])^2\}$$

LLSQ Coefficient of Determination = 0.9495

Amatex 20 [10] : Charge diameters: 102 mm to 17 mm

Critical diameter: ca. 20 mm.

$$[V, \text{meter } s^{-1}] = 7091.0 \{1 - (1.9732 \times 10^{-3} / [d, \text{meter}])\}$$

LLSQ Coefficient of Determination = 0.9896

$$[V, \text{meter } s^{-1}]^2 = (6954.3)^2 \{1 - (8.739 \times 10^{-3} / [d, \text{meter}])^2\}$$

LLSQ Coefficient of Determination = 0.9978

TABLE 1 (cont.)

RDX-based PBX-L#3 [24] : Charge Diameters: 10 to 30 mm.

Critical diameter : 6 mm.

$$[V, \text{meter } s^{-1}] = 8267.3 \{ 1 - (7.872 \times 10^{-4} / [d, \text{meter}]) \}$$

LLSQ Coefficient of Determination = 0.9536

$$[V, \text{meter } s^{-1}]^2 = (8035.5)^2 \{1 - (3.2406 \times 10^{-3} / [d, \text{meter}])^2 \}$$

LLSQ Coefficient of Determination = 0.9867.

RDX-based PBX-L#5 [24] : Charge Diameters: 10 to 30 mm.

Critical diameter: 7.5 mm.

$$[V, \text{meter } s^{-1}] = 7981.9 \{ 1 - (1.1781 \times 10^{-3} / [d, \text{meter}]) \}$$

LLSQ Coefficient of Determination = 0.9706

$$[V, \text{meter } s^{-1}]^2 = (7642)^2 \{1 - (3.950 \times 10^{-3} / [d, \text{meter}])^2 \}$$

LLSQ Coefficient of Determination = 0.9942

RDX-based PBX-M#C [25-27] : Charge Diameters: 20-50 mm.

Critical diameter $\geq$ 15 mm.

$$[V, \text{meter } s^{-1}] = 7787.7 \{ 1 - (2.378 \times 10^{-3} / [d, \text{meter}]) \}$$

LLSQ Coefficient of Determination = 0.9768

$$[V, \text{meter } s^{-1}]^2 = (7495.4)^2 \{1 - (8.160 \times 10^{-3} / [d, \text{meter}])^2 \}$$

LLSQ Coefficient of Determination = 0.9994

TABLE 1 (cont.)

RDX-based PBX-M#VF [25-27] : Charge Diameters: 10-50 mm.

Critical diameter < 10 mm.

$$[V, \text{meter } s^{-1}] = 7452.0\{1 - (0.1194 \times 10^{-3} / [d, \text{meter}])\}$$

LLSQ Coefficient of Determination = 0.9233

$$[V, \text{meter } s^{-1}]^2 = (7428.9)^2 \{1 - (1.344 \times 10^{-3} / [d, \text{meter}])^2\}$$

LLSQ Coefficient of Determination = 0.8102 ; linearity not deemed satisfactory.

PBXC-117A [28] : Charge Diameters: 39 mm to 16 mm.

Critical diameter < 16 mm, 12.5 mm (Cone test).

8 coordinates; 2 for each of 4 diameters #

$$[V, \text{meter } s^{-1}] = 8209.2\{1 - (1.131 \times 10^{-3} / [d, \text{meter}])\}$$

LLSQ Coefficient of Determination = 0.9471

$$[V, \text{meter } s^{-1}]^2 = (7989.0)^2 \{1 - (5.408 \times 10^{-3} / [d, \text{meter}])^2\}$$

LLSQ Coefficient of Determination = 0.9409

Were averaged values of each V(d) taken, it would be seen that each of the LLSQ coefficients of determination would have been very much closer to unity (>0.985).

PBXN-107A [28] : Charge Diameters: 16 mm to 39 mm.

Critical diameter < 10 mm, ca. 7.5 mm, (Cone test) [25]

8 coordinates; 2 for each of 4 diameters #

TABLE 1 (cont.)

PBXN-107A (cont.)

$$[V, \text{meter s}^{-1}] = 8281.5\{1 - (0.5763 \times 10^{-3} / [d, \text{meter}])\}$$

LLSQ Coefficient of Determination = 0.8556

$$[V, \text{meter s}^{-1}]^2 = (8196.4)^2 \{1 - (3.884 \times 10^{-3} / [d, \text{meter}])^2\}$$

LLSQ Coefficient of Determination = 0.8967.

[#] as for PBXC-117A.

Composition C-4 [7] **:** Critical diameter < 5 mm

$$[V, \text{meter s}^{-1}] = 8100.5\{1 - (0.4464 \times 10^{-3} / [d, \text{meter}])\}$$

LLSQ Coefficient of Determination = 0.9474

$$[V, \text{meter s}^{-1}]^2 = (8026.7)^2 \{1 - (2.894 \times 10^{-3} / [d, \text{meter}]^2\}$$

LLSQ Coefficient of Determination = 0.8777; trend satisfactory but linearity of plot not really satisfactory.

It was found, from a plot of a^* vs. d_c, taken from the experimental data in Table 1 and represented in Table 2 and adding the boundary condition that this plot passes through the origin (i.e., $a^* = 0$, $d_c = 0$), that a simple line of best fit can be obtained:

$$d_c = 2.208\, a^* \qquad [\text{Eq. } 5]$$

with a LLSQ coefficient of determination of 0.994.

From the right hand column in Table 2, it can be readily seen that there is very good agreement between the experimentally-determined d_c values and the calculated critical diameters for these RDX-driven composite formulations.

This leads to a practical outcome, namely:- that the critical diameter of an explosive formulation may be estimated without the need to prepare a large number of charges, very close to or less than the expected d_c, provided that it can be shown that the V(d) profile appears to follow Eq. 3 .

In addition, it may be interpreted that the larger the value of **a***, the more diffuse the reaction zone and the greater the critical diameter.

Furthermore, by combining Eq. 3 and Eq. 5, one obtains

$$[V(d) / D]^2 = 1 - [d_c / 2.208\, d]^2 \qquad [Eq.\ 6].$$

This enables the "lower threshold velocity" or "cut off velocity", $V(d_c)$, for an RDX-driven formulation whose V(d) profile follows [Eq. 3] to be estimated, thus:-

$$V(d_c) = 0.892\ D \qquad [Eq.\ 7],$$

a result which allows one to calculate the detonation energy [29] of an unconfined cylindrical charge of a heterogeneous explosive formulation at its critical diameter.

It should be appreciated that this analysis, derived from the experimental data summarised in Table 1, is based on results relating only to the RDX-driven component of the detonation reaction [14, 20, 22] ; more complete reaction, as in the case of PBXW-115, will involve detonative oxidation of Al by AP and probable reaction with the products from the detonation of RDX [20,22].

TABLE 2

Comparison of the Experimentally-determined and Calculated Critical Diameter for the various Unconfined Heterogeneous RDX-driven Explosives, listed earlier .

Formulation	V(d) Parameter, a*, mm [from Eq. 3]	Critical Diameter, d_c, mm (experimental)	Calculated d_c, mm ($d_c = 2.208\ a^*$) [Eq. 5]
PBXW-115 (Aust.)	35.25	80	77.8
PBXW-115 (USA)	18.33	37.6 ± 1.6	40.5
Amatex	8.74	ca. 20	19.3
PBX-M#C	8.16	≥15	18.0
PBXC-117A	5.41	12.5	11.9
PBX-L#5	3.95	7.5	8.7
PBXN-107A	3.88	ca. 7.5	7.9
PBX-L#3	3.24	6.0	7.2
Cyclotol	2.0	6.0	4.4
Comp. B [10]	1.66	4.3	3.4
Comp. B [6]	1.52	2.0	3.7

If one returns to Table 1, one sees that the formulations whose V(d) profiles better follow a linear V(d) vs (1/d) relationship (Eq. 1) than an elliptical relationship (Eq. 3) are formulations which have a large component of very fine RDX in the formulation (for example, Composition C4, Moulard's formulation PBX-M#VF and, perhaps, PBXC-117A and PBXN-107A).

To support this, one can look at the results in Table 2 for the two French research formulations, PBX-M#C and PBX-M#VF; they each consist of 70 % by mass of monomodal RDX in a cast-cured polyurethane binder. The V(d) profile of the formulation PBX-M#C, which is made with the relatively coarse RDX fraction (median particle size 134 μm), obeys Eq. 3 more closely than Eq. 1; on the other hand, the V(d) profile for PBX-M#VF made with very fine (6 μm) RDX is much better described by Eq. 1.

This trend can also be seen to be true by comparing the results from Composition C-4 [7] with those from the modified Composition A reported by James [4]. Composition C-4 consists of 91 % by mass RDX, containing between 25 and 50 % very fine (Class 5) material, which has a median particle size of between 5 and 20 μm [17], and its V(d) profile follows Eq. 1 better than Eq. 3, suggesting that it is behaving, *at least in a kinetic sense*, more like a "monomolecular" explosive formulation [22]. On the other hand, curve-fitting calculations for Composition A (91.8 % RDX, with less very fine RDX) suggest that the V (d) - d dependency follows Eq. 3 more closely than Eq. 1, even though this composition has a small critical diameter [4].

From Table 2, it is also apparent that the V(d) profile for Composition B is better described by Eq. 3 than Eq. 1 and this would appear to reinforce the notion

that particle-size plays an important role in determining detonation behaviour. An unclassified footnote in a recent, restricted compilation indicates that the RDX component of US-made Composition B is relatively coarse, being made up of less than 1% fine RDX (< 75 μm); from this, one may deduce that particle size as well as the distribution of RDX in the solidified TNT will influence the path of the energy releasing steps [2] in the detonation reaction of Composition B.

In short, the approach to ideal V(d) explosive behaviour of these RDX-driven detonation reactions in composite and heterogeneous explosives appears to be closely related to the particle size distribution of the RDX; the smaller the median particle size of the component RDX fractions, the larger the specific surface area of the detonation-driving component RDX, and, presumably, the greater its rate of reaction in the detonation zone [2] or its detonative pick-up and energy transfer [13, 30, 31]. With the coarser RDX-containing explosives containing a considerably less component of fine RDX, the kinetic processes in the reaction zone may be different, resulting subsequently in a different steady-state V(d) dependency. These variations may also be affected by differences in RDX particle shape [19, 32, 33].

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