Short Communication

Propellants, Explosives, Pyrotechnics

DOI: 10.1002/prep.202000280

A Computational Study on the Detonation Velocity of Mixtures of Solid Explosives with Non-Explosive Liquids

Thomas M. Klapötke*[a] and Muhamed Suceska*[b]

Dedicated in memoriam to Dr. Judah Goldwasser

Abstract: According to Urbanski's finding in a solid explosive with a density of less than the theoretical maximum density (TMD), the detonation velocity increases if the air contained in the explosive gets replaced by a non-explosive liquid. In order to quantify this observation, the detonation velocities for RDX in combination with ten non-explosive liquids were calculated using the EXPLO5 code (V6.05.04). It could be shown that pressing out the air of a high-explosive powder and replacing the voids with a non-explosive liquid such as ethylene glycol, water or glycerin helped to increase the final detonation velocity.

Keywords: Calculations · Detonation velocity · EXPLO5 · Hexogen · Mixtures (solid/liquid)

1 Introduction

Urbanski et al. published a paper in 1939 on the influence of the detonation velocity (VoD) if in a solid explosive with a density of less than the theoretical maximum density (TMD) the air contained in the explosive gets replaced by a non-explosive liquid [1]. The authors stated that replacing the air with a liquid that does not dissolve the explosive causes an increase in the detonation velocity. This seems to support the theory of Becker and Schmid which states that the VoD is equal to the sum of the speed of sound (C) and the particle velocity (U) at the CJ point [2–4]:

$$\mathrm{VoD} = C + U \tag{1}$$

In 1968, Hikita and Fujiwara proposed a method of calculation of the detonation velocity under the assumption that the inert liquid acts only as a shock transmitter during the reaction [5]. The authors have also reported that their proposed mechanism was proven by the experimental results [5].

In order to quantify these observations, the detonation velocities of RDX in combination with ten non-explosive liquids were calculated using the EXPLO5 code (V6.05.04).

2 Results and Discussion

In order to quantify Urbanski's finding, we calculated high explosives with non-explosive liquids using the EXPLO5 code (V6.05.04) [6].

RDX which has a theoretical maximum density of 1.8 g cm^{-3} was used as a high explosive. The results for the calculation of the detonation velocities for TMD and ρ = 1.35 g cm^{-3} are shown in Table 1.

If we assume a density ($\rho = m/V$) of 1.35 g cm^{-3}, the volume that 100 g occupy is ($V = m/\rho = 100/1.35$ cm^3) 74.074 cm^3. Therefore, a 100 g sample of RDX with a density of 1.35 g cm^{-3} and a total volume of 74.074 cm^3 contains 99.978 g of "net" RDX having density 1.800 g cm^{-3} (TMD) and occupying 55.543 cm^3 and 0.022 g of air occupying 18.531 cm^3. A calculation of a mixture of 99.978 mass-% RDX and 0.022 mass-% air resulted in a density of 1.35 g cm^{-3} and a VoD of 7319 m s^{-1} which is practically identical (difference is only 4 m s^{-1}, or 0.055 %) to the calculation (ρ = 1.35 g cm^{-3}) in Table 1.

We now calculated the detonation velocities in the above mixture but replaced the 18.531 cm^3 with various liq-

Table 1. Calculated VoD for RDX with different densities.

ρ [g cm^{-3}]	VoD [m s^{-1}]
1.80 (TMD)	8798
1.35	7315

[a] *T. M. Klapötke*
Dept. of Chemistry, LMU Munich, 81337 Munich, Germany,
**e-mail: tmk@cup.uni-muenchen.de*
[b] *M. Suceska*
Sveuciliste u Zagrebu Rudarsko-geolosko-naftni fakultet, Zagreb, CROATIA,
**e-mail: msuceska@rgn.hr*

Table 2. Calculated VoD for RDX with different non explosive liquids.

Non-expl. liquid	Speed of sound in non-expl.liq. [m s^{-1}] [7–9]	Density of non-expl. liquid [g cm^{-3}]	Mass ratio, RDX/non-expl. liquid	Density of mixture [g cm^{-3}]	VoD [m s^{-1}]
air (gas)	343	0.0012	99.978/0.022	1.351	7314
CCl_4 (l)	926	1.59	77.238/22.762	1.600	7714
CH_3–OH (l)	1123	0.79	87.228/12.772	1.665	7430
H_2O (l)	1497	1.00	84.363/15.637	1.555	7861
glycerine (l)	1923	1.26	81.068/18.933	1.544	7806
kerosene (l)	1324	0.82	86.807/13.193	1.609	7441
acetone (l)	1161	0.79	87.228/12.772	1.572	7509
aniline (l)	1640	1.02	84.100/15.900	1.590	7531
benzene (l)	1298	0.88	85.977/14.023	1.612	7365
cyclohexanol (l)	1465	0.96	84.894/15.106	1.547	7578
ethylene glycol (l)	1660	1.20	81.805/18.195	1.600	7762

Table 3. Calculated sound velocities (C), shock wave velocities (particle velocity, U), and VoD for different non-explosive liquids.

Non-expl. liquid	Mass ratio, RDX/non-expl. liquid	Particle velocity, U [m s^{-1}]	Sound velocity, C [m s^{-1}]	VoD [m s^{-1}]
benzene (l)	85.977/14.023	1795	5570	7365
CH_3-OH (l)	87.228/12.772	1848	5582	7430
kerosene (l)	86.807/13.193	1794	5647	7441
acetone (l)	87.228/12.772	1862	5647	7509
aniline (l)	84.100/15.900	1803	5728	7531
cyclohexanol (l)	84.894/15.106	1810	5768	7578
CCl_4 (l)	77.238/22.762	1892	5822	7714
ethylene glycol (l)	81.805/18.195	1869	5893	7762
glycerine (l)	81.068/18.933	1894	5912	7806
H_2O (l)	84.363/15.637	1914	5947	7861

uids of different density and sound velocity [7]. The mass of RDX was unchanged (99.978 g). The results are summarized in Table 2.

As we can see from Tables 2 and 3, the final detonation velocity does not correlate well with the density of the mixture nor with the sound velocity of the added non-explosive liquid but correlates well with the sound velocity in detonation products at the CJ point (Figure 1), while the particle velocity in these mixtures with similar composition is relatively constant. This is nicely in accord with Urbanski's finding and the theory of Becker and Schmid which states that the VoD is equal to the sum of the speed of sound (C) and the particle velocity (U) (eq. 1). Our results also compare nicely with the study by Hikita and Fujiwara [5] (this study: 18.9% glycerine, VoD = 7806 m s^{-1}; Hikita and Fujiwara [5]: 20% glycerine, VoD = 7850 m s^{-1}). The fact that the RDX/air mixture still shows a relatively high VoD can be attributed to the high mass ratio of RDX, while the other non-explosive liquids do not contribute to the energy output (but in many cases, contributed to increased sound velocities).

In summary, pressing out the air of a high-explosive powder and replacing the voids with a non-explosive liquid such as ethylene glycol, water or glycerin may help to increase the final detonation velocity.

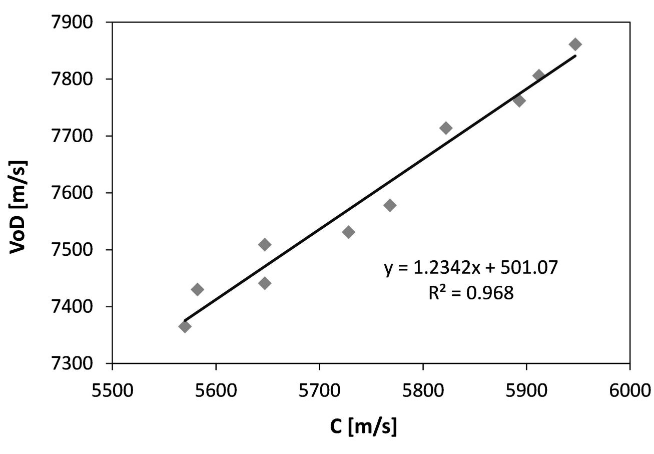

Figure 1. Correlation between the detonation velocity (VoD) and the sound velocity (C) in various mixtures (see Table 3).

Acknowledgement

Financial support of this work by Ludwig-Maximilian University (LMU), the Office of Naval Research (ONR) under grant no. ONR N00014-19-1-2078 and the Strategic Environmental Research and Development Program (SERDP) under contract no. W912HQ19C0033 are gratefully acknowledged. Open access funding enabled and organized by Projekt DEAL.

Data Availability Statement

No Data available.

References

[1] T. Urbanski, T. Galas, Sur la vitesse de détonation des mélanges d'explosifs solides avec des liquids non explosives, *Compt. Rend.* **1939**, *9th* October, 558–560.

[2] T. M. Klapötke, *Chemistry of High Energy Materials*, 5th edn., chapter 1.3, Walter de Gruyter, Berlin/Boston, **2019**.

[3] P. O. K. Krehl, Shock wave physics and detonation physics – a stimulus for the emergence of numerous new branches in science and engineering, *Eur. Phys. J. H* **2011**, *36*, 85–152.

[4] M. Suceska, *Test Methods for Explosives*, Springer, New York, **1995**.

[5] T. Hikita, S. Fujiwara, A Contribution to the Theory of Detonation of Solid Explosives Containing Inert Liquids, *Science and Technology of Energetic Materials*, **1968**, *29*, 432–437.

[6] M. Suceska, *EXPLO5-version V6.05.04*, OZM Research, **2020**, Czech Republic.

[7] http://hyperphysics.phy-astr.gsu.edu/hbase/Tables/Soundv.html (last accessed on October 14, 2020).

[8] https://www.engineeringtoolbox.com/sound-speed-liquids-d_715.html (last accessed on October 14, 2020).

Manuscript received: October 20, 2020
Revised manuscript received: December 7, 2020
Version of record online: January 27, 2021