Journal of Hazardous Materials 254–255 (2013) 214–220

Contents lists available at SciVerse ScienceDirect

Journal of Hazardous Materials

journal homepage: www.elsevier.com/locate/jhazmat

Studies on formation of unconfined detonable vapor cloud using explosive means

A. Apparao[a], C.R. Rao[b,*], S.P. Tewari[b]

[a] High Energy Materials Research Laboratory (HEMRL), Pune, India
[b] Advanced Centre of Research in High Energy Materials (ACRHEM), University of Hyderabad, Hyderabad, India

HIGHLIGHTS

- Parameters affecting explosive dispersion of propylene oxide in air was studied.
- Parameters studied are type of canister, nature and quantity of burster charge.
- Velocity of dispersion of fuel is found to be influenced by burster charge quantity.
- Theoretically estimated velocity of dispersion agrees with experimental values.
- The detonability of the fuel aerosols formed was tested.

ARTICLE INFO

Article history:
Received 22 July 2012
Received in revised form 7 December 2012
Accepted 26 February 2013
Available online 21 March 2013

Keywords:
Detonable aerosol
Propylene oxide
Ethylene oxide
Canister
Burster charge

ABSTRACT

Certain organic liquid fuels like hydrocarbons, hydrocarbon oxides, when dispersed in air in the form of small droplets, mix with surrounding atmosphere forming vapor cloud (aerosol) and acquire explosive properties. This paper describes the studies on establishment of conditions for dispersion of fuels in air using explosive means resulting in formation of detonable aerosols of propylene oxide and ethylene oxide. Burster charges based on different explosives were evaluated for the capability to disperse the fuels without causing ignition. Parameters like design of canister, burster tube, burster charge type, etc. have been studied based on dispersion experiments. The detonability of the aerosol formed by the optimized burster charge system was also tested.

1. Introduction

Certain organic liquid fuels like hydrocarbons, hydrocarbon oxides, when dispersed in air in the form of small droplets, mix with surrounding atmosphere, form vapor cloud (aerosol) and acquire explosive properties. The explodability of these aerosols depends upon the concentration of fuel in the aerosol, generally denoted by lower and upper explosive limits in air. The aerosols undergo detonation on suitable initiation by an external energy source and produce high temperature and high pressure gaseous products. Such situations can arise from the accidental release of fuels in storage, process or transport conditions resulting in severe consequences. These explodable fuel aerosols are also known as Fuel-Air-Explosives (FAE) which has found applications in military domain. The accurate modeling and estimation of conditions for formation and detonation of fuel aerosols are of extreme importance. Many researchers have studied the parameters affecting the formation of unconfined fuel aerosols and the initiation of the aerosol resulting in blast output [1–7]. The amenable conditions leading to explosive output are critically dependent on the characteristics of fuel – air cloud and the process by which the aerosol is formed. The formation of unconfined fuel aerosol, which depends on the structural aspects of fuel container (canister) and material properties of fuel and explosives, is complex phenomena and requires exhaustive experimentation.

Explosive means of fuel dispersion is the best suited for the purpose due to advantage of dispersing the fuel with extremely high speeds. However, it has got severe limitation of igniting the fuel because of the high energy associated with explosives and the flammable nature of the fuel. Hence, it is required to carry out in-depth study to establish the parameters of explosive charge vis-à-vis fuels for the formation of unconfined fuel aerosols without ignition. Fuel aerosols acquire explosive property, if the fuel vapor concentration is within the explosive limits of the particular fuel in air.

* Corresponding author. Tel.: +91 40 23134002; fax: +91 40 23012800.
E-mail addresses: vijaya_crr@yahoo.co.in, crrcs@uohyd.ernet.in (C.R. Rao).

0304-3894/$ – see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.jhazmat.2013.02.056

Table 1
Properties of propylene oxide and ethylene oxide [8,9].

Sl. no.	Property	Fuel	
		Propylene oxide	Ethylene oxide
1	Mol wt., g	58.08	44.05
2	Specific gravity (20 °C)	0.83	0.88
3	Boiling point, °C (1 atm)	34.2	10.4
4	Explosive limits, vol. %	2.3–37	3–100
5	Flash point, °C (open cup, ASTM method)	−37	<−18
6	Autoignition temp., °C (1 atm)	465	429
7	Heat of combustion (MJ/kg)	32.47	29.59

The explosives chosen for the study include Nitroguanidine (NQ), Trinitrotoluene (TNT) and RDX/wax (95/5). The fuel is filled in cylindrical container having a central tube. The explosive is filled in the central burster tube. The functioning of burster charge breaks open the container and disperses the fuel in air. The rate of fuel dispersion and the area coverage in terms of radius of aerosol were studied in the experiments by analyzing the video recordings of the dispersion events. The effect of burster charge to fuel weight ratio on velocities of fuel dispersion has been discussed and compared with that of theoretically estimated values. The details of the experiments to test the detonability of the aerosols are also presented in this paper.

2. Experimental

2.1. Materials/chemicals

Propylene oxide and ethylene oxide obtained from trade were selected and used as fuel in the study due to the wide range of explosive limits in air, high damage potential and high sensitivity to detonation [8,9]. The properties of propylene oxide and ethylene oxide are given in Table 1. Nitroguanidine, RDX/wax (95/5) and TNT were chosen for the preparation of burster charges on account of easy availability, well defined preparation methods and performance parameters. RDX/wax (95/5) was also selected as initiator charge for detonability tests.

2.2. Preparation of explosive charges

Nitroguanidine based burster charge is prepared by incremental filling method to achieve a uniform density of 410 kg/m^3. TNT is cast directly in the burster tube whereas RDX/wax (95/5) is used in the form of pellets. These pellets were made by pressing using a hydraulic press by applying a load of 1500 kg to have a pressed density of 1640 kg/m^3.

2.3. Canister and burster tube

Fuel container known as canister along with central burster tube is required for filling the fuel and fitment of burster charge respectively. The dispersion pattern of fuel is affected by the canister design. Ideally the canister should break open uniformly so that fuel is spread evenly around the central axis. Un-serrated and serrated canisters made of mild steel (MS) with dimensions $\phi 180 \times 225 \times 1.6$ mm with a provision for placing the central burster tube were selected for studying the fragmentation pattern. The serrated canister (Fig. 1) was provided with 24 equispaced vertical serrations of 0.6 mm thickness. The top and bottom lids of MS canister are of 1.6 mm thickness. Both the canisters are filled with water instead of fuel and fragmented with a central burster charge of 55 g NQ. Serrated canister was found to be suitable for fuel dispersion trials and the details are discussed in Section 3.1.

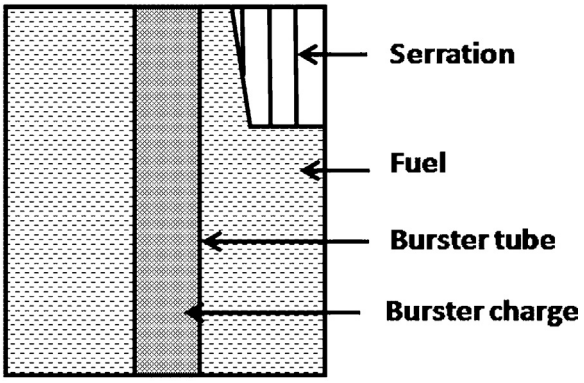

Fig. 1. Canister with burster charge.

2.4. Fuel dispersion trials

Serrated canisters were filled with fuel and different burster tubes of various diameters were used to accommodate various quantities of explosive burster charge. The experimental set-up is as shown in Fig. 2, is used for the fuel dispersion tests without using initiator. In these tests, the ignitability of the fuel and formation of unconfined aerosol were studied.

2.5. Detonation trials of unconfined aerosols

The optimised quantity of burster charge and fuel were used to form the unconfined aerosol and the aerosol was detonated by a separate initiator charge. The experimental set-up is shown in Fig. 2. The test parameters are as given below:

- Canister stand-off – 2.0 m
- Initiator stand-off – 2.1 m
- Separation between canister and booster – 0.5 m
- Initiator charge [RDX/wax (95/5)] – 200 g

The trial events were recorded using high speed digital video camera with a recording speed of 1000 frames per second. Wooden markers were positioned at either sides of the canister to measure the aerosol dimensions at different time intervals using video matrix system. Blast peak over pressures were measured using free field air blast transducers by placing at different distances from canister at a height of 2.0 m from ground.

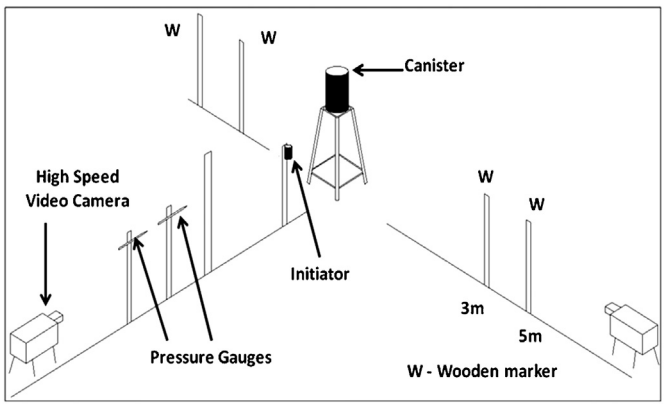

Fig. 2. Experimental set-up for aerosol formation and detonation.

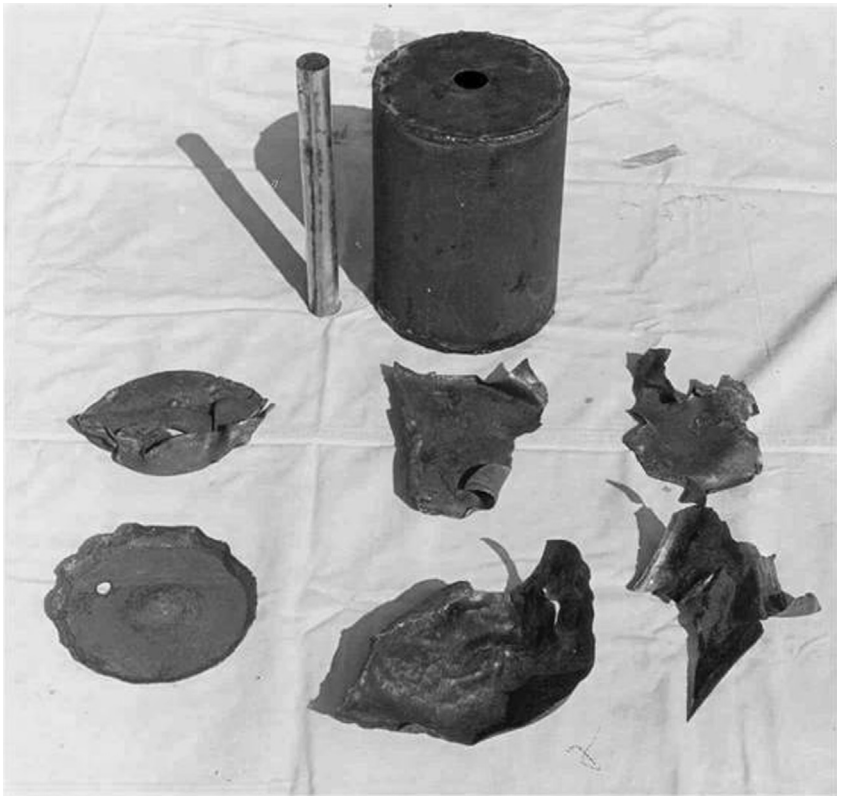

Fig. 3. Fragments obtained from breaking of un-serrated canister using NQ burster charge.

3. Results and discussion

3.1. Fragmentation pattern of serrated and un-serrated canisters

The fragments of water filled un-serrated and serrated canisters obtained with the burster charge of 55 g NQ were collected and analysed. It is found that unserrated canister was fragmented into six fragments of irregular shape (Fig. 3) whereas serrated canister produced more than ten regular rectangular fragments (Fig. 6). This indicates that uniform fuel dispersion is feasible with serrated canister and hence was used for fuel dispersion trials.

3.2. Dispersion of propylene oxide using different explosive charges

The results of experiments for the dispersion of propylene oxide fuel using burster charges based on different types of explosive charges, viz.; RDX/wax (95/5), TNT and NQ are given in Table 2. The quantity of burster charge and dimensions were chosen based on the critical diameter of the explosive and feasible method of processing. The radii of fuel dispersion w.r.t. time for different types of burster charges are given in Fig. 4.

Results of Table 2 indicate that the burster charges based on TNT and RDX/wax caused ignition of the fuel at the initial stages of dispersion and the remaining quantity of un-ignited fuel got dispersed but subsequently consumed in the expanding flame front. The ignition of fuel during dispersion can be attributed to the higher energetics of the explosives [10]. NQ with lower energetics and flashless nature had dispersed the fuel without causing ignition and formed aerosol as shown in Fig. 5. Based on the results, NQ was chosen as the explosive for burster charge in the further studies.

3.3. Effect of quantity of NQ as burster charge on canister fragmentation and dispersion of fuel

The fragmentation pattern of canisters with different quantities of NQ, viz., 30 g, 45 g, 55 g and 80 g have been analyzed and the fragments formed are shown in Fig. 6. The number of fragments formed using burster charge quantity less than 55 g were less and many fragments contained two to three serrations. Reasonably good fragmentation was observed with burster charge quantity of 55 g of NQ. For burster charge quantity of above 80 g, number of fragments is relatively more but with excess deformation in the fragments

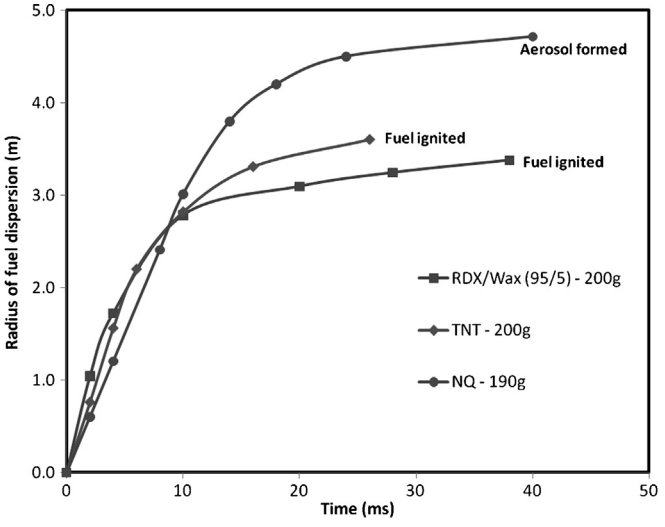

Fig. 4. Fuel dispersion pattern of 4.3 kg propylene oxide using RDX, TNT and NQ burster charges.

Table 2
Results of dispersion of propylene oxide fuel with different explosive charges. Canister: $\phi 180 \times 225 \times 1.6$ mm. Fuel: 4.3 ± 0.2 kg propylene oxide.

Sl. No.	Explosive	Burster charge			Observations
		Dimensions (mm)	Wt. (g)	Loading density (g/cc)	
1	Cast TNT	$\phi 28 \times 190$	200	1.63	Fuel ignited
2	RDX/wax (95/5)	$\phi 28 \times 190$	200	1.64	Fuel ignited
3	NQ	$\phi 58 \times 190$	290	0.41	Aerosol formed

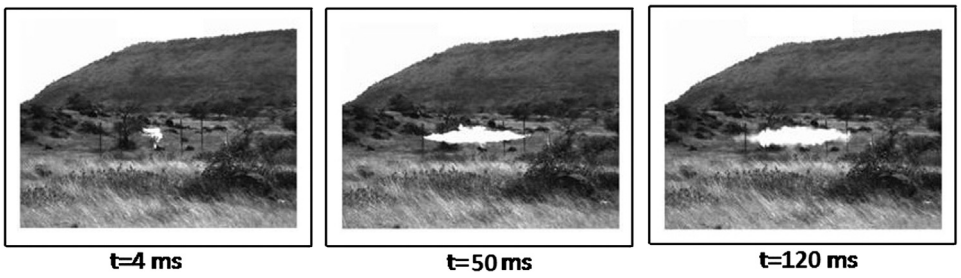

Fig. 5. Dispersion of 4.3 kg of propylene oxide fuel to form aerosol (Canister – $\phi 180 \times 225 \times 1.6$ mm, burster charge – 190 g NQ).

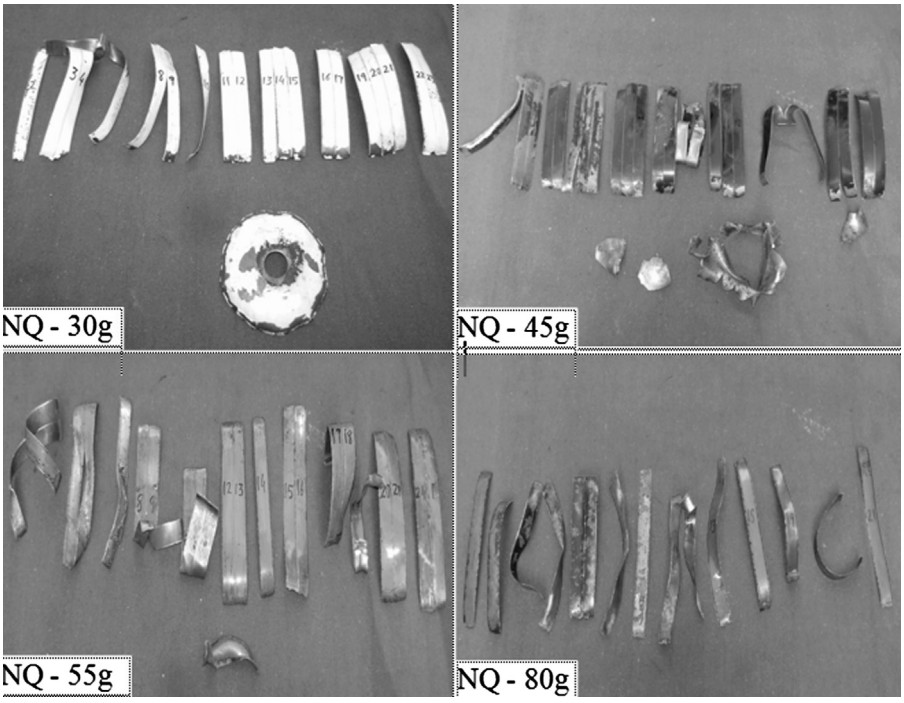

Fig. 6. Fragments obtained from breaking of serrated canisters for different quantities of NQ burster charge (Canister: $\phi 180 \times 225 \times 1.6$ mm, fuel: 4.3 ± 0.2 kg of propylene oxide).

indicating that the burster charge weight is higher than that required for optimum fragmentation.

The fuel dispersion pattern of propylene oxide (4.3 ± 0.2 kg) with different quantities of NQ using suitable burster tube have been presented in Fig. 7 in terms of radius of aerosol as a function of time. The increase in radius of aerosol formed with respect to time can be correlated with the forces acting on the fuel droplets as described by earlier researchers [11]. In the initial phase of dispersion, the explosive forces from the burster charge dominates resulting in break-up of fuel into small droplets and accelerates them thereby causing rapid vaporization of the fuel droplets. The initial spread of fuel in terms of radius is observed to be increasing with increase in weight of burster charge. For example, at 20 ms, the radii of the aerosol formed are 2.43, 2.72, 3.04, 3.50, 3.89, 3.95 and 4.30 m with 30, 45, 55, 80, 120, 150 and 190 g of NQ respectively.

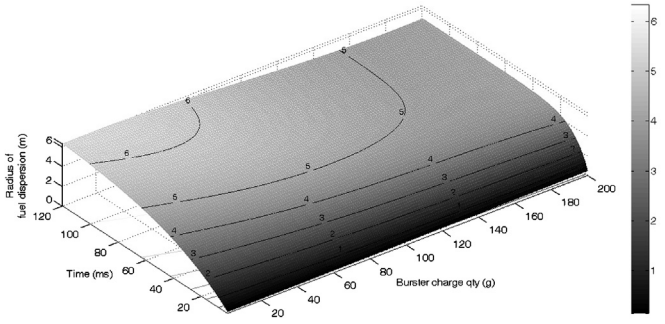

Fig. 7. Dispersion pattern of propylene oxide for different NQ burster charges (Canister: $\phi 180 \times 225 \times 1.6$ mm, fuel: 4.3 ± 0.2 kg of propylene oxide).

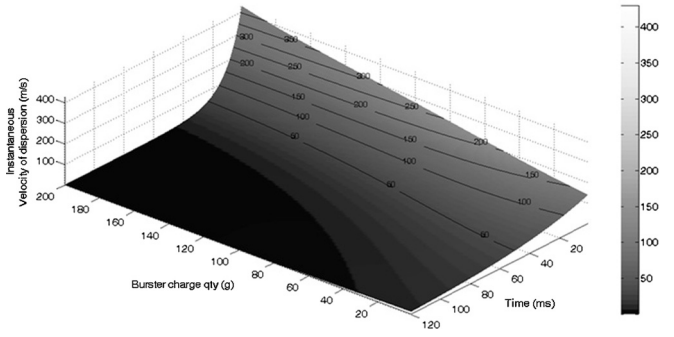

Fig. 8. Effect of NQ charge weight on velocity of dispersion of propylene oxide (Canister: $\phi 180 \times 225 \times 1.6$ mm, fuel: 4.3 ± 0.2 kg).

Further, there will be a transition phase where the explosive force on the fuel droplets is comparable to the aerodynamic forces acting on the fuel droplets. In the final phase, the aerodynamic drag forces predominate resulting in deceleration of the fuel droplets. Due to the higher aerodynamic forces acting on the speeding fuel droplets resulting from use of higher quantities of burster charge, the resultant radii of dispersion are relatively lower at 120 ms. In addition, video records indicate that the use of higher quantity of burster charge resulted in dilution of aerosol at distances near to canister as compared to that of farther distances probably due to excess dispersion velocity imparted to fuel droplets initially.

Based on the results of fuel dispersion and canister fragmentation, it is found that 55 g of NQ is suitable as burster charge for proper dispersion of fuel with reasonable number of fragments.

3.4. Effect of burster charge to fuel weight ratio on initial velocity of fuel dispersion

Analysis of the experimental data for propylene oxide fuel with varying quantities of burster charge showed that aerosol radius increases exponentially during the initial phase and the rate of growth decreases thereafter to follow an asymptote. Hence, the above behavior of cloud expansion can be represented by

$$r(t) = a(1 - e^{(-bt+ct^2)}) \quad (1)$$

where $r(t)$ – radius of aerosol at time, t and a, b and c are constants.

These constants have been calculated using the experimental data obtained with different weights of burster charge by using non-linear least squares method. The initial velocity of fuel dispersion is obtained by differentiating Eq. (1) and substituting $t = 0$. The velocity of fuel dispersion is given by Eq. (2)

$$V(t) = \frac{dr(t)}{dt} = -a(2ct - b)e^{(-bt+ct^2)} \quad (2)$$

The initial velocities of fuel dispersion with different quantities of burster charge are presented in Table 3. The results show that the initial velocity of fuel dispersion increases with increase in burster to fuel weight ratio. Moreover, for a given quantity of NQ, the velocity of fuel dispersion decreases with increase of time as is evident from the graphical representation of velocity of fuel dispersion with time (Fig. 8).

Similarly, limited fuel dispersion trials have been conducted with ethylene oxide (4.6 ± 0.1 kg) using different NQ burster charge weights, viz., 25 g, 55 g, 70 g and 95 g using the same experimental setup (Fig. 2). In these trials, it was observed that ethylene oxide fuel could be dispersed using NQ burster charge to form unconfined vapor cloud. The radii and velocities of fuel dispersion w.r.t. time for different weights of burster charge are shown in Fig. 9 and Fig. 10 respectively.

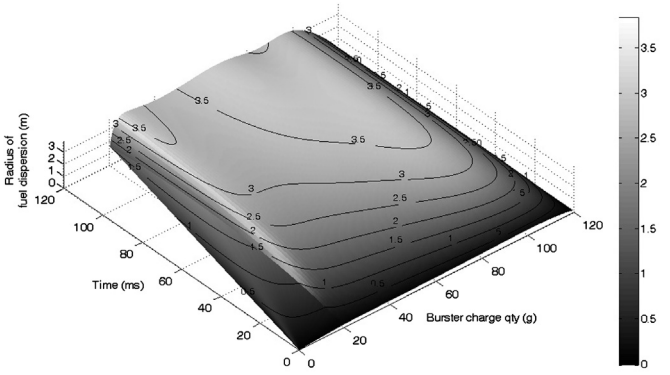

Fig. 9. Dispersion pattern of ethylene oxide for different quantities of NQ burster charges (Canister: $\phi 180 \times 225 \times 1.6$ mm, fuel: 4.6 ± 0.1 kg).

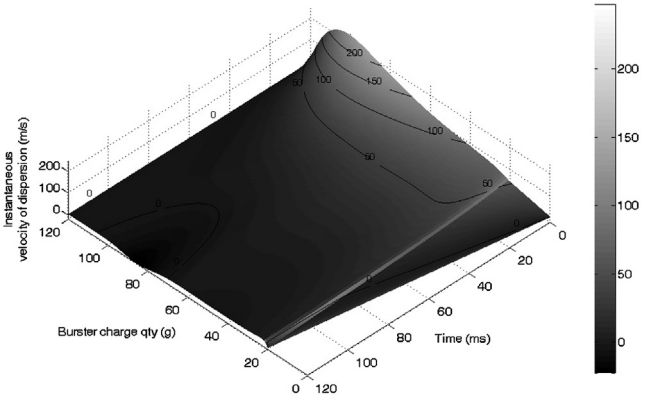

Fig. 10. Effect of NQ charge weight on velocity of dispersion of ethylene oxide (Canister: $\phi 180 \times 225 \times 1.6$ mm, fuel: 4.6 ± 0.1 kg).

The variation in radii of fuel dispersion and velocities of dispersion w.r.t. time for different quantities of burster charge have shown a similar trend as that of propylene oxide as explained in above paragraphs.

The initial velocities of fuel dispersion obtained using different burster charge quantities for propylene oxide and ethylene oxide are presented in Fig. 11. The results showed that the initial velocity of dispersion increased with increase in burster to fuel weight ratios for propylene oxide and ethylene oxide.

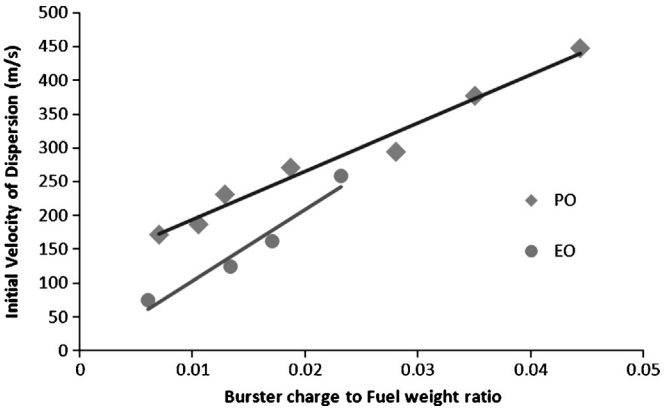

Fig. 11. Effect of burster charge to fuel weight ratio on the initial velocity of dispersion (Canister: $\phi 180 \times 225 \times 1.6$ mm, propylene oxide: 4.3 ± 0.2 kg, ethylene oxide: 4.6 ± 0.1 kg, burster charge: NQ).

Table 3
Comparative experimental and theoretical initial velocities of fuel dispersion for different NQ burster charges. Fuel: 4.3 ± 0.2 kg propylene oxide.

Sl. no.	Burster charge wt. (g)	Initial velocity of fuel dispersion (experimental) (m/s)	Theoretically calculated velocity (m/s)	
			Particle velocity	Plate velocity
1	30	171.77	97.05	191.45
2	45	186.96	110.72	225.10
3	55	230.89	118.11	243.79
4	80	270.75	133.12	282.74
5	120	293.98	151.27	331.62
6	150	376.92	162.17	361.90
7	190	447.77	174.47	396.87

3.5. Theoretical estimation of initial velocity of fuel dispersion

Assuming the behavior of propylene oxide similar to that of water, the initial velocity of dispersion of fuel due to burster charge detonation can be estimated by calculating the velocity of metallic plate of the fuel container by following the methods adopted in the case of underwater explosions and explosive working of metals [12,13]. The theoretical approach considers an infinite free metallic plate in a water medium subjected to explosive loading. The explosive shock travels through the liquid column, impacts on plate and gets reflected resulting in motion of the plate. The initial velocity of fuel dispersion is correlated with the initial plate velocity and particle velocity. Plate velocity is given by Eq. (3)

$$V_{plate}\ \ (\mathrm{m/s}) = \left[\frac{2P_m}{\rho_o C_o}\right](\beta^{1/(1-\beta)}), \tag{3}$$

where ρ_o is the density of the medium, 1000 kg/m^3; C_o is the velocity of sound in water, 1500 m/s; β is the $(\rho_o \cdot C_o \cdot \theta)/M$; M is the mass per unit area of plate, kg/m^2; P_m is the underwater shock pressure, kPa and is given as; $P_m = 72000\,[(q)^{1/2}/R]^{0.72}$, kPa; θ = time constant, s; $\theta = 10^{-4}(q)^{1/2}[R/(q)^{1/2}]^{0.45}$, s; R is the radius of canister, m; q is the weight per unit length of burster explosive, kg/m.

The particle velocity for shocks generated from different quantities of burster charges were computed using

$$P_m\ \ (\mathrm{kPa}) = \rho_o U_s U_p, \tag{4}$$

where U_p is the particle velocity, m/s; U_s is the shock velocity, m/s and is given as $U_s = a + b\,U_p$, m/s. a and b are constants. For water medium, $a = 1.647$, km/s and $b = 1.921$ [10].

The initial velocities of plate (fuel) velocity and the particle velocities were computed using Eqs. (3) and (4) and results are presented in Table 3. These values were compared with that of experimental initial velocities of dispersed fuel for different quantities of burster charge. As the resistance offered by burster tube and canister is negligible as compared to shock load, the value of initial velocity of fuel dispersion shall be in between the particle and plate velocities but closer to the plate velocity. The results of Table 3 indicate that the experimental values of initial velocities are comparable to that of plate velocity and higher than particle velocity for different quantities of burster charge. These minor differences in values can be attributed to the non-rigid nature of fuel droplets unlike metal plate. It can also be drawn from the results that the optimum weight of NQ burster charge lies between 55 g and 80 g as there was good agreement between experimental and theoretical values of velocities of dispersion.

3.6. Detonability of unconfined aerosols of ethylene oxide and propylene oxide

The detonability of the fuel aerosol formed using NQ burster charges for ethylene oxide (4.6 kg) and propylene oxide (4.3 kg) were evaluated by using experimental set-up shown in Fig. 2 and the recorded blast peak over pressures at 5 m and 7 m are given in Table 4. The results confirm the detonability of aerosols formed by dispersion of ethylene oxide and propylene oxide filled in serrated canisters using optimized quantity of NQ burster charge. Table 4.

Table 4
Comparative blast performances of ethylene oxide and propylene oxide using NQ based burster charges. Propylene oxide: 4.3 kg, ethylene oxide: 4.6 kg, burster charge: 55 g NQ, delay: 100 ms, initiator charge: 100 g RDX/wax.

Sl. No.	Fuel	Blast POP (kPa)	
		5 m	7 m
1	Ethylene oxide	248.2	145.2
2	Propylene oxide	150.1	64.8

The results of the study provide useful inputs for risk assessment and hazard analysis relevant to process or storage of similar class of fuels capable of forming detonable aerosols on release into atmosphere.

4. Conclusions

Serrated canister is found to fragment in a controlled manner facilitating uniform dispersion of fuel. Nitroguanidine (NQ) was found suitable for use as burster charge for dispersion and aerosol formation of propylene oxide and ethylene oxide for a wide range of explosive weight. The initial velocities of dispersed fuel increased with increase in burster charge to fuel weight ratio and are in good agreement with the theoretically estimated values. Based on the fuel dispersion and fragmentation pattern of canisters, 55 g of NQ burster charge was found optimum for use as burster charge for dispersion of 4.3 kg of propylene oxide. The aerosols of propylene oxide and ethylene oxide formed from serrated canisters using optimised burster charge were found to be detonable when suitably initiated at preset delay.

Acknowledgements

The authors are grateful to Director, HEMRL, Pune for his keen interest and encouragement throughout the course of this study. The support and help extended by Shri A.K. Vishwakarma, Dr. J. Saji and other members of FAE Division, HEMRL and ACRHEM, University of Hyderabad are also duly acknowledged.

References

[1] Z. Qi, W. Kezhen, L. Aimin, W. Denggui, Q. Bin, Numerical simulation on dispersal character of fuel by central HE, Def. Sci. J. 57 (4) (2007) 425–433.
[2] O.B. Kudryashova, B.I. Voroshtsov, E.G. Muravlev, I.R. Akhmadeev, A.A. Pavlenko, S.S. Titov, Physicomathematical modeling of explosive dispersion of liquid and powders, Propellants Explos. Pyrotechnol. 36 (2011) 524–529.
[3] G. Liu, F. Hou, B. Cao, L. Xie, Zh. Shen, T. Zhou, Experimental study of fuel air explosive, Comb. Expl. Shock Waves 44 (2) (2008) 213–217.
[4] Y. Dong, H. Li, H. Shi, I. Yi, Study of FAE explosive image analysis based on the fractional dimension, J. Math. Res. 1 (1) (2009) 102–107.
[5] L. Li, X. Ren, X. Lu, X. Yan, On the characteristics of liquid explosive dispersing flow, http://www.waset.org/journals/waset/v69/v69-109.pdf (accessed 21.07.11).

[6] L. Li, J. Cui, Y.C. Dong, Experimental investigations to the interfaces breakup during liquid explosive disseminations process, Chin. Sci. Bull. 54 (12) (2009) 1693–1700.
[7] F.D. Alonso, E.G. Ferrad, J.F.S. Perez, A.M. Aznar, J.R. Gimeno, J.M. Alonso, Characteristic overpressure–impulse–distance curves for vapor cloud explosions using the TNO multi-energy model, J. Hazard. Mater. A137 (2006) 734–741.
[8] R.O. Kirk, T. John Dempsey, Kirk-Othmer Encyclopedia of Chemical Technology, John Wiley and Sons Inc., New York, 1980.
[9] J.N. Cawse, J.P. Henry, M.W. Swartzlander, P.H. Wadia, Kirk-Othmer Encyclopedia of Chemical Technology, John Wiley and Sons Inc., New York, 1980.
[10] P.W. Cooper, Explosives Engineering, VCH Publishers, USA, 1996.
[11] D.R. Gardner, Near-Field Dispersal Modeling for Liquid Fuel-Air-Explosives, Report SAND90-0686, Sandia National Laboratories, New Mexico, USA, 1990.
[12] R.H. Cole, Underwater Explosions, Princeton University Press, New Jersey, 1948.
[13] J.S. Rinehart, J. Pearson, Explosive Working of Metals, Pergamon Press, London, 1963.