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Effect of Temperature, Density and Confinement on Deflagration to Detonation Transition of an HMX-Based Explosive

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Abstract: In order to obtain the characteristics of the deflagration-to-detonation transition (DDT) of PBX-2 (an HMX-based explosive) under different conditions, DDT tests were carried out as a function of charge density, temperature, and shell confinement. In these tests, the energetic materials were electrically ignited. The DDT response characteristics for PBX-2 with 53% and 99% of theoretical maximum density (TMD) were evaluated by different shell thickness confinements at ambient temperature and at 85 °C. The test results with different densities, confinements and temperatures exhibited a wide range of reaction violence. Firstly, at both ambient temperature and at 85 °C under 10 and 20 mm shell thickness confinement, PBX-2 did not undergo fully DDT at 99% TMD, only a low velocity detonation (LVD) occurred. Secondly, PBX-2 at 53% TMD underwent DDT, and significant influence on the minimum run distance to detonation by the shell confinement thickness was observed. Strong confinement is favorable for the transition of DDT but the confinement does not influence reaction degree. Thirdly, the reaction degree of PBX-2 at 85 °C was remarkably lower than that at ambient temperature. This insensitizing effect of temperature is induced by the melting and flowing of bonders which reduces the porosity and inhibits an important step of DDT, namely, high turbulent combustion.

Keywords: Explosion mechanisms · Explosive safety · Deflagration to Detonation Transition · HMX-based explosives

1 Introduction

The DDT (deflagration-to-detonation transition) test is an important method to evaluate the safety performance of explosives and can provide accurate evidence for safety estimation of explosives charge. In the past two decades, a lot of experimental and computational DDT investigations on explosives were carried out [1–9]. Bernecker and Price [1] studied the DDT behavior of 95/5 TNT/Wax to describe the sequence of events in confined burning of explosives that followed. Leuret et al. [4] investigated the DDT behavior of HMX 96% + polymer 4% formulation under high density of 1.823 $g\,cm^{-3}$ and low porosity rates (> 98% TMD) conditions. Recently, studies on the DDT characteristics of granulated HMX and RDX continue, some of which have given sufficient conditions of DDT [1, 5–7, 10–12]. Additional researches [5–7] demonstrated that DDT phenomena are highly dependent on the confinement and the scale of the sample.

Explosives may react severely when subjected to thermal environment heating conditions during transportation or operation. However, most current investigations mainly focus on DDT safety under the ambient temperature; research at varying temperatures is still very limited. Sandusky et al. [13] studied the temperature effect on DDT of HMX, concerning the temperatures of ambient, 160 °C (just below the temperature of pure HMX phase transition), and 190 °C (just above the temperature of pure HMX phase transition), but a wide range of temperature from 30–160 °C were not explored yet.

On the other hand, it is generally considered that DDT safety performance will get worse (namely DDT is easier to occur) with the increase of temperature. However, DDT response may be more complex because the thermal decomposition properties can be distinct at different temperatures. The result of Sandusky et al. [13] (51.3% TMD LX-04 did not lead to detonation at 160 °C, but did at 190 °C and at ambient temperature) is not sufficient to draw a persuasive conclusion because the lacking of data of 30–160 °C.

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Therefore, the DDT safety performance at different temperatures (e.g. 85 °C, which is close to the phase transition temperature of binders in PBX-2) remains to be studied.

In this paper, the safety performance of HMX-based PBX (named as PBX-2, with a rough formulation of 85–90 wt.-% HMX + 3–8 wt.-% TATB + a few binders + other components [14]) was investigated under thermal-confinement combined environment. The DDT characteristics of PBX-2 at ambient temperature and 85 °C as well as the transition conditions were obtained by DDT tests. Scanning electron microscopy (SEM) was used to observe the unreacted explosive. The low velocity detonation (LVD) phenomenon of PBX-2 was also observed in this work. According to our result, it was found that the DDT safety performance will be improved to some extent in certain heating ranges because of different response mechanisms.

2 Experimental Section

2.1 Test Principle

A cylindrical PBX-2 sample was confined in a DDT pipe and ignited by an electric igniter. The combustion wave was then formed inside the pipe and spread in the PBX. The combustion wave translated into the detonation wave under certain conditions. The running time and distance of combustion wave were measured to calculate the running velocity. The reaction degrees were judged by the running velocities and the wreckages of DDT pipes.

2.2 Test Devices

The schematic diagram and photograph of the DDT installation are shown in Figure 1. The test installation mainly included a DDT pipe, an electric igniter, a cylindrical explosive PBX and some electro-ionization probes. In high temperature tests, the electric thermo-couple and heating bands were installed. The DDT pipe was built from a steel cylindrical tube with a diameter of 30 mm.

During the test processes, the velocities of the reaction wave fronts were measured by the electro-ionization probes which were fixed at different locations in a line along the axial direction of PBX sample. The distance between two adjacent probes was 25 mm, see Figure 1. Hence the distance and time of DDT or slow reaction waves could be obtained and the reaction degrees could be estimated by the results. The temperature variations were measured by electric thermocouples.

2.3 Samples and Experimental Conditions

Information on samples and experimental conditions is listed in Table 1.

Table 1. The parameters of PBX-2 DDT tests.

Sample	density [$g\,cm^{-3}$]	Temperature [°C]	Confinement shell thickness [mm]
PBX-2	1.0 (approx. 53% TMD)	ambient	3
			13
	1.85 (approx. 99% TMD)	ambient	10
		85	10
		ambient	20
		85	20

3 Results and Discussion

3.1 Low Density (53% TMD) DDT Tests: Strong Confinement Shortens the Run Distance to Detonation

The DDT test results of low density (53% TMD) PBX-2 at ambient temperature are shown in Table 2. Under the confinement thickness of 3 mm, the minimum run distance from deflagration to detonation was approximately 170 mm and the stable detonation velocity was about 5.9 mm μs^{-1}. In contrast, under the confinement of 13 mm, the minimum run distance to detonation was approximately 90 mm and the stable detonation velocity was about

Table 2. Data measured for PBX-2 at approx. 53% TMD in DDT test.

Density [$g\,cm^{-3}$]	Temperature [°C]	Confinement thickness [mm]	Stable detonation velocity [$mm\,\mu s^{-1}$]	Run distance to detonation [mm]
1.0	ambient	3	5.9	170
		13	5.7	90

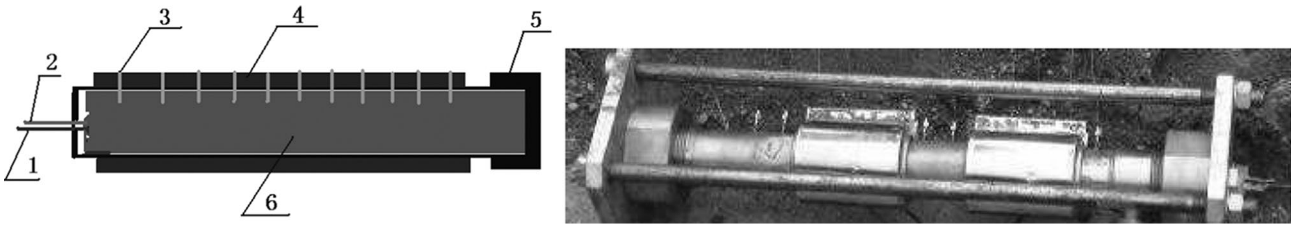


Figure 1. Diagram and photograph of DDT installation under heating. 1-Thermocouple, 2-igniter, 3-probes, 4-heating belt, 5-steel shell, 6-explosive sample.

Table 3. Data measured for PBX-2 at approx. 99% TMD in DDT test.

Density [$g\,cm^{-3}$]	Temperature [°C]	Confinement shell thickness [mm]	Running velocity [$mm\,\mu s^{-1}$]	Run distance to reaction [mm]	Reaction degree
1.85	ambient	10	4.3	400	LVD
	85		3.0	175	Deflagration
	ambient	20	4.2	400	LVD
	85		3.7	275	Deflagration

5.7 $mm\,\mu s^{-1}$. The shockwaves velocities were both high enough and stable, implying DDT occurred. The results also indicate that the thickness of the confinement has obvious effect on the minimum run distance to detonation. In low densities DDT tests, the DDT is easier to occur under stronger confinement, but the stable detonation velocities (5.9 and 5.7 $mm\,\mu s^{-1}$) show no obvious differences. In other words, the shell confinement thickness does not affect the reaction degree.

3.2 High Density (99% TMD) DDT Tests: High Density/Low Porosity Inhibits the Propagation of High Turbulent Combustion

The DDT test results of 1.85 $g\,cm^{-3}$ (99% TMD) PBX-2 under various conditions are shown in Table 3. The reaction spreading velocities before the fracture of the DDT pipes heated or unheated are both less than the detonation velocity (about 8.7 $mm\,\mu s^{-1}$ [14] at a density of 1.85 $g\,cm^{-3}$) that ignited by a detonator. So we can jump to a conclusion that DDT didn't occur in 1.85 $g\,cm^{-3}$ PBX-2, and what we observed in the tests is called LVD (low velocity detonation) phenomenon [1].

In fact, LVD can be observed during the DDT processes of gases, liquid explosives, powder explosives and even high density explosives [4,15–17]. Unstable compression shockwaves were generated by thermal ignition and combustion of explosive. The shockwaves lead to the breakage of the PBX structure and formation of cracks in the unreacted explosive [1,4]. The energy released from the combustion sustains the propagating of the unstable compression shockwaves. When the energy released and shockwave propagating reaches a balance state, the compression shockwave can propagate forwards steadily at a constant velocity [1,4]. Because of the changing of the shape and the crack of the pipe, the shape of the compression shockwave is unstable. Under the compression of the shockwave, the explosive is squeezed, sheared and crushed to make the combustion waves easier to spread through. Thus a stable mechanism of crushing-combustion-shockwave propagating comes into being. When this steadily propagating "LVD" phenomenon is disturbed by defects such as cracks and fractures in explosive, the balance of this "LVD" state will be broken very soon and DDT occurs consequently [1,4].

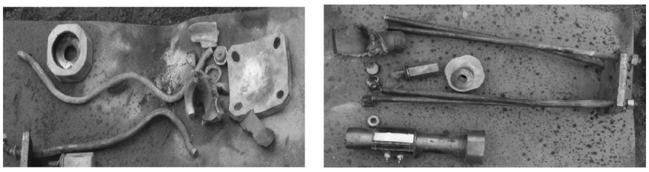
The results show that fully DDT did not occur in 99% TMD density explosive. In terms of low density explosive, after ignition, the reaction enters the stage of high turbulent combustion in which the reaction products of high temperature and high pressure transfer energy to the unreacted explosive by convection. Accumulation of reaction products results in higher and higher pressure, leading to the acceleration of high turbulent combustion [1,4,13]. In a weak confinement condition this acceleration will lead to a more unstable combustion processes. In a strong confinement condition, the acceleration will lead to a sharp rise in pressure and finally to a DDT process if the high turbulent combustion is not inhabited. In terms of high density explosive high turbulent combustion cannot take place as a result of the short number of holes and interspace in PBX, namely, a lower porosity is not beneficial to high turbulent combustion. The combustion area is quite small so that the generating rate of gases and energy release rate are both limited. As a result, the pressure condition is not sufficient for DDT to occur.

On the other hand, high density explosive needs higher shock ignition pressure than low density ones. Reaction will turn into detonation only when the pressure generated in the combustion zone is equivalent to the critical pressure. The DDT process of high density explosive has one more stage of materials breakage and formation of gaps, which give the explosive the property and performance like polyporous explosives. After this extra stage, the subsequent DDT process is just similar to the DDT process of low density explosive.

The shock ignition pressure for high density HMX-based PBX is higher than 1 GPa, and the strength of the 20 mm DDT pipes is about 0.4 GPa. As a result, our high density tests resulted in pipes breakage rather than DDT.

3.3 Temperature Effect on DDT Reaction Degree

Table 3 also tells that in 10 mm tests, the stable running velocity is about 4.3 $mm\,\mu s^{-1}$ at ambient temperature. When the temperature of the explosive is heated to 85 °C, the stable running velocity reduces to 3.0 $mm\,\mu s^{-1}$. In 20 mm tests, the stable running velocity is about 4.2 $mm\,\mu s^{-1}$ at ambient temperature. When the temperature of explosive is heated to 85 °C, the stable running velocity reduces to 3.7 $mm\,\mu s^{-1}$. These results obviously show that the reaction degree of PBX-2 heated to 85 °C is much lower than that at



a. ambient b.85°C

Figure 2. Photographs of recover wreckages of PBX-2 and confinements at approx. 99 % TMD.

ambient temperature in both 10 mm and 20 mm confinement tests.

The observation of the recover wreckages of PBX-2 and confinements, presented in Figure 2, supports the typical DDT behavior of 10 mm shell confinement. At ambient temperature the DDT pipe was torn into large pieces and some indents appeared on the surface of the witness board, with the entire sample consumed, indicating a violent reaction. At 85 °C after the test the front section of the pipe broke while the middle and tail sections remained unchanged, with large amount of PBX-2 remained, indicating a much less violent reaction. So it is obviously that the rising of the temperature from ambient temperature to 85 °C can reduce the DDT reaction degree if other conditions keep the same. The reason might be the changing of the porosity while the temperature rises.

In order to find out the answer, the samples at ambient temperature and from 75–85 °C were compared by scanning electron microscopy (SEM) [15]. The mechanical performances under different temperatures were also studied. The data of the tension, compression modulus and tensile strength under various temperatures are given by Dari et al. [15]. The tensile strength of PBX-2 is reducing with the rising of temperature, which is no more than 0.2 MPa above 85 °C. Both the tension modulus and compression modulus of PBX-2 have the same trend with the tensile strength. The lower modulus and tensile strength make it much easier to transform or extend and behavior as viscous flow almost without strength. This viscous flow property is attributed to the low phase transition temperature of binders in PBX-2 which is much close to 85 °C [14]. The original holes and the interfaces of the grains in PBX-2 can be filled due to that viscous flow property, leading to a lower porosity.

The SEM pictures of PBX-2 at ambient temperature and at 75 °C were also previously presented [15]. From the SEM pictures we can see that the holes in the unheated PBX-2 are clear-cut and the grains of explosive are wrapped by binder. The interfaces of the grains and the binder are quite clear. When the explosive is heated to 75 or 85 °C, flow occurs obviously in the binder due to the viscous flow property of PBX-2, and the original holes of explosive are filled. As a result, the interfaces of the grains and the binder mix together and are almost not recognizable. Compare to unheated explosive, the PBX-2 heated to 85 °C is unlikely to produce high turbulent combustion due to the absence of original holes and low porosity. So the area of combustion is relatively less and the gases generating rate and energy release rate are both limited. Hence the relatively higher rate of pressure increase, which is needed by DDT is not provided. The pressure generated in the combustion area is unable to maintain its spreading forward. When the generated pressure is higher than the strength of DDT pipe confinement, the pipe will break, leading to a time advance of the 85 °C PBX-2 than the unheated PBX-2. Therefore, in the DDT test, the PBX-2 reaction degree at 85 °C is lower than that at ambient temperature.

4 Conclusions

Our tests exhibited a wide range of reaction violence including DDT, LVD, and Deflagration. PBX-2 at approx. 53 % TMD undergoes DDT, and there is significant influence on the minimum run distance to detonation by the shell confinement thickness. Strong confinement is favorable for DDT but it does not affect the reaction degree.

PBX-2 does not undergo DDT at approx. 99 % TMD, although it still results in a low velocity detonation. There is also no influence on reaction degree by the shell confinement thickness in high density tests. DDT did not occur in high density explosive because the high density or low porosity inhibits the propagation of high turbulent combustion.

The reaction degree of PBX-2 heated to 85 °C is remarkably lower than that of ambient temperature in both 10 mm and 20 mm confinement tests. The mount of porous beds for PBX-2 at 85 °C is less than at ambient temperature. The original holes and the interfaces of the grains in PBX-2 can be filled due to the viscous flow property at 85 °C whereas the binders melts and flows, leading to a lower porosity. This lower porosity inhibits the propagation of high turbulent combustion.

The results of tests with approx. 53 % and approx. 99 % TMD show that most porous beds in high confinement is favorable for DDT. The existence of sufficient space that high turbulent combustion needs is one of the reasons.

References

[1] R. R. Bernecker, D. Price, Studies in the Transition from Deflagration to Detonation in Granular Explosives – I. Experimental Arrangement and Behavior of Explosives which Fail to Exhibit Detonation, *Combust. Flame* **1974**, *22*, 111.

[2] Q. M. Liu, C. H. Bai, J. Li, W. X. Dai, Deflagration-to-Detonation Transition in Nitromethane Mist/Aluminum Dust/Air Mixtures, *Combust. Flame* **2010**, *157*, 106.

[3] M. R. Baer, R. J. Gross, J. W. Nunziato, E. A. Igel, An Experimental and Theoretical Study of Deflagration-to-Detonation Transition (DDT) in the Granular Explosive, CP, *Combust. Flame* **1986**, *65*, 15.

[4] F. Leuret, F. Chaissé, H. N. Presles, B. Veyssière, Experimental Study of the Low Velocity Detonation Regime During the Deflagration-to-Detonation Transition in a High Density Explosive, *11th Symposium (International) on Detonation*, Snowmass Village, CO, USA, August 31–September 4, **1998**, p. 693.
[5] R. Verbeek, A. C. van der Steen, E. de Jong, The Influence of Parameter Variations on the Deflagration-to-Detonation Transition, *10th Symposium (International) on Detonation*, Boston, MA, USA, July 12–16, **1993**, p. 685.
[6] B. W. Asay, J. M. McAfee, Temperature Effects on Failure Thickness and the Deflagration-to-Detonation Transition in PBX9502 and TATB, *10th Symposium (International) on Detonation*, Boston, MA, USA, July 12–16, **1993**, p. 485.
[7] P. E. Luebcke, P. M. Dickson, J. E. Field, Experimental Investigation into the Deflagration-to-Detonation Transition in Secondary Explosives, *10th Symposium (International) on Detonation*, Boston, MA, USA, July 12–16, **1993**, p. 242.
[8] J. R. Peterson, C. A. Wight, An Eulerian–Lagrangian Computational Model for Deflagration and Detonation of High Explosives, *Combust. Flame* **2012**, *159*, p. 2491.
[9] D. A. Kessler, V. N. Gamezo, E. S. Oran, Simulations of Flame Acceleration and Deflagration-to-Detonation Transitions in Methane–Air Systems, *Combust. Flame* **2010**, *157*, 2063.
[10] T. H. Zhao, X. Y. Zhang, B. Li, Experimental Study on the Deflagration-to-Detonation Transition for Granular HMX, RDX, *Chin. J. Energ. Mater.* **2003**, *11*, 187.
[11] T. H. Zhao, S. Q. Zhang, X. Y. Zhang, An Experimental Study of the Effects of DDT Tube Materials on the Deflagration-to-Detonation Transition in Granular RDX Bed, *Chin. J. High-Pressure Phys.* **2000**, *14*, 99.
[12] Y. M. Huang, C. G. Feng, X. P. Long, Deflagration to Detonation Transition Behavior of Explosive JOB-9003, *Chin. J. Explos. Propellants*. **2002**, *24*, 54.
[13] H. W. Sandusky, R. H. Granholm, D. G. Bohl, K. S. Vandersall, D. E. Hare, F. Garcia, Deflagration to Detonation Transition in Lx-04 as a Function of Loading Density, Temperature, and Confinement, *13th Symposium (International) on Detonation*, Norfolk, VA, USA, July 23–28, **2006**, p. 920.
[14] H. S. Dong, F. F. Zhou, *Properties of High Explosives and their Relatives*, Science Press, Beijing, **1989**, p. 380.
[15] X. G. Dai, Y. S. Wen, H. Huang, P. J. Zhang, M. P. Wen, Impact Response Characteristics of a Cyclotetramethylene Tetranitramine-Based Polymer-Bonded Explosives under Different Temperature, *J. Appl. Phys.* **2013**, *114*, 114906.
[16] V. I. Manzhalei, Low-Velocity Detonation Limits of Gaseous Mixtures, *Combust. Explos. Shock Waves.* **1999**, *35*, 296.
[17] R. F. Chaiken, Mechanism of Low-Velocity Detonation in Liquid Explosives, *Appl. Mech. Rev.* **1972**, *17*, 575.

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