Effect of Pore in Composition-B Explosive on Sensitivity under Impact of Drop Weight

Qi Zhang\*, Shaoqiao Hu, and Huimin Liang

State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology, Beijing-100081, China \*E-mail: qzhang090417@126.com

#### ABSTRACT

Experiment impacting explosive sample with a drop weight is a standard approach in China. Pores in explosive have a significant effect on its sensitivity under impact of a drop weight. In the experiments impacting explosive samples with a drop weight, it is difficult to observe the dynamic responding and igniting process around a pore by using a measurement approach. This work developed an approach to predict the effect of pore in explosive on sensitivity under impact with drop weight. The effect of pore in composition-B explosive on the sensitivity under impact with a drop weight was investigated by using numeral simulation in this work. Through a series of numerical calculation, it was found that when the sizes of pore in composition-B explosive are less than 0.3 mm, its effect on sensitivity under impact of a drop weight can be ignored. This result agrees with the experimental data.

Keywords: Safety performance of explosive, impact sensitivity, drop weight, launch process, numerical simulation

#### 1. INTRODUCTION

Detonation in condensed explosives has been important to the scientific community for many decades, and there have been numerous publications on theoretical, experimental, and numerical investigations<sup>1,2</sup>. Detonations in solid explosives are believed to be facilitated by the presence of defects, known as 'hot spots,' because of enhanced chemical reactivity when a shock wave passes over and possibly interacts strongly with them<sup>3</sup>.

Experiment impacting explosive sample with a drop weight is a standard approach in China. Pores in explosive have a significant effect on its sensitivity under impact of a drop weight. The sensitivity under impact of a drop weight here is referred as the probability initiating explosion. It is used to examine safety performance of explosive charged in a warhead under launching process<sup>4,5</sup>. In the experiments impacting explosive samples with a drop weight, it is difficult to observe the dynamic responding and igniting process of pore. The effect of pore in Composition B explosive on the sensitivity under impact with a drop weight was investigated in this work by using numerical simulation.

Under impact of drop weight, the pore deforms and the local temperature around the pore increases. This process is commonly called into hot spot growth. About shock initiation and ignition models, there are a large number of document reports<sup>6-8</sup>. Tran and Udaykumar performed simulation of void collapse in an energetic material<sup>9</sup>. Tarver, *et al.* estimated critical hot spot to initiate detonation for HMX and TATB<sup>10</sup>.

Compared with shock initiation, the load generated by drop weight is less and the action duration is longer. Therefore, the ignition model used in shock initiation should be revised to carry out numerical simulation on initiation explosion in explosive under impact from a drop weight. The result obtained in study of shock initiation cannot used to understand the phenomenon initiating explosion of explosive sample under impact from a drop weight. The process initiating explosion around pore in explosive under impact from a drop weight was simulated by using numerical method to examine the factors and condition affecting ignition in this work. Mechanical impacts are a main cause of ignition of explosive atmospheres in the industry<sup>11</sup>. This research can be applied to estimate the risk of ignition of explosive under impact with other drop weights instead of conduct of experiments also.

### 2. NUMERICAL MODEL

#### 2.1 Geometry

The geometry for calculation is shown in Fig.1. The 40 mm diameter by 40 mm long explosive cylinder is charged in a shell made of steel, shown in Fig.1. When a weight at a height drops the explosive cylinder will be impacted. The load strength depends on the weight and its drop height. The mass of drop weights commonly used in the experiments are 200 kg and 400 kg respectively.

### 2.2 Material Model and Parameters

A 5 mm thick PMMA shim was placed on the top end of the explosive cylinder. The material density for PMMA was 1.18 g/cm<sup>3</sup> and its shear modulus and yield strength were 1.5 GPa and 0.5 GPa respectively.

Received 01 January 2012, revised 20 December 2012, online published 24 January 2013



Figure 1. Schematic of geometry for calculation.

For PMMA shim, Mie-Gruneisen equation of state was used in the numerical simulation:

$$p = \frac{\rho_0 C^2 \mu \left[ 1 + \left( 1 - \frac{v_0}{2} \right) \mu - \frac{a}{2} \mu^2 \right]}{\left[ 1 - (S_1 - 1) \mu + S_2 \frac{\mu^2}{\mu + 1} - S_3 \frac{\mu^3}{(\mu + 1)^2} \right]^2} + (\gamma_0 + a\mu) E_T$$
(1)

where  $\mu = \rho / \rho_0 - 1$ ;  $\rho$  and  $\rho_0$  are the current and initial densities of material respectively;  $E_{\rm T}$  is the thermal energy,  $C_s S_1, S_2, S_3$ ,  $\gamma_0$ , and *a* are the constants listed in Table 1.

The drop weight and the shell were made of gun steel. For gun steel, Plastic-Kinematic model was used in this numerical simulation:

$$\sigma_{y} = \left[1 + \left(\frac{\dot{\varepsilon}}{C_{s}}\right)^{\frac{1}{P}}\right] \left(\sigma_{0} + \beta E_{P} \varepsilon_{P}^{eff}\right)$$
(2)

where  $\sigma_0$  is the yield stress;  $\dot{\varepsilon}$  is the stain rate; *C* and *P* are the parameters for strain ratio;  $\varepsilon_P^{eff}$  is the effective plastic strain;  $E_P$  is the plastic hardened modulus.

$$E_P = \frac{E_{\rm tan}E}{E - E_{\rm tan}} \tag{3}$$

where *E* is the elastic modulus,  $E_{tan}$  is the tangent modulus. Because the effect of  $\dot{\epsilon}$  was ignored in this numerical simulation *C* and *P* were taken as the omitted values.

Table 1. Gruneisen equation of state parameters for PMMA

$ ho_0$ , gcm <sup>-3</sup>	C, cm	$\mathbf{S}_{1}$	$\mathbf{S}_2$	$S_3$	$\gamma_0$	a
1.18	0.25661	1.595	0	0	1.000	0

Table 2. Material parameters for gun steel

$ ho_0$ , gcm <sup>-3</sup>	E/100GPa	Poisson's ratio	Yield stress/100GPa	E <sub>tan</sub> /100GPa
7.83	2.1	0.284	0.0053	0.1

The ignition and growth reactive flow model uses two Jones–Wilkins–Lee (JWL) equations of state, one for the un-reacted explosive and one for its reaction products, in the temperature dependent form

$$P = ae^{-R_1 V} + be^{-R_2 V} + \frac{gT}{V}$$
(4)

where p is pressure, V is relative volume, T is temperature,  $g=wC_v$ , w is the usual Gruneisen coefficient,  $C_v$  is the average heat capacity, and a, b,  $R_1$ , and  $R_2$  are constants (listed in Table 3).

The density for Composition-B is 1.717gcm<sup>-3</sup>, the tangent modulus 0.035 (100GPa) and the yield strength 0.2GPa. The equation of state for the air in the pore is

$$p = C_0 + C_1 + C_2 v^2 + C_3 v^3 + \left(C_4 + C_5 v + C_6 v^2\right) E_0$$
(5)

The initial density of air is 0.00129gcm<sup>-3</sup>.  $C_0$ ,  $C_1$ ,  $C_2$ ,  $C_3$ ,  $C_4$ ,  $C_5$ , and  $C_6$  are the coefficients in the equation of state:  $C_0 = C_1 = C_2 = C_3 = 0$ ,  $C_4 = C_5 = 0.4 \cdot v = \rho / \rho_0 - 1$ 

( $\rho$  and  $\rho_0$  are the current and initial densities of the air in the pore);  $E_0$  is the initial inner energy for the air in the pore:  $E_0 = 2.50 \times 10^{-6}$  J. Ignition and growth reactive flow model parameters have been developed for SDT in many solid explosives. Much progress has been made in study on shock initiation in recent years. The investigation aiming at the effect of pore on sensitive of Composition-B under impact of drop weight is nevertheless scarce in the published literature. The detailed information of igniting process induced by a pore in the explosive cylinder under impact with a drop weight is investigated by numerical simulation in this paper.

In the numerical simulation of igniting process for explosives it is a key to determine the ignition and growth reactive flow model suitable for the explosive examined under the impact of drop weight. The ignition and growth reactive flow model of shock initiation and detonation has been used to model many shock initiation and detonation studies of solid explosives. But the previous parameters<sup>12</sup> of ignition and growth reactive flow model were calibrated on the high pressure and short load duration. Therefore, the parameters in the equation of reaction rate for shock initiation need to be revised to adapt to the low pressure and long load behavior in this study.

Based on the previous report<sup>12</sup>, the binomial expression of reactionrate issuitable for lower pressure with long action duration.

$$\frac{\partial F}{\partial t} = I \left(1 - F\right)^b \left(\rho / \rho_0 - 1 - a\right)^x + G_1 \left(1 - F\right)^c F^d p^y \tag{6}$$

Table 3. Equation parameters of state for Composition-B

Parameter	Unreacted JWL	Product JWL
<i>a</i> ,10 <sup>2</sup> GPa	778.1	5.42
<i>b</i> ,10 <sup>2</sup> GPa	0.0531	0.07678
$R_1$	11.3	4.2000
$R_2$	1.13	1.1000
8	2.2390×10-5	3.4×10 <sup>-6</sup>

The main factor influencing initiation process is  $G_1$ . The parameter  $G_1$  can be calibrated by the result of experiments (13).  $G_1=110\times10^{15}$  Pa s<sup>-1</sup> is suitable in this study<sup>14</sup>. The other parameters in the chemical reaction equation were taken as: I = 44.0×10<sup>6</sup> s<sup>-1</sup>; a = 0.010; b = 0.222; c = 0.222; d = 0.667; x = 4.00; y = 2.

# 3. EFFECT OF GRID SIZES ON CALCULATION ACCURACY

Grid sizes in the numerical simulations have a significant contribution to the calculated results. In the trial calculations three grid sizes (0.05 cm, 0.025 cm, and 0.01 cm) were taken. The calculated results for the three grid sizes were shown in Fig. 2. The comparison of the calculated results shows that the pressure at the initiating location for 0.025 cm was very near that for 0.01 cm. Therefore, the grid size was taken as 0.025 cm in the numerical simulation of this work.



Figure 2. Pressure time histories at initiating location in explosives or three grid sizes.



Figure 3. Pressure history initiating explosion for 0.0 cm diameter of pore.

#### 4. SIMULATION RESULTS AND ANALYSIS

#### 4.1 Effect of Pore Size on Process Initiating Explosion

To examine the characteristics of Composition-B explosive with a pore against impact of a drop weight at given height, numerical simulations were performed in this work. A spherical pore was located at x = 0.3 cm, y = 3.5 cm (shown in Fig.1). The following condition was taken to calculate: Weight mass is 400 kg, and drop height 3 m; Shell thickness is 1.8 cm; Height and radius of cylindrical explosive are 4 cm and 2 cm respectively. The location of pore in the explosive sample is at (0.3 cm, 3.5 cm), as shown in Fig. 1.

The effect of pore in the process of initiation was examined by using numerical simulation. The four sizes of pore were used in the calculation. The processes initiating explosion for various pore sizes are shown in Figs. 3-6. For the three cases with pores the explosion was initiated also around the pore.

From Figs. 3-6, we can find that before the chemical reaction is initiated the values of local pressures in the explosive sample are approximately equal. When explosion is imitated, the local pressures are different clearly. This is because the impact load from a drop weight is far less than the explosion load from chemical reaction of explosive. Minimum loads in Figs.3-6 are the original pressures initiating explosion and the corresponding locations and times are the original locations and times initiating explosion.

Table 4.Comparison of original locations and times initiating<br/>explosion for various pore sizes

Diameter of pore/mm	Original locations initiating explosion/cm	Original times initiating explosion/µs
0.0	2.9	415.5
0.3	3.5	412.8
0.7	3.4	386.8
1.0	3.3	352.2



Figure 4. Pressure history initiating explosion for 0.03 cm diameter of pore.



Figure 5. Pressure history initiating explosion for 0.07 cm diameter of pore.



Figure 7. Pressure histories at initiating location for 400 kg weight at 3 m height.

The original location initiating explosion for 0.0 cm diameter of pore is at (0.3 cm, 2.9 cm), as shown in Fig. 3. Similarly, the original locations initiating explosion for 0.03 cm, 0.07 cm, 0.1 cm diameter of pores were obtained. The original locations and times initiating explosion are shown in Fig. 7 and listed in Table 4.

To compare, the pressure time histories at the initiating locations were shown in Fig. 7. 0.0 mm, 0.3 mm, 0.7 mm, and 1 mm in Fig. 7 represents the diameters of the pores in composition-B explosive respectively. Fig. 7 shows that the histories for the 0.0 mm and 0.3 mm pores are coincident.

This result illustrates that when the size of pore is less than 0.3 mm the effect on initiation of composition-B explosive can be ignored, which agrees with the experiential data<sup>12</sup>.

Table 4 shows that the original time initiating explosion decreases as the pore size increase. Meanwhile, pore in explosive sample has an impact on the original location initiating explosion.



Figure 6. Pressure history initiating explosion for 0.1 cm diameter of pore.



Figure 8. Pressure histories in Composition-B with 0.0 mm pore under impact of 400 kg weight at 1.9 m.

#### 4.2 Minimum Height Initiating Explosion

For given drop weight, the probability initiating explosion increases with the drop height. When the height is less than a critical value, explosion cannot be initiated by the impact of the drop weight. The critical value is called into the minimum height in this work. Through the numerical simulation, the minimum heights of the 400 kg drop weight were obtained for the pores with various sizes which were 0.0 mm, 0.3 mm, 0.7 mm, and 1.0 mm. For Composition-B explosive with the 0.0 mm pore under impact of the 400kg drop weight the minimum height is 1.9 m. In this case the pressure time histories at the various locations on axis Y are shown in Fig. 8. In Figs. 8 and 9, units of X-axis (time) is given as ms. The pressure histories in Fig.8 show that explosion was not initiated.

In the similar way the minimum height was obtained for composition-B explosive with the 0.3 mm pore under impact of the 400 kg drop weight. It is 1.85 m. The pressure time histories in composition-B explosive at the various locations on axis Y in this case are shown Fig. 9. Fig. 9 shows that explosion was not initiated in composition-B explosive with 0.3 mm pore under impact of the 400 kg drop weight at 1.85.

In the similar way the minimum height is 1.6 m for composition-B explosive with the 0.7 mm pore under impact of the 400 kg drop weight. The pressure time histories in composition-B explosive at the various locations on axis Y in this case are shown Fig. 10.

In the similar way the minimum height is 1.4 m for composition-B explosive with the 1.0 mm pore under impact of the 400 kg drop weight. The pressure time histories in composition-B explosive at the various locations on Y-axis in this case are shown Fig. 11.The comparison between the minimum heights for the four cases is listed in Table 5.

In the similar way, the minimum heights were obtained for composition-B explosive with the various size pores under impact of the 200 kg drop weight. The comparison between the minimum heights for the four size pores is listed Table 6.

Under impact of 400 kg and 200 kg drop weights, the minimum heights for the composition-B explosive with the 0.3 mm pore are very close to those with the 0.0 mm pore.



Figure 9. Pressure histories in composition-B with 0.3mm pore under impact of 400 kg weight at 1.85 m.

Table 5.Minimum heights for composition-B explosive with<br/>various size pores under impact of 400kg drop<br/>weight

Diameter of pore, mm	Minimum height, m	Maximum pressure/GPa
0.0	1.9	0.84742
0.3	1.85	0.81457
0.7	1.6	0.78413
1.0	1.3	0.72916



Figure 10. Pressure histories in composition-B with 0.7 mm pore under impact of 400 kg weight at 1.6 m.



Figure 11. Pressure histories in composition-B with 1.0 mm pore under impact of 400 kg weight at 1.4 m.

Table 6.Minimum heights for composition-B explosive with<br/>various size pores under impact of 200 kg drop<br/>weight

Diameter of pore, mm	Minimum height, m	Maximum pressure/GPa
0.0	3.55	0.86884
0.3	3.4	0.85984
0.7	2.8	0.82821
1.0	2.1	0.78704

Therefore, when the sizes of pore in the composition-B explosive are less than 0.3 mm, the effect of pore on impact sensitivity can be ignored.

## 5. CONCLUSION

This work developed an approach to predict the effect of pore in explosive on sensitivity under impact with drop weight. The sensitivity under impact with drop weight represents the safety performance of explosive in launching process. The numerical results in this work showed that when the sizes of pore in composition-B explosive are less than 0.3 mm, its effect on sensitivity under impact of a drop weight can be ignored. This result agrees with experimental data.

The detail information in the process initiating explosion in explosive sample under impact from a drop weight can be obtained by using numerical simulation. The numerical result shows that pore in explosive sample has an impact on the original locations and times initiating explosion. The original time initiating explosion decreases as the pore size increase.

## ACKNOWLEDGMENTS

The research presented in this paper was supported by the National Science Foundation of China (11072035) and Foundation for Doctor Dissertation of China (20111101110008).

## REFERENCES

- Hamate, Y. & Horie, Y. Ignition and detonation of solid explosives: A micromechanical burn model. *Shock Waves*, 2006, 16, 125–147.
- Hunt, E.M.; Malcolm, S.; Pantoya, M.L.; Davis, F. Impact ignition of nano and micron composite energetic materials. *Int. J. Impact Eng.*, 2009, 36, 842–846.
- Holian, B.L.; Germann, T.C.; Maillet, J.B. & White, C. T. Atomistic mechanism for hot spot initiation. *Physical review letters*, 2002, 89(28), 285501-1-285501-4.
- Zhang, Q. & Xiang, C. Void generation between shell and charge of warhead under the projection load. *Def. Sci. J.*, 2008, **58**(6),715-720.
- Zhang, Q.; Lin, D.C. & Bai, C.H. Motion state of fuel with shell in projection acceleration process. *Def. Sci. J.*, 2003, 53(3), 259-265.
- Kapila, A.K.; Schwendeman, D.W.; Bdzil, J.B. & Henshaw, W.D.A study of detonation diffraction in the ignition-and-growth model. *Combust. Theory Modell.*, 2007, **11**(5), 781-822.
- 7. Sharpe, G.J.; Gorchkov, V. & Short, M. Shock initiation of explosives: The idealized condensed-phase model. *IMA J.*

Applied Mathe., 2008, 73(2), 361-373.

- Herring, S.D.; Germann, T.C. & Grønbech-Jensen, N. Effects of void size, density, and arrangement on deflagration and detonation sensitivity of a reactive empirical bond order high explosive. *Physical Review B* (*Condensed Matter and Materials Physics*), 2010, 82(21), 214108-4120.
- 9. Tran L. & Udaykumar H.S. Simulation of void collapse in an energetic material, Part 2: Reactive Case. *J. Propulsion Power*, 2006, **22**(5), 959-974.
- Tarver, C.M.; Chidester, S.K. & Nichols, A.L. Critical conditions for impact- and shock-induced hot spots in solid explosives. *J. Phys. Chem.*, 1996, **100**, 5794-5799.
- Hawksworth, C.P.; Rogers, S.; Beyer, R.M.; Lakic, D.; Raveau, D.; Herve P.; Pina,V.; Petitfre're, C. & Lefebvr X. Development of a method for predicting the ignition of explosive atmospheres by mechanical friction and impacts (MECHEX). *J. Loss Prev. Process Ind.*, 2007, 20, 349–365.
- Murphy, M.J.; Lee, E.L.; Weston, A.M. & Williams, A.E. Modeling shock initiation in Composition B. Paper Presented at the 10<sup>th</sup> Detonation Symposium, Boston, MA, 12-16 July1993, 8.
- Rui, X.T.; Yun, L.F.; Wang. G.P.; Chen, T.; Gu, J.L.; Yang, F. & Zhang, C. Direction to launch safety of ammunition. National Defense Industry Press, Beijing, 2009. pp.219.
- 14. Zhang, Q. & Hu, S. Factors influencing ignition and explosion characteristics of explosives under drop weight impact. *Inter. J. Energ. Mater. Chem. Propul.*, 2013, (In press).

### Contributors

**Dr Qi Zhang** received his PhD from China University of Mining and Technology, Beijing, presently working as a Professor at State Key Laboratory of Explosion Science and Technology. His research interests areas include: Explosion mechanics and its applications.

**Mr Shaoqiao Hu** received his ME from Beijing Institute of Technology in 2011. He is a engineer at the No.208 institute in Beijing. His research interest includes : Engineering mechanics and explosion blast.

**Dr Huimin Liang** received her PhD from Beijing Institute of Technology in 2006. She is a lecturer at Beijing Institute of Technology. Her research interest includes : Explosive and its applications.