Reactive Flow Modeling of Density Effect on Diverging JB-9014 Detonation Impelling

Xin Yu, Kuibang Huang and Miao Zheng Institute of Applied Pyhsics and Computational Mathematics, Beijing Beijing, China

1 Introduction

Difference of original density has a remarkable effect on detonation performance of IHE (Insensitive High Explosive), which attracts much interesting of researchers. It's highly valuable to find out how detonations respond to the physical properties' variety in engineering design and application. Hill and Aslam^[1] presented a method to scale the detonation shock dynamics Dn(k) function to accommodate variations in high explosive. Their results show the original density of the high explosive effect the detonation velocity and detonation pressure remarkably in the case of steady detonation. Other theoretical and experimental investigations also post the density effect on the shock to detonation procedure, propagation, the velocity, the pressure and the other impact behavior^[2-3].

This paper present our experimental and numerical work on the density effect of Insensitive High Explosive named JB-9014 which composed of 95% TATB and 5% F_{2314} . The experimental results reveal the original density effect the hemispherical detonation impact performance, and the numerical work show the effect should consider not only in Chapman-Jouguet detonation speed or pressure but also in the parameters of products equation of state in the theoretical analysis.

2 Experimental Set

The experimental assembly consisted of a hemispherical shell charge of JB-9014 confined between the inner hemispherical booster and the outer hemispherical OFHC shell as shown in Fig. 1. A plexiglass under prop was equipped to support the VISAR probes. The radius of the booster is 18mm, which is designed to make sure the JB-9014 could be detonated unfailingly, and the radial thickness of OFHC shell was set as 2mm. We change both the radial thickness and the original density of JB-9014 in order to observe the varieties of the OFHC free surface velocity with VISAR probes. Three sets of VISAR probes are equipped in different angles, hence the free surface velocity of OFHC could be recorded at different location to avoid the information missing only with one set of VISAR. Table 1 displays the radius thickness and the shot density of JB-9014 in our experiments.



Figure 1. Cross-section of the assembly 2D view showing booster, IHE and the locations of VISAR probes.

Table 1: Shot sizes and the density

Radius thickness	10mm	15mm	20mm	25mm
density				
higher	1.90	1.899	1.901	1.900
regular	1.887	1.883	1.885	1.885

3 Experimental Results

Figure 2 shows two typical velocity histories in our experiments with regular density and the higher density with the same thickness of JB-9014, in which the first jump of velocity could be explained by the entering of detonation wave and the following flat roof could be understood as spallation of OFHC by the free surface rarefaction wave (It is clear that the OFHC surface reflect a rarefaction after the entering the detonation wave and the strength of this rarefaction wave is strong enough to cause the spallation.). As to the in succession velocity increase of the curve, it is theimpelling result by the detonation product. The first jump in velocity in the higher density shot was apparently higher than the one with regular density, so as to the following parts of the curves. It reveals that the density of JB-9014 should affect not only the properties of detonation wave but also the equation of state of the products.



Figure 2. Velocity curve with different density in shot of JB-9014 radial thickness 20mm.

Fig. 3 shows the velocity history of different radial thickness of JB-9014, the increase of the first jump with the increase of the radial thickness could be easily understood by the DSD theory as the curvature decrease with the radius in diverging detonation, which we will not discuss in this paper, neither to the spallation.



Figure 3. Velocity curve with different JB-9014 radial thickness 20mm in regular density.

4 Numerical modeling and discussion

4.1. models and parameters

An improved, combined reaction rate for JB-9014 was taken in this work and the Jones-Wilkins- Lee (JWL) equation of state was chosen for the reactant and the product. The Ignition and Growth reactive flow model derived from Lee and Tarver^[4] contains three-term rate law (seen in Equation 1) as three stages of reaction generally observed in shock initiation and detonation of heterogeneous solid explosives. For detonation, the first term represents the ignition of the explosive, or the formation of the hot spots, as it is compressed by the leading shock wave. The second term represents the growth of these hot spots in the main reaction. The third term is used to describe the relatively slow performance of energy release and the end of high explosive burn. The typical I&G reaction rate is given by

$$\frac{\partial \lambda}{\partial t} = I(1-\lambda)^b (v-1-a)^x + G_1(1-\lambda)^c \lambda^d p^v + G_2(1-\lambda)^e \lambda^g p^z,$$
(1)

Where λ is the fraction reacted, *t* is time in μs , *v* is the relative volume, *p* is pressure in *Mbars*, and *I*, *G*₁, *G*₂, *a*, *b*, *c*, *d*, *e*, *g*, *x*, *y*, and *z* are constants. In order to match a wide variety of experiments with one set of reactive parameters, Wescott, Steward and Davis improved former term with two different pressure sensitivities in the growth term, one for shock initiation and another for full detonation ^[5]. The improved, combined reaction rate is given as following

$$\frac{\partial \lambda}{\partial t} = r_I S_I(\lambda) + r_G S_G(\lambda) + [1 - S_G(\lambda)] r_B, \qquad (2)$$

$$r_{G} = \{ r_{IG} W(\rho_{SH}) + r_{DG} [1 - W(\rho_{SH})] \},$$
(3)

$$Y_{I} = K_{I} \left(\frac{\rho}{\rho_{0}}\right)^{2} (1-\lambda)^{2/3} H \left(\frac{\rho}{\rho_{0}} - 1 - a\right), \qquad (4)$$

$$r_{IG} = K_{IG} \left(\frac{p}{p_{CJ}}\right)^{z_1} \lambda^d (1-\lambda), \tag{5}$$

$$r_{DG} = k_{DG} \left(\frac{p}{p_{CJ}}\right)^{z_2} \lambda^g (1-\lambda), \tag{6}$$

Yu X

$$r_B = K_B \left(\frac{p}{p_{CJ}}\right) (1-\lambda)^{1/2}, \qquad (7)$$

$$S_{I}(\lambda) = \frac{1}{2} \{1 - \tanh[200(\lambda - 0.025)]\},$$
(8)

$$S_G(\lambda) = \frac{1}{2} \{1 - \tanh[30(\lambda - 0.9)]\},$$
(9)

$$W(\rho_{SH}) = \frac{1}{2} \left\{ 1 - \tanh\left[50 \left(\frac{\rho_{SH}}{\rho_c} - 1 \right) \right] \right\}.$$
 (10)

Where ρ_0 is the initial density in g/cm^3 , ρ_{SH} is the shock density or von-Neumann (V-N) spike density in g/cm^3 , ρ_c is the critical density sensitive to the failure diameter in g/cm^3 , p_{CJ} is the pressure at the Chapman–Jouguet (C-J) point in *Mbars*, and the functions $S_I(\lambda)$, $S_G(\lambda)$ and $W(\rho_{SH})$ are tanh functions which switch the initiation and detonation growth terms. r_I is the ignition term and K_I is a constant sensitive to the ignition. r_G is the detonation growth or the fast reaction term, here r_{IG} and r_{DG} represent the shock initiation part and the detonation part, respectively. r_B is the completion of the whole reaction. The parameters of JB-9014 were calculated by fitting the one dimensional Pop plots, which illustrated in the table 2.

Table 2: Reactive flow model parameters ^[6]

$K_I \ (\mu s^{-1})$	K_{IG} (μs^{-1})	Z_1	Z_2	а	d	g
3.00e06	22.0	2.7	2.0	0.0214	0.667	0.333

The model uses two Jones-Wilkins- Lee (JWL) equations of state, one for the unreacted explosive and one for the detonation products, in the temperature dependent form as

$$p = Ae^{-R_{1}v} + Be^{-R_{2}v} + \omega C_{v}T/v$$
(11)

where *p* is pressure in *Mbars*, *v* is relative volume, *T* is temperature in *K*, ω is the Gruneisen coefficient, *C_v* is the average heat capacity, and *A*, *B*, *R₁*, and *R₂* are constants (seen in Table 3). The JWL product equation of state was fitted by the cylinder tests, in which the parameters are adjusted with Tang's modification ^[8]. Gruneisen equation of state was taken in this work for the OFHC, and the Li's equation of state was taken for the state p<0 to simulate the spallation phenomenological ^[7].

Numerical tests about artificial viscosity and mesh size were taken to independent the results of calculation method. The mesh sizes used in these calculations are 20 zones per mm in high explosive and 10 zones per mm in OHFC. The results are independent of mesh size so the modeling has converged to consistent answers.

Unreacted JWL		$ ho_{ heta}$ (g/cm ³)	A _e (Mbar)	$B_e(Mbar)$	R _{1e}	R_{2e}	ω _e	C _e (Mbar/K)
		1.890	746.556	-0.11544	11.29	2.0	0.85	2.487e-5
	$E_{\theta}(Mbar)$		$A_p(Mbar)$	$B_p(Mbar)$	R_{Ip}	R_{2p}	ω_p	$C_p(Mbar/K)$
Products JWL	Higher density	0.07058	7052.15	2.8209	17.5	3.225	0.35	1.0e-5
	Regular density	0.07025	190.89	2.712	12.5	3.245	0.35	1.0e-5

Table 3: JWL EOS parameters of reactant and detonation products [6]

4.2. result comparison and discussion

Yu X

Fig. 4 shows the calculated velocity history of a 20mm radial thickness shot with higher density in our simulation, and the experimental data is illustrated for comparison. The first jump of the velocity in our work agrees well with the experimental result and unload adjustment equation of state could suitably describe the experimental spallation flat roof, so as to the succession curve.



Figure 4. Comparison of calculated Velocity curve with the experimental data in shot of higher density JB-9014 with radial thickness 20mm.



Figure 5. Comparison of calculated Velocity curves of higher density JB-9014 with radial thickness 20mm.

Fig. 5 presents the modeling work with and without EOS parameter adjustments. In this simulation, the Chapman-Jouguet detonation velocity and pressure were adjusted with the density referencing the method of Sources et al ^[8]. It shows that the first jump was decided by the entering detonation shock or the pressure of detonation and the following curve was decided by the EOS of detonation products. The curve without EOS parameter adjustment could fit only the first jump, and the work with comprehensive adjustment could agree well with the characterizations obtained from experiments (seen the red line in Fig. 5).

5 Conclusion and future work

The experimental work reveals the effect of high explosive density on the divergence detonation shell impelling. The numerical simulation investigates the density effect on detonation properties and EOS of products, separately. The numerical results show the original density affect not only the Chapman-Jouguet detonation properties but also the EOS of detonation products.

There are some details of the velocity curve which could not be repeated by the present numerical modeling after the flat roof. Future work will pay attention to spall model with consideration of reactive flow to score the velocity curve accurately.

6 Acknowledgement

The authors thank the support of the experimental team. This work was supported by the national nature science foundation of 11002029 and 11202033.

References

[1] Hill LG, Aslam TD. (2010). Detonation Shock Dynamics Calibration for PBX 9502 with Temperature, Density, and Material Lot Variations. LA-UR-10-10428.

[2] Tang PK. (2000). Temperature effect on PBX 9502 Equation of State. LA-UR-XXXX.

[3] Yu X, Huang KB, Wei L, Zheng M. (2014) Numerical Study of Density Effect on JB-9014 Equation of State of Detonation Product. The 9th International Colloquium on Pulsed and Continuous Detonation.

[4] Wescott B, Steward D, Davis W. (2005). Equation of state and reaction rate for condensed-phase explosives. J. Appl. Physics. 98:1.

[5] Lee E, Tarver C. (1980). Phenomenological model of shock initiation in heterogeneous explosives. Phys. Fluids, 23:2362.

[6] Yu X, Huang KB. (2013). Reactive Flow Modeling of Detonation Propagation JB-9014 in 2D Semispherical Shell. The 4th Asian Symposium on Computational Heat Transfer and Fluid Flow, Hong Kong.

[7] Li MS, Chen DQ. (1988). An applied equation of state for elastic-plastic fluid (II). High Pressure Physics Transaction. 2:153.

[8] Souers PC, Wu B, Haselman LC. JR. (1996). EOS of Detonation Product in LLNL. UCRL-ID-119262.

Yu X