High-Resolution Numerical Simulation of Dead Zones in the Insensitive Explosive Detonation

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1 Introduction

Insensitive High Explosive (IHE) is the most influential energetic material, which have good thermal stability and other insensitivity in many other aspects, such as shockwave or electricity. For IHE, dead zones in the corner-turning is a significant phenomenon, and many researches have been conducted to it. Souers et al [2, 3] took pin and X-ray corner-turning data on ambient LX-17 and PBX9502, and simulated them with JWL++ code. Tarver [1] proposed a "hockey pucks" experiment, and simulated it with a three-reaction-channel ignition-and-growth reaction rate model. Kapila et al [4, 5, 6] simulated corner-turning in the LX-17 with different boundary condition, and proposed a desensitization model used to calibrate dead zone formation of LX-17 in the hockey puck experiment.

In this paper, the fifth-order WENO method is used to simulate air-corner turning of LX-17 in the hockey puck configuration with level set method, and the simulation result is compared with rigid-corner turning with the same configuration based on the desensitization model [4]. In the result of weak-confinement corner simulation, the position and the size of dead zone are both consistent with the experiment result in [3].

2 Numerical Model

Two-dimensional Eulerian governing equations with reaction and desensitization model are

$$\frac{\partial \boldsymbol{U}}{\partial t}+\frac{\partial \boldsymbol{F}}{\partial x}+\frac{\partial \boldsymbol{G}}{\partial y}=\boldsymbol{S} \tag{1}$$

$$\boldsymbol{U}=\left(\rho,\rho u,\rho v,\rho E,\rho\lambda,\rho\varphi\right)^{T} \tag{2}$$

$$\boldsymbol{F}=\left(\rho u,\rho u^{2}+p,\rho uv,\rho u\left(E+p/\rho\right),\rho u\lambda,\rho u\varphi\right)^{T} \tag{3}$$

$$\boldsymbol{G}=\left(\rho v,\rho uv,\rho v^{2}+p,\rho v\left(E+p/\rho\right),\rho v\lambda,\rho v\varphi\right)^{T} \tag{4}$$

$$\boldsymbol{S}=\left(0,0,0,0,0,\rho\dot{\lambda},\rho\dot{\varphi}\right)^{T} \tag{5}$$

$$E=e+\left(u^{2}+v^{2}+w^{2}\right)/2+\left(1-\lambda\right)Q \tag{6}$$

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where ρ is density, p is pressure, and u,v,w are velocities in x,y,z directions respectively; e is specific internal energy, λ is reaction progress, φ is desensitization progress, and Q is reaction heat.

In this paper, p, e, ρ and other variables are treated as mixture parameter of unreacted explosive and reaction products, which means mixture rules are necessary. We assume that the total volume and total internal energy are respectively equal to the weighted sum of those two materials, and they have the same temperature and pressure. The equations are listed below:

$$\frac{1}{\rho} = v = (1-\lambda)v_e + \lambda v_p \tag{7}$$

$$\rho e = \frac{e}{v} = (1-\lambda)\frac{e_e}{v_e} + \lambda \frac{e_p}{v_p} \tag{8}$$

$$p = p_e = p_p \tag{9}$$

$$T = T_e = T_p \tag{10}$$

where e (subscripts) represents unreacted explosive, and p (subscripts) represents reaction products.

Equations of states of unreacted explosive and reaction products employed in this article are both JWL equations. The equation is listed below, and the parameters are listed in Table 1.

$$p = A\left(1-\frac{\omega}{R_1 V}\right)\exp(-R_1 V) + B\left(1-\frac{\omega}{R_2 V}\right)\exp(-R_2 V) + \frac{\omega E}{V} \tag{11}$$

$$V = \frac{v}{v_0} = \frac{\rho_0}{\rho} \quad , \quad E = \rho_0 e \tag{12}$$

where p is pressure, e is specific internal energy, ρ is density, ρ_0 is initial density of unreacted explosive. T is temperature. C_v is specific heat. A,B, R_1, R_2 and ω are constants of EOS.

Table 1: JWL EOS Parameters for unreacted LX-17 and reaction products

	Value		
	Reactant	Product	Units
A	77810	1481.05	GPa
B	-5.031	63.79	GPa
R_1	11.3	6.2	-
R_2	1.13	2.2	-
ω	0.8938	0.5	-
C_v	2.487	1.0	10^{-3} GPa/K
ρ_0	1.905	1.905	g/cm^3
E_0	-	6.9	10^9 J/m^3

The reaction rate model used in this paper is a pressure-driven ignition-and-growth reaction model with three reaction channel, proposed by C. M. Tarver in 2005 [1]. The equation is listed below, and the parameters are listed in Table 2.

$$\begin{aligned}\frac{\mathrm{d}\lambda}{\mathrm{d}t} &= I(1-\lambda)^b\left(\frac{\rho}{\rho_0}-1-a(\varphi)\right)^x && 0<\lambda<\lambda_{Ig\max}\\ &+ G_1(\varphi)\cdot(1-\lambda)^c\lambda^d p^y && \lambda_{G_1\min}<\lambda<\lambda_{G_1\max}\\ &+ G_2\cdot(1-\lambda)^e\lambda^f p^z && \lambda_{G_2\min}<\lambda<1\end{aligned} \tag{13}$$

where λ is reaction progress, t is time, ρ_0 is initial density of unreacted explosive, and ρ is density of unreacted explosive under shock. I, G_1, G_2, b, c, d, e, f, x, y and z are constants of reaction rate. $\lambda_{Ig\max}$, $\lambda_{G_1\max}$ and $\lambda_{G_2\min}$ are threshold of three reaction channel.

Table 2: Ignition and Growth Parameters for LX-17

	Value	Units		Value	Units
b	0.667	-	I	4.0×10^6	μs^{-1}
c	0.667	-	G_1	0.0045	$GPa^{-y}\mu s^{-1}$
d	1.0	-	G_2	0.30	$GPa^{-z}\mu s^{-1}$
y	3.0	-	$\lambda_{Ig\max}$	0.02	-
e	0.667	-	$\lambda_{G_1\max}$	0.8	-
f	0.667	-	$\lambda_{G_2\min}$	0.8	-
z	1.0d0	-			

The desensitization rate model used in this paper is a pressure-driven equation, similar to the , proposed by G. DeOliveira, A. K. Kapila and et al in 2006 [4]. The equation is listed below, and the parameters are listed in Table 3.

$$\frac{\mathrm{d}\varphi}{\mathrm{d}t} = S\cdot p\varphi(1-\varphi) \tag{14}$$

$$a(\varphi)=(1-\varphi)a_0+\varphi a_1 \tag{15}$$

$$\lambda_{G_1\min}=\lambda_t\varphi \tag{16}$$

where φ is the desensitization progress, a_0, a_1, x, y, z, S, λ_t are constants, and $a(\varphi)$ as well as $\lambda_{G_1\min}$ would be used in the reaction rate model.

Table 3: Desensitization Parameters for LX-17

	Value	Units
S	5.4	$GPa^{-1}\mu s^{-1}$
a_0	0.22	-
a_1	0.5	-
λ_t	0.01	-

3 Numerical method

In this paper, the fifth-order WENO finite difference scheme and the third-order TVD Runge–Kutta scheme are employed to discretize Eulerian equations with reaction and desensitization source. The scheme is as follows:

$$\boldsymbol{U}_t = \boldsymbol{L}(\boldsymbol{U}) = -\left(\frac{\hat{\boldsymbol{F}}_{i+1/2,j,k} - \hat{\boldsymbol{F}}_{i-1/2,j,k}}{\Delta x} + \frac{\hat{\boldsymbol{G}}_{i,j+1/2,k} - \hat{\boldsymbol{G}}_{i,j-1/2,k}}{\Delta y} + \frac{\hat{\boldsymbol{H}}_{i,j,k+1/2} - \hat{\boldsymbol{H}}_{i,j,k-1/2}}{\Delta z} \right) + \boldsymbol{S} \tag{17}$$

Third-order TVD Runge–Kutta scheme employed for temporal discretization is as follows:

$$\begin{cases} \boldsymbol{U}^{(1)} = \boldsymbol{U}^n + \Delta t \cdot \boldsymbol{L}\left(\boldsymbol{U}^n\right) \\ \boldsymbol{U}^{(2)} = \dfrac{3}{4}\boldsymbol{U}^n + \dfrac{1}{4}\left[\boldsymbol{U}^{(1)} + \Delta t \cdot \boldsymbol{L}\left(\boldsymbol{U}^{(1)}\right)\right] \\ \boldsymbol{U}^{n+1} = \dfrac{1}{3}\boldsymbol{U}^n + \dfrac{2}{3}\left[\boldsymbol{U}^{(2)} + \Delta t \cdot \boldsymbol{L}\left(\boldsymbol{U}^{(2)}\right)\right] \end{cases} \tag{18}$$

Level set method is used to track the interface between explosive and air, and the governing equation is written as

$$\frac{\partial \varphi}{\partial t} + u\frac{\partial \varphi}{\partial x} + v\frac{\partial \varphi}{\partial y} = 0 \tag{19}$$

where φ is a signed normal distance function from the interface. The sign of φ represents the type of material. Plus represents explosive, and minus represents air.

The RGFM (Real Ghost Fluid Method) is used for interface treatment, which solves the Riemann problem at the interface first, and then extrapolate the Riemann solution to adjacent ghost nodes and real nodes.

4 Numerical Example: Hocky Puck

The configuration of the hocky-puck model is referred to Souers et al 's work in [3] and DeOliveira et al 's work in [4] , shown in Figure 1. The boundaries of the corner are treated as rigid, while the others are treated with outflow conditions. At $t = 0$ μs, $p = 31.46$GPa, $\rho = \rho_0$, $\lambda = 1.0$ in the circle region, which radius is 7.68mm. The coordinate of the center of the initial ignition is [21.5, 0].

The simulation results with rigid-confinement corner are shown in Figure 2. The detonation wave reached the corner at $t = 1.6$ μs . In Figure 2, The dead zone is not really "dead" without desensitization model. The detonation wave flow around the dead zone, and reignite it with high pressure. While the desensitization model inhibit the detonation at the corner due to the decrease of the local pressure, which would weaken the reaction rate in the ignition process and the growth process. When the desensitization model is used, dead zone is larger, but the result is not consistent with the simulation result in [6].

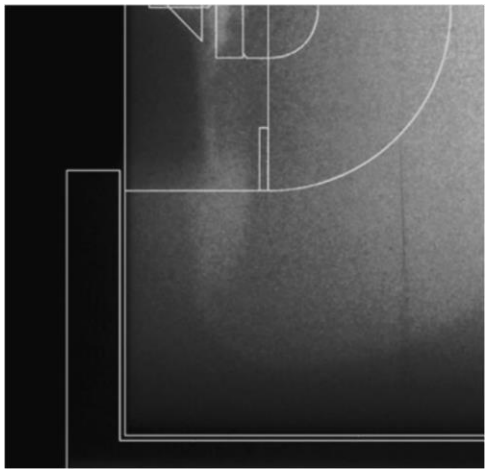

Figure 1. X-ray taken 7.74μs after the optical pin, from [3]

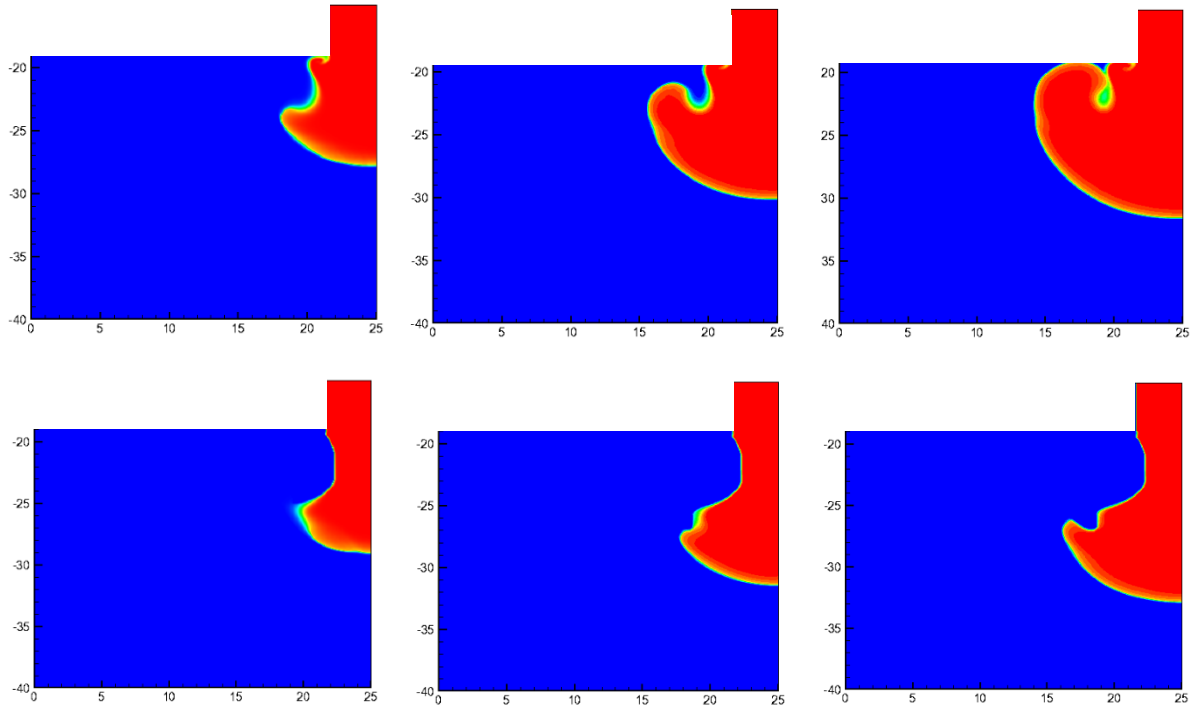

Figure 2. Zoomed reaction progress λ contours without desensitization model (Up) and with desensitization model (Down) for rigid-corner turning, t = 2.84μs (Left), 3.16μs (Middle), and 3.36μs (Right).

The simulation results with air-corner are shown in Figure 3. The detonation wave reached the corner at $t = 1.32\ \mu s$. The reaction products flow out into the intial air region, which is marked with black line in Figure 3. The detonation wave flow around the dead zone from beneath, and the dead zone is obvious at $t = 2.72\ \mu s$, and it is at the position of 1.8 ~ 5.6 mm from the initial corner point, which is consistent with the experiment of [6].

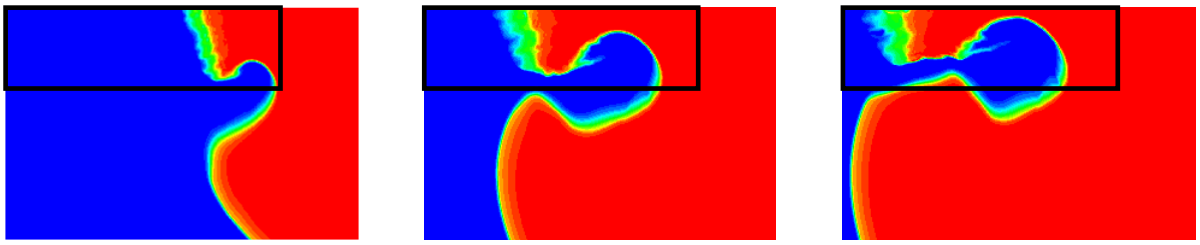

Figure 3. Zoomed reaction progress λ contours with level set method for air-corner turning, t = 1.97 μs (Left), 2.72μs (Middle), and 3.12μs (Right).

5 Conclusions

In this paper, the desensitization model is used to simulate the rigid-corner turning of LX-17 in the hockey puck experiment, and level set method is used for the air-corner turning. The result of rigid-corner turning with desensitization model is not consistent with the simulation result of Banks's work in [6], while the multi-material simulation with air-corner turning is consistent with the experiment result of Souers's work in [3]. For condensed explosive, the rigid boundary is too idealistic, and multi-material model could simulate the corner-turning problem better.

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