Numerical Modeling of Detonation Properties for Cast TNT

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Abstract: Referring to the data of reaction rate and JWL equation of state reported by Lee, E. L. and Tarver, C. M., we compute the detonation wave structure and numerically simulate the shock initiation and detonation proceeding around a corner of cast TNT by using the 2D Lagrangian FCM code. We also compare the results obtained from computation with those given by experiment, and find both of them well agreeable with each other.
Keywords: Cast TNT Detonation property Numerical modeling

1 Detonation Wave Structure of Cast TNT

1.1 JWL equation of state and reaction rate

In this paper, detonation properties of cast TNT are investigated. The JWL equation of state used is as[1]

$$p_i = A_i(1-\frac{\omega_i}{R_{1i}V})\exp(-R_{1i}V) + B_i(1-\frac{\omega_i}{R_{2i}V})\exp(-R_{2i}V) + \frac{\omega_i E_i}{V} \tag{1.1}$$

Where, i=1 or 2, i=1 indicates reactant, while i=2 indicates product, $A_i, B_i, \omega_i, R_{1i}, R_{2i}$ are EOS parameters, p_i is pressure, V is specific volume, and , E_i is internal energy.
The function of reaction rate is

$$\frac{\partial f}{\partial t} = I(1-f)^{\frac{2}{9}}\eta^4 + G(1-f)^{\frac{2}{9}}f^{\frac{2}{3}}p^{1.2} \tag{1.2}$$

Where, t is time, f is the process variable of reaction, $\eta = \frac{V_0}{V} - 1$, V_0 is initial specific volume, I and G are two experiment constants.

1.2 The steady detonation structure in 1-D planar case

Connecting the physical quantities on both sides of the wave front with Hugonoit relation as

$$(1-f)E_1 + fE_2 - fQ - E_0 = \frac{1}{2}(p+p_0)(1-V) \tag{1.3}$$

Where, Q is the energy released in chemical reaction. Let E_0 and E_1 denote the internal energies of the reactant ahead and behind the wave, and E_2 denote the internal energy of the product.
Put (1) into (3), then can get

$$\begin{aligned} p\left\{(1-f)\frac{V}{\omega_1} + \frac{fV}{\omega_2} - \frac{1}{2}(1-V)\right\} = \left\{(1-f)\left[\frac{A_1V}{\omega_1}(1-\frac{\omega_1}{R_{11}})\exp(-R_{11}V) + \frac{B_1V}{\omega_1}(1-\frac{\omega_1}{R_{21}})\exp(-R_{21}V)\right]\right. \\ \left. + f\left[\frac{A_2V}{\omega_2}(1-\frac{\omega_2}{R_{12}})\exp(-R_{12}V) + \frac{B_2V}{\omega_2}(1-\frac{\omega_2}{R_{22}})\exp(-R_{22}V)\right] + fQ + \frac{1}{2}p_0(1-V) + E_0\right\} \end{aligned} \tag{1.4}$$

which can be derived from the assumption of local pressure eqilibrium. p is the pressure of both reactant and product.

For different values of f, solving equation (1.4) numerically, then get Hugoniot relation as shown in table 1.1 and Fig.1.1.

Table 1.1 Hugoniot relation of cast TNT in prtial reaction

	Pressures vs different volumes/GPa							
f	1.00	0.95	0.90	0.85	0.80	0.75	0.70	0.65
0.0	0.00	0.62	1.62	3.19	5.66	9.48	15.41	24.69
0.1	1.86	2.71	3.95	5.74	8.35	12.15	17.74	26.05
0.3	4.19	5.32	6.82	8.84	11.58	15.30	2.043	27.57

0.5	5.59	6.87	8.52	10.66	13.44	17.10	21.94	28.41
0.7	6.53	7.91	9.65	11.86	14.66	18.26	22.90	28.94
0.9	7.20	8.65	10.45	12.70	15.52	19.07	23.57	29.30
1.0	7.47	8.94	10.77	13.04	15.86	19.39	23.83	29.45

Hugoniot curves of cast TNT for different f are in Fig.1.1, Where four values of f(0, 0.3, 0.7, and 1.0 respectively) are given. In Fig.1.1, let Rayleigh line be tangential to the Hugoniot curve of the product f=1 at point(p_0,V_0) and intersect the Hugoniot curve of f=0, then can get Von Neumann spike and C-J point. Table 1.2 gives C-J and Von Neumann values.

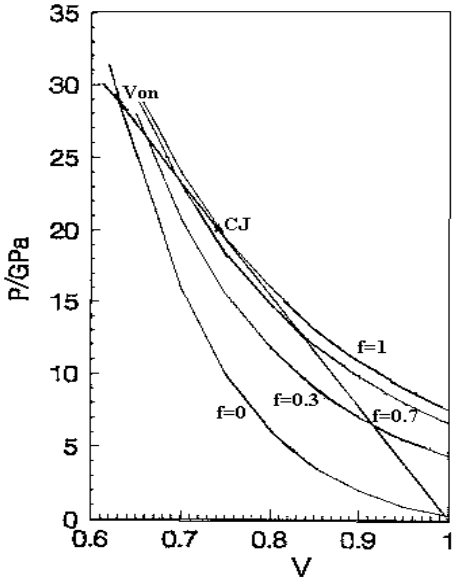

Fig.1.1 Hugoniot curves of cast TNT

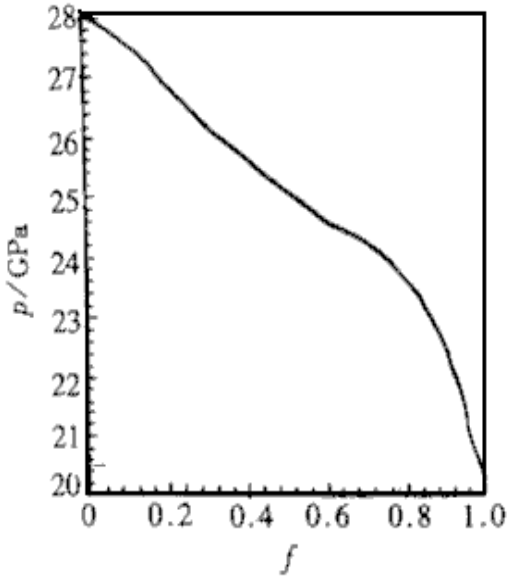

Fig.1.2 Pressure in detonation wave for cast TNT

Table 1.2 Von Neumann spike and Chapman-Jouguet conditions of cast TNT

	Von Neumann values				C-J values		
	D/(m/s)	p_s/GPa	V_s/V_0	u_s/(m/s)	p_{CJ}/GPa	V_{CJ}/V_0	u_{CJ}/(m/s)
Reference[1]	6.85	28.1	0.63	2.55	21.0	0.73	2.28
FCM*	6.67	28.2	0.64	2.50	20.2	0.74	2.30

* computed by 2-D lagrangian particle method FCM(Free Cell Method).

Fig.1.2 is the pressure curve of cast TNT in detonation wave.

2 1-D Calculating Results

Shock initiation probrem of cast TNT is studied numerically by using FCM program. Fig.2.1 and Fig.2.2 show the calculation results and experimental POP curve respectively. Fig.2.2 shows the calculated and experimental pressure histories at several manganin gage locations for the initiation of cast TNT by a sustained pulse of 6.5GPa. The solid line in Fig.2.2 is experimental values. Fig.2.1 is calculated by FCM code. The time of build up to detonation for cast TNT is 2.4μs, the distant is 11.5mm. The comparision shows that calculation by FCM gives good agreement to experament.

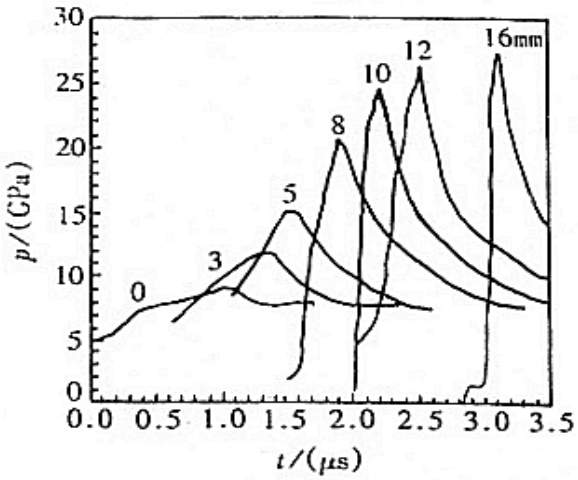

Fig.2.1 Pressure history in cast TNT calculated by FCM

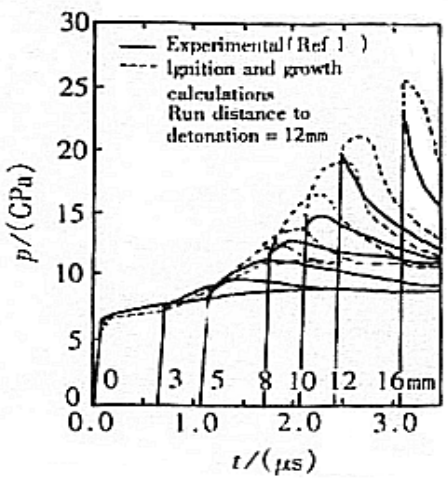

Fig.2.2 Calculated and experimental pressure histries in cast TNT from reference [1]

3 2-D Calculating Results

For the axisymmetry model in Fig.3.1, the proceeding process of detonation wave going around a corner in a cylindrical cast TNT charge after being initiated is calculated, Fig.3.2 shows the calculating results of the detonation wave at 0μs, 18μs and 40μs respectively. For the 2-D plane model in Fig.3.3, the proceeding process of detonation wave passing around a hollow tube in a plane cast TNT charge after being initiated is calculated. Fig.3.4 shows the calculated results of the detonation wave at 0μs,43μs and 50μs respectively.

References

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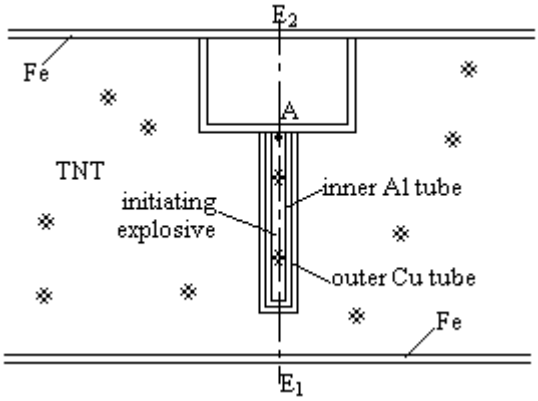
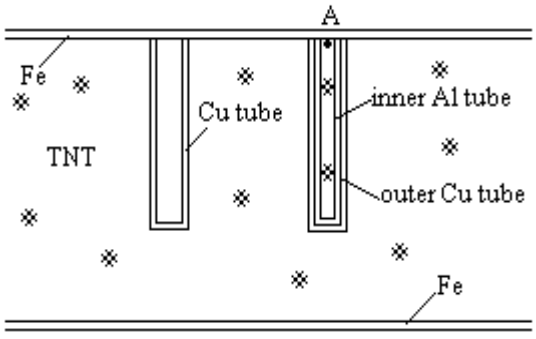
2 Cao Juzhen, Numerical simulating of detonation properties for insensitive exsplosive, Explosion and Shock, 1995, 15(1) pp28-36.



$\overline{E_1E_2}$ is axisymmetry axis, A is initiating point

Fig.3.1 Initial axisymmetry model structure



A is initiating point

Fig.3.3 Initial plane model structure

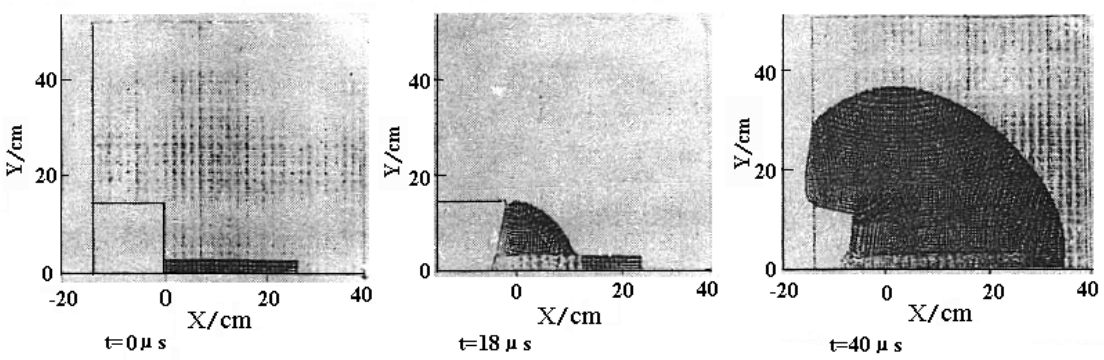


Fig.3.2 Computational results of axisymmetry model

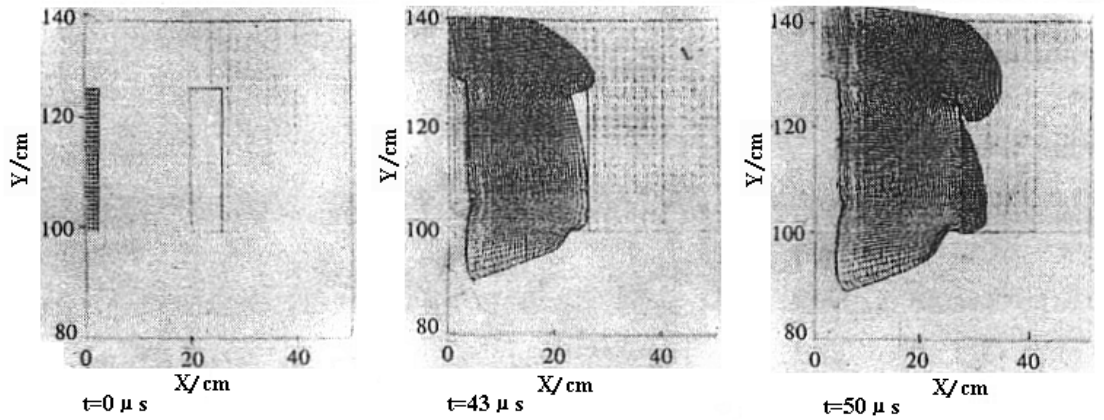


Fig.3.4 Computational results of plane model