Theoretical calculation for overpressure of air shock wave of explosion induced reaction of reactive material case

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Abstract. In order to study the power of the air shock wave produced by the reactive material driven by explosion, the reaction behavior of the reactive material driven by explosion was analyzed by AUTODYN@ software, and the reaction law of the reactive material was obtained. Considering the chemical energy released by the reactive material, the calculation model of shock wave initial parameters is improved. Combined with dimensional analysis, the theoretical calculation model for overpressure of air shock wave generated by the reactive material driven by explosion is studied. The results show that, under the driving of explosion, the casing made of the reactive material does not react completely. The velocity of air shock wave produced by the charge with reactive material casing is higher than that of the charge with inert material casing. The predicted value of the theoretical calculation model is in good agreement with the experimental results, and the established model can well describe the attenuation law of the air shock wave overpressure generated by the reactive material driven by the explosion.

Nomenclature

- \( P_{\text{H}} \): the C-J pressure of detonation
- \( E_a \): the apparent activation energy
- \( P_k \): critical pressure
- \( \rho \): reference density
- \( P_X \): pressure of initial shock wave front
- \( T \): environment temperature
- \( P_0 \): environment pressure
- \( A \): the pre factor of apparent index
- \( r_0 \): the charge radius
- \( c \): the velocity of detonation product
- \( t \): the reaction duration

1. Introduction

Reactive material is usually composed of two or more non explosive materials, such as polymer/metal or metal/metal mixture. reactive material has been used in various high energy devices[1, 2]. It mainly depends on the exothermic reaction among the components of the reactive material to improve the energy density and total energy output. Compared with inert material, reactive material reacts chemically and releases a lot of heat after being driven by explosion, which can strengthen the
overpressure of initial air shock wave and improve the damage ability to the target.

Scholars at home and abroad have carried out a lot of experimental research work in characterizing the energy release characteristics of impact reaction of reactive material [3, 4], but the existing research has not paid enough attention to the calculation model of overpressure of air shock wave produced by reactive material driven by explosion. Clemenson et al. [5, 6] studied the enhanced reaction characteristics of aluminum based casing driven by explosion, and thought that the fine particles less than 10μm produced during the initial crushing of casing played a key role in the enhanced reaction. Through the static explosion test, it is found that the pressure effect of the reactive material is significantly improved under the explosion driving. Guadarrama et al.[7] made an experimental study on the peak overpressure of shock wave produced by powder materials commonly used as pyrotechnic agents under the driving of explosion. Compared with inert materials, pyrotechnic materials can improve the peak overpressure of air shock wave. Wang et al. [8] conducted an experimental study on the energy output characteristics of active fragments, and obtained the peak overpressure generated by active fragment of three different formulations in the target container. Xiong [9] and Ames[10] analyzed the impact energy release characteristics of reactive material from the point of end-point effect and quasi closed secondary impact reaction experiment. Compared with inert materials, the quasi-static pressure of reactive material increased significantly. Although a lot of experimental research work has been carried out on the peak overpressure of shock wave generated by reactive material at home and abroad, there is little research on the calculation model of shock wave overpressure generated by reactive material.

In this paper, the reaction behavior of reactive material casing driven by explosion is studied by numerical simulation to find out the reaction law of reactive material. In this paper, the chemical energy released by the reactive material is introduced to calculate the initial parameters of the air shock wave generated by the reactive material driven by the explosion, and then calculate the relative volume of the initial detonation product. Finally, based on dimensional analysis, the theoretical model of overpressure of air shock wave generated by reactive material driven by explosion is established, and the test results of peak overpressure of air shock wave are compared, which provides reference for the engineering application of reactive material such as Al/PTFE.

2. Numerical simulation

2.1. Numerical model

Due to the symmetrical characteristics of the load, boundary conditions and structure, a quarter model of warhead structure is established. The numerical model established is consistent with the structure of the test device. In the numerical model, the explosive charge named 8701 is a cylinder of Φ30mm×37mm with a density of 1.7g/cm³ and a charge mass of 44g, the casing is Al/PTFE with an outer diameter of 50mm and an inner diameter of 34mm, the spacer is a nylon cylindrical shell with a wall thickness of 1.7mm. The numerical model is shown in figure. 1, where point labeled by 1-12 is the pressure observation point.
In this paper, the Lagrange/Euler coupling method is used to calculate the whole change process of the casing driven by explosion. The mesh of explosive and air is divided by Euler method. Johnson cook strength model and shock equation of state are used to describe the high temperature, high pressure and high strain rate of PTFE/Al casing, detonator base and lower cover plate. The material model are shown in table 1[11]. In addition, Stochastic model in AUTODYN@ software is used to simulate the fracture process of Al/PTFE shell under the action of explosive detonation.

| Component                              | Material       | $\rho$/(g.cm$^{-3}$) | Equation of state | Strength model | Erosion of standard |
|----------------------------------------|----------------|---------------------|-------------------|----------------|---------------------|
| Casing                                 | Al/PTFE        | 2.27                | Shock             | Johnson Cook   | Principal Strain    |
| Detonator and bottom cap               | Steel 1006     | 7.83                | Shock             | Johnson Cook   | Johnson Cook        |
| Spacer                                 | Nylon          | 1.14                | Shock             | Von Mises      | Hydro               |
| Explosive                              | 8701           | 1.71                | JWL               | -              | -                   |
| Air                                    | /              | 0.001225            | Ideal Gas         | -              | -                   |

2.2. Numerical results
In order to verify the effectiveness of the numerical simulation method, scholars [12, 13] conducted numerical simulation and experimental research on the impact of active fragments on the target plate. When the peak stress of the observation point is lower than the critical reaction threshold, the chemical reaction can not take place in the reactive material. The simulation results are consistent with the test results, which can show the validity of the numerical model.

The peak stress distribution in the reactive material during the explosion driving process is shown in figure 2. It can be seen from the figure that the internal stress peaks of observation points 1, 5 and 9 are higher than the critical response threshold, and the internal stress peaks of other observation points do not reach the critical response threshold. It shows that the shell of the reactive material does not react completely under the driving of explosion in the test, that is to say, some of the reactive material close to the explosive react and release energy, while the rest of the reactive material do not react chemically. The peak value of internal stress at observation points 1 and 9 is significantly higher than that at observation point 5, which is due to the restriction of cover plate at both ends of the explosive.
device and the reflection of stress wave.

3. Theoretical derivation
In this paper, the initial parameters of shock wave produced by the explosion of reactive material are calculated, and then the peak value of air shock wave overpressure is deduced.

3.1. Initial parameters of air shock wave
After the explosive charge in the air is detonated, the explosive detonation produces detonation products and high pressure. The detonation product expands outward at a very high speed and pressure, and compresses the adjacent air medium strongly, making its pressure, density and temperature jump suddenly, forming the initial shock wave. When the detonation product is separated from the initial shock wave, the pressure of the detonation product is equal to the pressure of the initial shock wave front, and the velocity of the detonation product is equal to the velocity of the air behind the initial shock wave front[14, 15]. The schematic diagram of the initial shock wave parameters is shown in figure 3, where $P_0$ is the air pressure without disturbance.
When the pressure of explosive product expands from \( P_{\text{H}} \) to \( P_x \), the velocity of product increases from \( u_{\text{H}} \) to \( u_x \), which satisfies the following relationship[15].

\[
    u_x = u_{\text{H}} + \int_{P_{\text{H}}}^{P_x} \frac{\rho_x v_x}{c} \, dp
\]

(1)

Where \( u_{\text{H}} \) is the velocity of detonation product behind the detonation wave front, \( u_x \) is the particle velocity of initial shock wave front, \( v_x \) is the volume of detonation product, \( c \) is the velocity of detonation product, \( P_x \) is the pressure of initial shock wave front, and \( P_{\text{H}} \) is the C-J pressure of detonation.

Assuming that the expansion process of explosive detonation product is divided into two stages[16], the second stage pressure (critical pressure) is \( P_s \), and considering the chemical energy released by the reactive material, the expression of \( P_s \) can be obtained as follows.

\[
    P_s = \frac{P_m}{2} \left[ \frac{K-1}{\gamma-1} \left( \frac{Q_{\text{ch}}}{Q_m} + \frac{Q_{\text{m}}}{Q_m} \right) \right] \left( \frac{\gamma-1}{K-1} \right)^{\frac{K}{\gamma}}
\]

(2)

Where, the explosive product parameter \( k \) is 1.4, \( \gamma = 3 \), \( Q_{\text{ch}} \) is the explosive heat of the charge, \( Q_{\text{m}} \) is the heat per unit volume released by the reaction of the reactive material, \( y \) is the degree of reaction, and \( v_{\text{H}} \) is the initial volume of the charge.

Based on the detonation theory [15] and formula (1), the following formula can be obtained

\[
    u_x = \frac{D}{\gamma + 1} \left[ 1 + \frac{2\gamma}{\gamma - 1} \left( 1 - \frac{P_{\text{H}}}{P_{s}} \right) \right] + \frac{2C_x}{K - 1} \left[ 1 - \left( \frac{P_{\text{H}}}{P_{s}} \right)^{\frac{K}{\gamma}} \right]
\]

(3)

According to the above formula, the relationship between the velocity \( u_x \) of the wave front particle of the initial shock wave and the pressure \( P_x \) of the wave front can be determined. Since the initial shock wave of explosion is strong shock wave, the strong shock wave relation is satisfied.

\[
    u_c = \left[ 2P_x/\rho_a(K_\alpha + 1) \right]^{1/2}
\]

(4)

Where, \( K_\alpha \) is the isentropic index of undisturbed air, taking 1.2, \( \rho_a \) is the density of undisturbed air, taking 1.225\,\text{kg}\cdot\text{m}^{-3}.

According to the above formula, the initial parameters \( P_x \) and \( u_x \) of shock wave in air explosion can be calculated.

For 8701 and other ideal explosives, the pressure form of JWL equation of state is as follows[14].

\[
    p = A(1-\omega R_1 V^1)e^{R_1 V} + B(1-\omega R_2 V^1)e^{R_2 V} + \omega e V^1
\]

(5)

The isentropic equation through point C-J is as follows.

\[
    p_s = A_0 e^{R_1 V} + B_0 e^{R_2 V} + C_0 (\omega + 1)
\]

(6)

Where: \( A, B, C, R_1, R_2 \) and \( \omega \) are linear coefficients, \( R_1, R_2 \) and \( \omega \) are non-linear coefficients, \( e \) is the internal energy of detonation product per unit volume, \( V = \rho V_0 \) is the relative specific volume of detonation product (volume of detonation product / volume of unexploded explosive), and \( p_s \) is the pressure of detonation product.

The parameters of JWL state equation of the charge named 8701 are shown in table 2. The calculated initial parameters of air shock wave are shown in table 3.
Table 2. JWL Equation of State Coefficient of 8701 Explosive

| A/GPa | B/GPa | R₁ | R₂ | ω |
|-------|-------|----|----|---|
| 881.45 | 10.459 | 4.8 | 1 | 0.31 |

For the reactive material, the improved JWL equation of state is used to describe it.

\[ p = A(1 - \omega R_1 V^{-1})e^{R_1 V} + B(1 - \omega R_2 V^{-1})e^{R_2 V} + \omega (e + yQ_0)V^{-1} \]  

(7)

Arrhenius model [17] can accurately describe the reaction kinetics of reactive material. Arrhenius model combined with Avrami-Erofeev's n-dimensional nuclear / growth control reaction model [18] can obtain the reaction rate of reactive material.

\[ \frac{dy}{dt} = Ae^{-E_u/RT}n(-\ln(1-\gamma))^{(n-1)/n} \]  

(8)

Where: \( A \) is the pre factor of apparent index, \( t \) is the reaction duration, \( E_u \) is the apparent activation energy, \( T \) is the absolute temperature, \( R_0 \) is the molar gas constant, and \( n \) is the time index related to the reaction mechanism.

Table 3. Reaction parameters Al/PTFE typical reactive material

| Material type | Mass fraction % | \( Q_m \) (kJ·g⁻¹) | \( \rho \) (g·cm⁻³) | \( E_u \) (kJ·mol⁻¹) | \( n' \) |
|---------------|----------------|---------------------|-------------------|-----------------|------|
| Al/PTFE-[19]  | 24.0:76.0      | 3.38                | 2.27              | 50.8            | 0.63 |

Guadarrama et al. [7] carried out the research on the coupling effect of reactive material and explosives, and measured the peak overpressure of air shock wave generated by reactive material driven by explosion. In combination with the above formula, the initial shock wave parameter \( p_s \) and the relative specific volume \( V_s \) of the initial detonation product can be determined as shown in table 4.

Table 4. Initial shock wave parameters of different materials driven by explosion

| Material type               | No.       | \( m/g \) | \( Q_m/KJ\cdot g^{-1} \) | Test value/kPa | \( p_s/MPa \) | \( V_s \) |
|-----------------------------|-----------|-----------|--------------------------|----------------|--------------|--------|
| Alumina[7]                  | Al₂O₃     | 8.91      | 0                        | 91.5           | 90.0         | 38.67  |
| Mechanically alloyed powder[7] | Al-Mg (NJIT)-1 | 11.30     | 16.1                     | 137.5          | 144.5        | 31.32  |
|                             | Al-Mg (NJIT)-2 | 9.95      | 16.9                     | 139.9          | 147.0        | 31.46  |
| Flake aluminum[7]           | Al(Flake) | 9.70      | 15.5                     | 135.2          | 142.5        | 31.97  |
| Spherical aluminum powder(repeats) [7] | Al H-2-1 | 9.95      | 16.8                     | 120.6          | 146.8        | 28.99  |
|                             | Al H-2-2 | 10.83     | 15.5                     | 123.9          | 142.6        | 30.04  |
|                             | Al H-2-3 | 10.02     | 16.8                     | 125.4          | 146.7        | 29.30  |
| Atomized alloy powder[7]    | Al-Mg(Valimet) | 9.62      | 18.3                     | 130.6          | 144.6        | 30.74  |

3.2. Calculation of overpressure peak value of air shock wave caused by explosion of reactive material

Firstly, the empirical formula of the peak overpressure of air shock wave can be obtained by dimensional analysis method as follows[20].

\[ p_s = \frac{m}{A}\frac{Q_m}{V_m} \]
\[ \frac{\Delta p}{p_s} = f\left(\frac{\beta V}{R}, \frac{p_0}{p_s}\right) \]  

(9)

Where, \( \Delta p=p-p_0 \) is the front pressure of air shock wave, \( p_0 \) is the air pressure without disturbance, \( R \) is the distance from the explosion center, \( V=(r_x/r_0)^3 \), \( r_0 \) is the charge radius, \( r_x \) is the distance from the explosion center when the initial shock wave is formed.

Based on dimensional analysis, it is found that the peak overpressure of air shock wave should follow the law of geometric similarity. That is to say, the non dimensional peak overpressure of air shock wave generated by the explosion of reactive material in the air is a function of the wave front pressure of the initial shock wave and the relative volume of the detonation product. The physical equation of peak overpressure of air shock wave is as follows

\[ \Delta p = p_x f\left(\frac{\beta V}{R}\right) \]  

(10)

In general, the empirical formula of peak overpressure of air shock wave [14] is used to describe the variation of blast wave pressure with distance.

\[ \Delta p = f\left(\frac{\sqrt{\omega}}{R}\right) \]  

\[ \Delta p = 0.082\frac{\sqrt{\omega}}{R} + 0.265\left(\frac{\sqrt{\omega}}{R}\right)^2 + 0.686\left(\frac{\sqrt{\omega}}{R}\right)^3 \]  

(12)

Where, \( 1 \leq R = R/\omega^{1/3} \leq 15 \) is called relative distance, \( \omega=MQ_v/Q_{\text{TNT}}, Q_0 \) is the detonation heat of 8701, \( Q_{\text{TNT}} \) is the detonation heat of TNT, \( H/\omega^{1/3} \geq 0.35 \) (\( H \) is the height of the explosive center from the ground).

The final form of equation (10) is as follows.

\[ \Delta p = p_x (A_1\frac{\beta V}{R} + A_2\left(\frac{\beta V}{R}\right)^2 + A_3\left(\frac{\beta V}{R}\right)^3) \]  

(13)

Where, the coefficients \( A_1, A_2 \) and \( A_3 \) are fitted by the test data in Table 5.

Therefore, the peak value of air shock wave overpressure is as follows.

\[ \Delta p = p_x (0.0222\frac{\beta V}{R} - 0.524\left(\frac{\beta V}{R}\right)^2 + 6.788\left(\frac{\beta V}{R}\right)^3) \]  

(14)

4. Explosion experiment

4.1. Experimental principle

The explosive driving device is mainly composed of detonator base, booster charge, explosive charge, nylon spacer, casing and lower cover plate. The material of casing is Al/PTFE (the mass percentage is 26.5:73.5). The detonator base is mainly used to fix the detonator and booster column and constrain the detonation product together with the lower cover plate, so as to control the direction of detonation product dispersion. The structure diagram of the explosion driving device is shown in figure 4. In the preparation of Al/PTFE materials, the pressing sintering process is used. The sintering process is an important means to obtain the final structural strength of Al/PTFE. This method has the advantages of low cost and simple process. The average particle size of Al powder is about 75μm, and PTFE is a flocculent material. The explosive driving device of reactive material is shown in figure. 5.
In the experiment, the charge was placed on the PVC plastic pipe support, 1.5m from the ground. YD-202 piezoelectric pressure sensor is used to measure the peak overpressure of free field air shock wave driven by explosion. The dynamic process of the fireball is photographed by high-speed photography at the speed of 5000 frames per second to capture the transient evolution of the fireball in the explosion driving process of the Al/PTFE casing and measure the instantaneous velocity of the detonation wave at each point in the whole detonation process. The horizontal distance between explosion driving device and pressure sensor is 1.8m, and the horizontal distance between explosion driving device and high-speed photography is 22m. In order to ensure the scientifi city and rationality of the experiment results, the experiment is repeated twice.

4.2. Experimental results
Driven by the explosion, the explosive products of high density and high pressure expand rapidly, and the surrounding medium is impacted and compressed to form a sudden interface, and then the shock wave front is formed.

Figure 6 and figure 7 show the propagation of air shock wave generated by Al₂O₃/PTFE and Al/PTFE materials driven by explosion respectively. It can be seen from figure 6 and figure 7 that the air shock wave is separated from the detonation product, and gradually propagates outward with the increase of time. figure 6(a) and figure 6(c) are the test phenomena of Al₂O₃/PTFE material fragments before and after reaching the steel plate. It can be found that Al₂O₃/PTFE material does not produce fire light after hitting the steel plate. figure 7(a) and figure 7(c) are the test phenomena of Al/PTFE material fragments before and after reaching the steel plate. It can be found that the Al/PTFE material produces fire light after hitting the steel plate. On the other hand, the fire light of Al/PTFE material increases obviously at different time. The reason is that the Al/PTFE materials do not react completely under the detonation pressure, only some of the reactive material participate in the reaction and release energy, and the unreacted fragments fly around. The simulation results are in good agreement with the test results, both of which show that the Al/PTFE material does not react completely under explosive driving. According to figure 6 and figure 7, the shock wave velocity at different distance from the explosion center can be measured.
According to figure 6 and figure 7, the shock wave velocity at different distance from the explosion center can be measured. Figure 8 shows the curve of shock wave velocity changes with time. It can be seen from figure 8 that the overall trend with time of air shock wave velocity of the two reactive material is the same. With the increase of time, the velocity of shock wave decreases. At different times, the velocity of shock wave generated by Al₂O₃/PTFE is lower than that by Al/PTFE. From 0.8ms to 1.4ms, the velocity of shock wave produced by the two materials decreases linearly, and the difference between them is small. After 1.4ms, the velocity of shock wave generated by Al₂O₃/PTFE decreases faster than that by Al/PTFE, and the difference between them increases gradually. This is because driven by the explosion, part of Al/PTFE undergoes chemical reaction and releases energy, which strengthens the air shock wave.

Based on the theoretical model of overpressure peak of blast air shock wave, the overpressure peak of air shock wave generated by 8701 ideal explosive, Al/PTFE and Al₂O₃/PTFE is calculated as shown
in table 5 with experimental results. From the data in table 5, it can be seen that the relative error between the theoretical calculation results of the peak overpressure of air shock wave and the actual experimental results is within 6%, which meets the engineering application requirements.

| Material type | No. | R/m  | m/g  | $Q_0$/KJ.g$^{-1}$ | Experimental results/kPa | Theoretical calculation results/kPa | Relative error% |
|---------------|-----|------|------|-------------------|--------------------------|-----------------------------------|----------------|
| 8701          | 1   | 2.2  | 44.0 | 5.12              | 27.1                     | 28.7                              | 6.0            |
| Al/PTFE       | 2   | 1.8  | 87.78| 8.87              | 43.3                     | 41.8                              | 3.6            |
| Al$_2$O$_3$/PTFE | 3 | 1.8  | 87.45| 0                 | 30.2                     | 30.7                              | 1.7            |

5. Conclusion
In this paper, the typical reactive material Al/PTFE is taken as the research object. By calculating the initial parameters of the air shock wave generated by the explosion of the reactive material in the air, the peak value of the shock wave overpressure is deduced, and the following conclusions are obtained:

1) The casing made by Al/PTFE material does not react completely under explosive driving. The numerical simulation results are consistent with the experimental results, which shows that the numerical simulation method and material model parameters used in this paper are reliable. The unreacted fragments fly around, impact the steel plate during the process of flying and react subsequently. The velocity of air shock wave produced by the charge with reactive material casing is higher than that of the charge with inert material casing.

2) The calculation model of the peak value of air shock wave overpressure established in this paper can well describe the propagation law of air shock wave generated by reactive material, and provide theoretical support for the evaluation of the power of air shock wave produced by reactive material driven by explosion.

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