Study on theoretical calculation of quasi-static pressure for aluminized explosive in confined space

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Abstract. The process of the explosion damage in confined space mainly involves two parts, shock wave pressure effect and quasi-static pressure effect. A complicated afterburning reaction occurs in the internal explosion of aluminized explosives, not only enhancing the intensity of the shock wave, but also having a great influence on the final quasi-static pressure. A theoretical calculation model of final quasi-static pressure for aluminized explosive in confined space considering afterburning effect was proposed, based on the analysis of chemical reaction, the law of conservation of energy and the improved Jones-Wilkins-Lee equation of state. The factor that the volume of gaseous explosive products decreases in the afterburning reaction was also taken into consideration. The results of RDX-based and HMX-based charges calculated by the model were then analyzed and compared with the references’ experimental results as well as Anderson’s empirical formulas to verify the reliability and correctness of the proposed model. The results show that: the final quasi-static pressure of aluminized explosive calculated by the theoretical calculation model is in good agreement with the results of experimental measurement in the papers and the relative error doesn’t exceed 10%; the Anderson’s empirical formula is inapplicable to predict the final quasi-static pressure of the aluminized explosive in confined space. The study in this paper can provide a better theoretical calculation model to predict the final quasi-static pressure of aluminized explosives and provide some reference and guidance for the assessment of internal explosion damage of aluminized explosive and the design of explosive-resistant structures.

1. Introduction

With the rapid development of modern military technology, the range of combat and defense has extended from ground operations on land to the target naval ships and underground fortifications. Under this circumstance, aluminized explosive is applied to get better damage of the confined space. Aluminized explosive are composed of high-energy explosive, aluminum power, binders and oxidizer. The process of the explosion damage in confined space mainly involves two parts, shock wave pressure effect and quasi-static pressure effect. After the explosion, the shock wave first acts on the target, causing the structure to be pre-damaged and the multiple reflections of the shock wave in the confined space cause the aluminum power to fully mix with the explosion products and air. Then the
afterburning reactions occur which has a great influence on the quasi-static pressure. The quasi-static pressure formed causes substantial damage to the surrounding structure.

The influence of afterburning effect on the quasi-static pressure has been extensively investigated. Anderson [1] fitted an empirical formula that can predict the quasi-static pressure of some high-energy explosives, based on the dimensional analysis and a large number of experimental data. The quasi-static pressure effect has a long acting time and a large impulse and the total energy released is the only parameter of the final quasi-static pressure [2], so that the US Naval Surface Weapon Center [3] used quasi-static pressure as the only power assessment parameter when comparing the power of different explosives in confined space. Waldemar A. Trzcin´ski [4] performed explosion experiment with RDX-based aluminized explosives containing 15%-60% aluminum power in the 0.15 and 7 m³ chambers which confirmed the influence of the afterburning reactions of aluminized explosive to quasi-static pressure and the experimental results show that the shape and content of the aluminum power affect the actual performance of the internal explosion of the aluminized explosive.

Zhang Yulei et al. [5] measured the intensity of shock wave, impulse and quasi-static pressure of the thermobaric explosive and TNT charge in the confined space, then through the theoretical calculation and experiment analysis, it was concluded that these parameters of the thermobaric explosive are higher than the same mass TNT charge. Duan Xiaoyu [6] made a study on RDX-based aluminized explosive containing 15%-45% 50μm aluminum powder, which concluded that the quasi-static pressure of internal explosion showed a trend of increasing first and then decreasing with the content of aluminum powder and began to decrease when the content was 40%. Wang Xinglong [7] studied the completeness of the reaction of aluminum powder in the explosion of the thermobaric explosive, and concluded that the reaction degree of aluminum powder increased with the increase of the confined space volume and the rate of increase gradually decreased. When the confined space volume exceeded 1.8m³, it had no effect on the reaction degree. Zhengbo et al. [8] observed the dispersal process of explosive products of the high-energy explosive, aluminized explosive and thermobaric explosive, indicating that the explosive range of thermobaric explosive had been formed during the detonation period and early afterburning period of the explosion. During the expansion process, the explosive products and metal particles had already reacted with the oxygen in the confined space.

A large number of experiments have been carried out on the internal explosion of aluminized explosives at home and abroad, but there is still no good theoretical calculation model of final quasi-static pressure in the internal explosion of aluminized explosives. Therefore this paper established such a model, based on the chemical reaction analysis, the law of conservation of energy and the improved Jones-Wilkins-Lee equation of state, and then verified the reliability and accuracy of the model according to the experimental data in the references.

2. Reaction stage analysis of the internal explosion

Aluminized explosive is one of the typical non-ideal explosives and the aluminum powder it contains doesn’t react on the C-J plane. At present, there are three main explosion mechanism: secondary reaction theory, the inert thermal dilution mechanism and the chemical heat dilution theory [9].

Based on the three theories, A.Hahma and K.Palovuori et al. [10] divided the reaction process of
the aluminized explosive into three stages:

1) The first stage: anoxic detonation of high-energy explosive, lasting about 0.1 μs

2) The second stage: anaerobic combustion, lasting about hundreds of microseconds. The explosion products like CO, CO₂, H₂O produced in the first stage react with the aluminum powder under the high temperature and high pressure environment. There is no oxygen in the air to participate in the reaction at this stage.

3) The third stage: aerobic combustion, lasting about tens of milliseconds. The explosion products and aluminum powder react with the oxygen in the air, increasing the temperature and pressure of the gaseous explosion products.

In this paper, the explosion heat of aluminized explosive is divided into two parts. The first part is detonation heat, which is produced in the stage of anoxic detonation of high energy explosive. The second part is afterburning heat, which consists of the energy released by anaerobic combustion and aerobic combustion. And because aluminized explosives are mixed explosives, having no fixed molecular formula, the explosion heat of aluminized explosive is often calculated according to its atomic composition.

The atomic number of each element of the aluminized explosive can be calculated by the formula (1):

$$n_s = \sum \frac{n_{s,i} w_i}{M_i}$$

Where $n_s$ is the number of $s$ atom in the composition of aluminized explosive; $w_i$ is the mass percentage of the $i$-th component; $M_i$ is the molar mass of the $i$-th component; $n_{s,i}$ is the number of $s$ atom in the $i$-th composition.

Thus the atomic composition expression of aluminized explosive is $C_aH_bN_cO_dAl_f$.

During the anaerobic detonation phase, reactions take place in the molecule of the high-energy explosive, generating explosive products. The detonation heat can be calculated based on the atomic composition expression of aluminized explosive and Hess’s law, regardless of the physical charge structure, only considering the chemical charge structure.

$$C_aH_bN_cO_d \rightarrow \frac{b}{2}H_2O + \frac{c}{2}N_2 + \left(d - \frac{b}{2} - a\right)CO_2 + \left(2a - d + \frac{b}{2}\right)CO$$

The equation is only applicable when the negative oxygen balance value is small. If there is no more oxygen, the excess C forms a single substance. According to the Hess’s law, the detonation heat can be calculated by the formula (3).

$$Q_v = \sum n_{p,i} \Delta H_{f,p,i}^0 - \sum n_{m,j} \Delta H_{f,m,j}^0 - n_g RT$$

Where $n_{p,i}$ is the molar quantity of the explosive product $i$; $\Delta H_{f,p,i}^0$ is standard enthalpy of formation for explosive product $i$, J/mol; $n_{m,j}$ and $\Delta H_{f,m,j}^0$ are the molar quantity and the standard enthalpy of formation of the high-energy explosive $j$; $n_g$ is the total mole number of gaseous explosive products; $R$ is the universal gas constant, 8.314J/(mol*kJ); $T$ is ambient temperature, 298.15K.

$$n_g = \frac{b}{2} + a + \frac{c}{2} (mol)$$

In the afterburning reaction phase, aluminum powder is considered to react firstly with explosive products and then with oxygen in the air. However, actually, explosive products and aluminum powder...
have reacted with oxygen in confined space in the expansion process, so the anaerobic combustion and aerobic combustion cannot be separated for analysis. For the simplicity of calculation, it is assumed that the four oxidizing gases in the secondary reaction of aluminum powder participate in the reaction in the same proportion as their initial molar ratio (i.e. after the detonation of the main explosives), and the following reaction formula is formed like equation (5):

\[
\frac{2n_1+4n_2+2n_3+4n_4}{3} Al + n_1H_2O + n_2CO_2 + n_3CO + n_4O_2 \rightarrow \frac{n_1+2n_2+n_3+2n_4}{3} Al_2O_3 + n_4H_2 + (n_2 + n_3)C + \frac{1}{3}(950n_1 + 2171n_2 + 1344n_3 + 3348n_4)
\] (5)

Where \(n_i\) (i=1,2,3) is the mole number of H\(_2\)O, CO\(_2\) and CO generated by high energy explosives per unit mass, and \(n_4\) is the mole number of oxygen of the air in the confined space.

3. Theoretical calculation model for internal explosion

The Jones-Wilkins-Lee (JWL) equation of state has been used to accurately describe the pressure-volume-energy behavior of the detonation products of explosives, which can describe both the high pressure and low pressure sections of the explosive impact load. As is well known, aluminized explosive has the secondary reaction. To describe the effects of the energy release of the secondary reaction, a late energy release term \(\lambda Q\) was already added into the traditional JWL EOS, yielding \(\frac{\omega(E + \lambda Q)}{\theta}\), making it as an improved form to fit for an aluminized explosive, the expression is:

\[
p = A(1 - \frac{\omega}{R_1\theta})e^{-\frac{R_1\theta}{E}} + B(1 - \frac{\omega}{R_2\theta})e^{-\frac{R_2\theta}{E}} + \frac{\omega(E + \lambda Q)}{\theta}
\] (6)

Where \(p\), \(\theta\) and \(E\) are the pressure, relative volume and relative energy of the detonation products, respectively; \(A\), \(B\), \(R_1\), \(R_2\), \(\omega\) are the adjustable parameters; \(\lambda\) is the mass fraction of the aluminum powder which finish reaction and \(Q\) is the total heat released by the secondary reaction of the aluminum powder.

According to Reference [11], the afterburning reaction not only releases a large amount of energy, but also results in the decrease of the quantity of gaseous detonation products, which has an influence on the final quasi-static pressure. Based on such a conception a new EOS is proposed.

\[
p = A(1 - \frac{\omega}{R_1\theta})e^{-\frac{R_1\theta}{E}} + B(1 - \frac{\omega}{R_2\theta})e^{-\frac{R_2\theta}{E}} + \frac{\omega(E + \lambda Q(1 - \lambda z))}{\theta}
\] (7)

Where \(z\) is the total decreasing percentage of gaseous explosion products when the afterburning reaction comes to an end.

In this paper, the first and second exponential high-pressure terms on the right-hand side of the equation (7) are abbreviated as A+B term. And the value of the (A+B) term as a function of the density of the final gaseous explosion products is shown in the figure 1.
Figure 1. The value of (A+B) term as a function of the density of gaseous explosion products.

It can be concluded that the pressure of (A+B) term decreases rapidly with the decrease of the density of the final gaseous explosion products. When it is less than 500 kg/m$^3$, the pressure of (A+B) term is approximately equal to 0, and when it is happened in a confined space, it always far less than 500 kg/m$^3$.

And in the formula:

$$\begin{aligned} E &= \rho_0 e \\
Q &= \rho_0 q \\
\theta &= \rho_0 / \rho \end{aligned}$$

So the new EOS can be simplified as follows:

$$P = \rho \omega \left[ e + \lambda q(1 - \lambda z) \right]$$  \hspace{1cm} (8)

Where $\omega = \gamma - 1$; $\gamma$ is the adiabatic indexes of the air-explosion gas mixture; $e$ is the detonation heat of the aluminized explosive, e=-Q,$\text{KJ/Kg}$; $q$ is the total afterburning heat of the aluminized explosive, KJ/Kg.

When the internal explosion in the confined space is complete and the gaseous explosion products fill the whole confined space, according to the law of conservation of mass, equation (9) can be obtained.

$$\rho = m/V$$  \hspace{1cm} (9)

Where $m$ is the mass of the aluminized explosive, Kg; $V$ is the volume of the confined space, m$^3$.

According to reference (12), in the mixed multi-component case, the calculation of $\lambda$ can be written as follows:

$$\gamma = \frac{\sum_{i=1}^{N} n_i \times C_{p,m,i}}{\sum_{i=1}^{N} n_i \times C_{p,m,i} - R \sum_{i=1}^{N} n_i}$$  \hspace{1cm} (10)

Where $C_{p,m,i}$ is the molar constant pressure specific heat ratio of component $i$.

Therefore $\gamma$ can be calculated by the equation (10) and the final molar quantities of the explosive
products.

4. Analysis on calculation model of the afterburning reaction of aluminized explosive

For the afterburning reaction phase of the aluminum powder, two situations need to be discussed.

1) The oxidizing gases in the explosion products and the oxygen in the air can completely react the aluminum powder ($\lambda = 1$). The situation meets the following condition:

\[ f < \frac{2n_1 + 4n_2 + 2n_3 + 4n_4}{3} \]  \hspace{1cm} (11)

Where $f$ is the number of aluminum atoms of aluminized explosive.

According to the equation (5), the energy $q$ (kJ) released by the afterburning reaction of aluminized explosive per unit mass can be written:

\[ q = \frac{f}{2(n_1 + 2n_2 + n_3 + 2n_4)} \times (950n_1 + 2171n_2 + 1344n_3 + 3348n_4) \]  \hspace{1cm} (12)

Meanwhile,

\[ \begin{cases} z = \frac{\Delta n}{n_g} \\ \Delta n = \frac{3f(n_2 + n_3)}{2(n_1 + 2n_2 + n_3 + 2n_4)} \end{cases} \]  \hspace{1cm} (13)

2) The oxidizing gases in the explosion products and the oxygen in the air can not completely react the aluminum powder ($\lambda < 1$). The situation meets the following condition:

\[ f > \frac{2n_1 + 4n_2 + 2n_3 + 4n_4}{3} \]  \hspace{1cm} (14)

The energy $q_R$ (kJ) released by the afterburning reaction of aluminized explosive per unit mass can be written:

\[ q_R = \frac{1}{3} (950n_1 + 2171n_2 + 1344n_3 + 3348n_4) \]  \hspace{1cm} (15)

The remaining mole number of aluminum powder after the final afterburning reaction is:

\[ n_{Al} = f - \frac{2(n_1 + 2n_2 + n_3 + 2n_4)}{3} \]  \hspace{1cm} (16)

The extent of aluminum powder is:

\[ \lambda_{max} = \frac{n_{Al}}{f} \]  \hspace{1cm} (17)

And

\[ \begin{cases} z_R = \frac{\Delta n}{n_g} \\ \Delta n = \frac{3f(n_2 + n_3)}{2(n_1 + 2n_2 + n_3 + 2n_4)} \end{cases} \]  \hspace{1cm} (18)

However, the $q_R$ in equation (15) and the $z_R$ in equation (18) are the values when the extent of aluminum powder reaches the actual maximum value $\lambda_{max}$, not the cases when the aluminum powder reaction degree $\lambda$ reaches 1. Therefore, when the two characters are used in the equation (8), they need to be corrected:
When aluminized explosive of different mass explode in the confined space of different volume, corresponding \( \omega, \rho, e, q, z, \lambda \) can be obtained, substituted into equation (8) and then the final quasi-static pressure can be calculated.

However, it should be noticed that the theoretical calculation model of the quasi-static pressure for aluminized explosive in this paper is only applicable to the aluminized explosive without oxidants. The total amount of the gaseous detonation products of aluminized explosive with oxidants is closely related to the decomposition rate of oxidants. But this model doesn’t take into account the decomposition rate of the oxidant. And the influence of the aluminum powder size on the quasi-static pressure is also not included, which will be the following work.

5. Analysis on the references of the quasi-static pressure of aluminized explosive in internal explosion

In this section, the experimental data of the quasi-static pressure of RDX-based and HMX-based charges with different aluminum contents in some references are selected.

In reference [6], an internal explosion experiment of 0.1kg RDX-based aluminized explosive was carried out in a 500L cylindrical explosion tank which is composed of a spherical cap on the top and a welded plate on the sides and bottom. And the corresponding quasi-static pressures were measured.

| Number | RDX/% | Al/% | Bind/% | Quasi-static pressure/Mpa |
|--------|-------|------|--------|--------------------------|
| HL-15  | 80    | 15   | 5      | 0.6798                   |
| HL-25  | 70    | 25   | 5      | 0.7959                   |
| HL-30  | 65    | 30   | 5      | 0.8869                   |
| HL-35  | 60    | 35   | 5      | 0.9057                   |
| HL-40  | 55    | 40   | 5      | 1.0343                   |
| HL-45  | 50    | 45   | 5      | 0.8348                   |

In reference [13], an internal experiment of 1kg HMX-based thermobaric explosive was carried out in an explosion tank with an inner diameter of 2.6m and a volume of 26m\(^3\). The corresponding quasi-static pressure was measured.

| Components | Gaseous environment | Quasi-static pressure/Mpa | Calculation result/Mpa | Relative error/% |
|------------|---------------------|---------------------------|------------------------|-----------------|
| HMX: Al: Bind | 64.4: 30: 5.6 | \( \text{空气} \) 0.194 | 0.191 | 1.55 |
|            |                    | \( \text{氮气} \) 0.108 | / | / |
In reference [14], an internal experiment of 40g RDX-based aluminized explosive was carried out in an cubic explosion tank with sides of 0.6m. The corresponding quasi-static pressure was measured.

| Components         | \( \rho/(g/cm^3) \) | Quasi-static pressure /Mpa | Calculation result /Mpa | Relative error /% |
|--------------------|----------------------|----------------------------|-------------------------|-------------------|
| RDX/Al/wax(80/15/5) | 1.757                | 0.65                       | 0.613                   | 5.69              |
| RDX/wax(95/5)      | 1.675                | 0.53                       | 0.465                   | 12.26             |

In reference [4], internal experiments of RDX-based aluminized explosive were carried out in explosion tanks with the volume of 0.15m³ and 7m³ respectively. The corresponding quasi-static pressures were measured.

| V/m³   | m/g | RDX/% | Al/% | Bind/% | Quasi-static pressure /Mpa |
|--------|-----|-------|------|--------|---------------------------|
| 0.15   | 25  | 79.9  | 15   | 5.1    | 0.564                     |
|        |     | 65.8  | 30   | 4.2    | 0.61                      |
|        |     | 51.7  | 45   | 3.3    | 0.64                      |
|        |     | 37.6  | 60   | 2.4    | 0.632                     |
| 7      | 200 | 79.9  | 15   | 5.1    | 0.138                     |
|        |     | 65.8  | 30   | 4.2    | 0.160                     |
|        |     | 51.7  | 45   | 3.3    | 0.171                     |
|        |     | 37.6  | 60   | 2.4    | 0.183                     |

The quasi-static pressure in different references may have some deviations, because there is no accepted method for determining the value of quasi-static pressure in an internal explosion and the experiment test technology has a great influence. Therefore we introduced the Anderson empirical formula which was summarized based on a large number of experimental data for comparative analysis. This can also make up for the lack of experimental data.

\[
\tilde{p} = \begin{cases} 
1.336 \left( \frac{W}{p_0 V} \right)^{0.6717} - 1 \right) p_0, & \frac{W}{p_0 V} \leq 350 \\
[0.1388 \left( \frac{W}{p_0 V} \right) - 1] p_0, & \frac{W}{p_0 V} > 700
\end{cases}
\]

Where \( p_0 \) is the atmospheric pressure, Pa; \( V \) is the volume of the confined space, m³; \( W \) is the total energy released when the explosive reaction reaches its final state, J.
6. **Comparative analysis of quasi-static pressure among theoretical model results and experimental results**

In order to test the reliability of the quasi-static pressure calculation model established in this paper, the quasi-static pressures among the experimental measurements, theoretical model calculation and equation (20) are compared in this section, as shown in figure 2-4.

**Figure 2.** Comparisons of quasi-static pressure among theoretical calculation, experimental measurements and Anderson formula [6].

**Figure 3.** Comparisons of quasi-static pressure among theoretical calculation, experimental measurements (0.15m³) and Anderson formula [4].
Figure 4. Comparisons of quasi-static pressure among theoretical calculation, experimental measurements (7m$^3$) and Anderson formula [4].

From figure 2-4, it can be seen that when the theoretical calculation model established in this paper is applied to RDX-based charges, the calculated value of quasi-static pressure is in good agreement with the experimental value.

As shown in figure 2, for the internal explosion of 0.1 kg RDX-based explosive (m/V=0.2 kg/m$^3$), the quasi-static pressure first increases and then decreases with the increase of aluminum powder content, reaching its maximum when the content is 40%. When the content is less than 40%, the results of Anderson formula is in good agreement with the experimental result. But when the content is more than 40%, there is a large deviation.

As shown in figure 3, for the internal explosion of 0.025kg RDX-based explosive in 0.15m$^3$ confined space (m/V=0.17kg/m$^3$), the quasi-static pressure first increases and then decreases with the increase of aluminum powder content, reaching its maximum when the content is 45%. However, according to the results of Anderson formula, the quasi-static pressure reaches its maximum when the content is 30%, which differs from the trend of experimental results. And when the content is 60%, the relative error between the theoretical calculation model results and experimental results is relatively large, which may be caused by the experimental measurement error and other accidents of chemical reactions in the internal explosion.

As shown in figure 4, for the internal explosion of 0.2kg RDX-based explosive in 7m$^3$ confined space(m/v=0.03kg/m$^3$), the quasi-static pressure increases with the increase of aluminum powder content and gradually tends to be stable. The difference between the Anderson formula results and experimental results are more and more large. In the case of a small mass-volume ratio, there is enough oxygen in the space, if the temperature required for the afterburning reactions can be met, a large amount of energy will be released. However, due to heat conduction and other factors, the temperature in the confined space keeps decreasing and then the reaction condition cannot be reached. Only taking into consideration the total energy released in the explosion reaction makes the calculated value much higher than the experimental value. Based on this assumption, it is more necessary to
consider the impact of the reduction of gaseous explosion products in the afterburning reaction.

In figure 2-4, there are cases where the results of theoretical calculation model are less than the experimental results in references. The possible reasons are: ① In the actual reaction process, the aluminum powder cannot be fully reacted and the actual reduction of the gaseous explosion products is smaller than the reduction in the calculation process. The influence of the gas reduction calculation term on the quasi-static pressure is greater than that of the energy $Q$ released in the afterburning reaction. ② In the confined space, other substances that may exist in gaseous form and the influence of other small amounts of gaseous explosion products are ignored. ③ There is no recognized method for defining the value of the quasi-static pressure in the experimental measurement. And both the experimental error and the error of the method need to be considered.

According to figure 2-4 and table 2-3, it can be seen that the relative error among most of the measured quasi-static pressures in the references and the theoretical calculation results does not exceed 10% and only a few cases have large errors. Therefore, the theoretical calculation model established in this paper is proved to be reliable and correct. It can be applied to predict the quasi-static pressure of RDX-based and HMX-based aluminized explosive in internal explosion. Meanwhile there is larger error when Anderson empirical formula is applied to predict quasi-static pressure of aluminized explosive.

7. Conclusion
In this paper, by studying the afterburning reaction of aluminized explosive and establishing the theoretical calculation model of quasi-static pressure, it is found that:

1) The results of quasi-static pressure of the theoretical calculation model for internal explosion of aluminized explosive established in this paper is in good agreement with the experimental measurement results in references. And the model is reliable and right, which can be applied to predict the value of the quasi-static pressure of RDX-based and HMX-based aluminized explosive for internal explosion in a certain range of mass-volume ratio.

2) There is larger error when Anderson empirical formula is applied to predict quasi-static pressure of aluminized explosive. And in some cases the trend of calculated quasi-static pressure is inconsistent with that of the experiment data.

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