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# Numerical Simulation of High Energy Solid Propellant Explosion

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## Abstract

**Aiming at the engineering deployment of a high-energy propellant charge motor stored in a confined space, based on the assumption of instantaneous detonation, the propagation of explosion shock wave of a single high-energy solid propellant is numerically simulated, the propagation law of explosion shock wave in the confined space is obtained, and the characteristics of high-pressure area with large risk coefficient in the confined space are analyzed, The critical burst distance of the engine in the typical direction is further obtained. The results show that due to the reflection superposition of the wall, there are many areas with high pressure near the corner, and the corner reinforcement should be paid attention to in engineering construction. Affected by the shape of the engine, the critical burst distance is larger in the axial direction than in the radial direction. When the engine is stored, the axial distance between the engines should be greater than the radial distance. Combined with the critical burst distance, it is suggested that the front and rear spacing of engines placed coaxially should be greater than 2.5 m, and the spacing of engines placed radially in parallel should be about 2.8 m.**

## Keywords

**Explosion impact, Critical burst distance, Pressure distribution law, numerical simulation.**

## 1. Introduction

Although China has carried out the research on the storage reliability of general ammunition earlier, it has also established the storage reliability model and the traditional ammunition storage reliability theory. However, with the continuous development of weapons and equipment in recent years, a large number of new types of missiles have been put into service. Compared with traditional missiles, these missiles have adopted many new materials and technologies, and their failure mechanism and initiation conditions have changed. The traditional detection, test and simulation evaluation methods are difficult to apply, and mature and complete theoretical and engineering standards have not been formed [1]. There is no unified specification for the storage standard of magazine in position engineering construction, and the number and spacing of weapons stored in magazine cannot be determined, There is not enough theoretical support.

At present, the propagation law and impact load of explosion shock wave in confined space or other confined space have been studied at home and abroad, and the corresponding theoretical guidance and empirical formula have been obtained. According to the similarity law, Pokrovsky [2] fitted the empirical formula of overpressure peak value of air shock wave propagation in the tunnel, and its overpressure peak value is expressed as a function of the ratio of TNT mass to the product of tunnel cross-sectional area and explosion center distance; Yang Kezhi et al. [3] used the three-dimensional chemical explosion internal flow field calculation program to numerically simulate the explosion in the tunnel, adopted the same fitting formula format as Pokrovsky, obtained the overpressure peak value and impulse formula, and obtained more universal fitting parameters by changing the tunnel section and the explosive charge of the explosion source.

American Welch CR et al. [4] proposed the attenuation law of peak overpressure of shock wave in tunnel and the expression form of proportional distance and mass size (tunnel diameter, TNT equivalent mass). However, due to the different geometry of different confined spaces such as section shape and length width ratio, the reflection law will also change, and the difference of explosion source geometry will also lead to the difference of shock wave propagation law. Therefore, the universality of the above formula needs to be improved.

In terms of storage safety test, many complete machine explosion safety tests have been carried out abroad. An air force research laboratory in California conducted a martyrdom test using two small intercontinental ballistic missile (SICBM) rocket engines in order to observe the propellant impact to detonation (SDT) behavior and predict the engine response to impact and debris stimulation [5]. The US Navy has conducted safety tests on standard missiles, ESSM missiles and rattlesnake missiles with full ammunition and engines. The data of these tests provide a reference basis for ammunition storage protection. At present, there is no report on the safety test of the whole machine in China, but some scholars have carried out small-scale tests and simulations in terms of martyrdom [6,7,8]. Firstly, a large number of fragment impact initiation tests and simulation calculations are carried out, and the initiation threshold and influencing factors of shell impact velocity are mainly analyzed; The second is the research on shock wave initiation. Many experiments and numerical simulations have been carried out to determine the impact sensitivity of various energetic materials in China. Jia Xiangrui et al. [9] obtained through numerical calculation that the critical initiation pressure of high-energy solid propellant with filling density of 83.5% is 1.8GPa. Wu Junying et al. [10] tested solid propellant (composition: HMX, AP, Al) and obtained that the critical initiation pressure of shock wave is 2.0 ~ 3.0 GPa and the detonation velocity is 5717km/s.

Based on the above research, it is found that the safety test of the whole machine has been carried out abroad, and a variety of initiation forms of impact initiation have been studied. The SDT behavior of some energetic materials has been tested and simulated in China, and the critical initiation pressure threshold has been obtained. However, there is little research on XDT behavior, and there is no systematic research on the explosion performance of large-size charges such as engine. In this paper, taking a high-energy propellant charge engine as the research object, aiming at the safety and explosion-proof problem in the storage warehouse, the initiation mechanism and critical initiation conditions of martyrdom explosion under the engine storage conditions are analyzed by using the methods of theoretical analysis and numerical simulation, the variation law of internal explosion pressure field is obtained, and the corresponding damage effect is analyzed. It provides a theoretical basis for solving the layout and protection design of single warehouse project in the current position engineering construction.

## 2. Numerical Calculation Model

### 2.1. Geometric Model

In the actual engineering construction, most of the storage warehouses are in the shape of straight wall and circular arch, which is hundreds of meters long. The influence of the position of the explosion engine in the warehouse on the propagation of shock wave can not be ignored. If the engine located in the middle of the garage explodes, the reflection of the front and rear walls need not be considered; If an explosion occurs near the reservoir bottom, the shock wave propagation is greatly affected by the reservoir bottom wall, and the reflection of the reservoir

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bottom wall must be considered. Therefore, two kinds of models are established: one is the explosion model in the middle of a long and narrow confined space; The second is the explosion model near the wall. When considering the propagation law of engine pressure field exploding near the bottom of the reservoir, because the front wall has little influence on it, in order to save the calculation space, the axial length of the confined space is shortened when establishing the geometric model.

Based on the above analysis, two sizes of confined spaces are established in this chapter. The shape is a straight wall circular arch structure. The control width, height and arch height are the same. The size difference is only reflected in the length. The length of model 1 is 120.0 m to study the law of engine explosion pressure in the library; The second model is 20.0m long, and the variation law of engine explosion pressure field near the bottom of the reservoir is studied. The geometric model is shown in Figure 1. The side and front and rear walls are specified in the figure for the analysis and description of subsequent pressure nephogram.

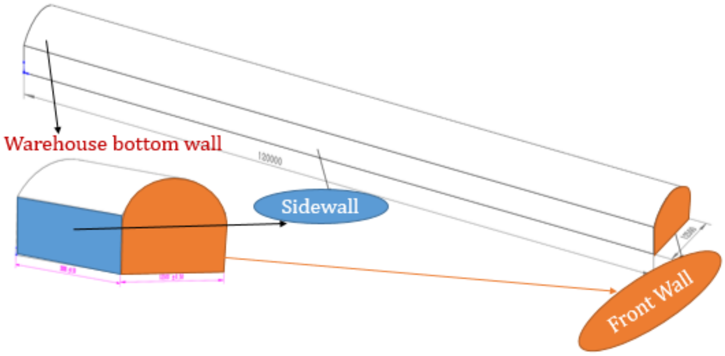


Figure 1: Schematic diagram of geometric model of confined space

## 2.2. Computational model

The shock wave overpressure field after explosion in engine confined space is simulated by fluent simulation software. The following assumptions are made for the model:

(1) The density distribution of propellant is uniform and the explosion process is isotropic;

(2) The explosion process of propellant is completed instantly. At the end of explosion, it can be regarded as that the detonation gas has not expanded, and the heat released by explosion is concentrated in the volume occupied before explosion. Therefore, the cylindrical propellant is equivalent to uniform high temperature and high pressure detonation products;

(3) The composition of explosive gas remains unchanged and no chemical reaction occurs in the flow process.

According to the above instantaneous detonation and other model assumptions, the explosion moment of the engine is regarded as an equal volume of high-temperature and high-pressure explosive gas, and the propagation of explosion shock wave in a confined space is simulated. Because the outflow field generated by explosion is a high-speed compressible flow and there is a diffusion process of detonation products, it needs to be solved by density based coupling, that is, the coupled equations of continuity equation, momentum equation, energy equation and component transport equation are solved at the same time, and then the turbulence equation is solved according to the results of the coupled equations. The turbulence model adopts k-e model. In order to converge quickly, the implicit scheme with good stability is used for calculation. Finally, combined with the change of pressure field, some suggestions on the storage safety of engine are put forward.

## 2.3. Material model

The propellant adopts JWL equation of state, and the relationship between detonation product pressure, specific internal energy and specific volume is as follows:

Isentropic condition:

Where $p$ is the pressure of detonation product, GPa; $V$ is the relative specific volume of detonation products $V=\rho_0/\rho$, and $\rho_0$ is the initial density of propellant; $E$ is specific internal energy (Absolute internal energy $E_a=mc_vT$, Specific internal energy $E=E_a/V$, unit $J/m^3$); $A$, $B$, $R_1$, $R_2$, $\omega$ are undetermined coefficients determined by relevant explosion tests.

The parameters of JWL equation are different with different explosive types and densities. The parameters are determined by combining the fitting method [11] proposed by Zhao Zheng et al. And the empirical formula established by Shen Fei et al. [12]. The equation of state of detonation products can be determined only by explosive density and detonation velocity.

For HMX explosive, its density is $1891\text{kg/m}^3$. $E=1.9\times10^{10}\text{J/m}^3$, $A=7.783\times10^2\text{GPa}$, $B$=7.1GPa, $R_1$=4.1, $R_2$=1.0, ω=0.35. At the same time, refer to the relevant parameters adopted by sun Baizheng [13] and others in the numerical simulation of NEPE propellant, $A=5.574\times10^2\text{GPa}$, $B$=3.59GPa, $R_1$=4.52, $R_2$=1.53, ω=0.33.

The air adopts the polytropic gas state equation. According to Boyle's law and the experimental law of gasification and volume (the volume of various gases participating in the same reaction at the same temperature and pressure is a simple integer ratio), the polytropic gas state equation is expressed as:

$$p=(\gamma-1)\rho e \tag{1}$$

Where: $p$ is the gas pressure, and the initial pressure $p_0$ is atmospheric pressure; $\gamma$ is the isentropic index, usually 1.4; $\rho$ is the current density of air; $e$ is the internal energy per unit volume.

## 2.4. Initial and boundary conditions

Based on the model assumption, the solid wall boundary condition is adopted as the boundary condition. The explosion moment of the engine is a mass of high-pressure and high-temperature detonation products. The types and contents of detonation products are set according to the propellant chemical reaction equation. The explosion reaction equation of RDX is

$$C_3H_6N_6O_6=3H_2O+3CO+3N_2 \tag{2}$$

Chemical decomposition reaction formula of ammonium perchlorate(AP):

$$4NH_4ClO_4=6H_2O+4HCl+2N_2+5O_2 \tag{3}$$

Since there are no reliable experimental values for the specific components of detonation products so far, combined with the above chemical equations, refer to group IV of solid composite propellant studied by he Ning et al. [14] in the development of TNT equivalent calculation software, and assume that there is no carbon solid residue. See Table 1 for the components and contents of detonation products.

$$\begin{gathered}2.9C_3H_6N_6O_6+7NH_4ClO_4+6Al= \\ 7HCl+19.2H_2O+0.2CO+8.5CO_2+7.85N_2+3Al_2O_3\end{gathered} \tag{4}$$

Table 1: Composition and content of detonation products of Propellants

| $H_2O$ | $CO_2$ | HCl | $N_2$ |
|---|---|---|---|
| 0.45 | 0.20 | 0.16 | 0.18 |

The detonation product has been obtained. In the next step, the temperature and pressure at the moment of explosion are calculated. In this paper, the detonation temperature and detonation pressure of the propellant are used instead. Referring to detonation physics, taking

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the detonation temperature as 3000K, combined with the detonation parameter determination method [15], the final detonation pressure is 26.5 GPa.

## 3. Shock wave initiation mechanism

In the introduction, it has been found that the critical initiation pressure of direct initiation of NEPE Propellant by strong shock wave is about 1.8 GPa, but it is not comprehensive to judge whether the charge is detonated only by the critical pressure of direct initiation. This section introduces the explosive initiation standard from the perspective of energy, and determines the critical initiation conditions of the research object in combination with the test experience of scholars at home and abroad.

### 3.1. Initiation conditions

The high-speed fragments produced after the explosion of shell explosive will cause damage to the adjacent engine shell and produce a gap, which makes the shock wave directly reach the propellant surface at the gap without attenuation through the shell, and even reflect and converge at the gap [16]. If the pressure exerted on the charge is lower than the critical detonation pressure, the detonation will occur only when the long-term pressure acts on the charge.

The initiation of explosives must meet the conditions of ignition and development into detonation or explosion. Considering the ignition stage of explosion, the induction period is analyzed qualitatively. Considering the initial pressure variation, after the explosive reaches the critical initiation condition, there are two regions in the explosive, the combustion product region and the unreacted region. It is assumed that the pressures in the two areas are equal, i.e

$$\frac{dP}{dt}=\frac{dP_1}{dt}=\frac{dP_2}{dt} \tag{5}$$

Subscripts 1 and 2 represent the reactant phase and the product phase, respectively.

It is assumed that the volume remains unchanged during the initiation process caused by shock wave. The energy change during ignition start can be expressed as:

$$(1\text{-}F)\frac{dE_1}{dt}+F\frac{dE_2}{dt}=Q\frac{dF}{dt} \tag{6}$$

$F$ represents the reaction fraction and $Q$ is the heat of combustion. The rate of pressure rise is expressed by the derivative of, i.e

$$\frac{dP}{dt}=\frac{dP_1}{dt}=\frac{\partial P_1}{\partial E_1}\frac{dE_1}{dt}+\frac{\partial P_1}{\partial V_1}\frac{dV_1}{dt} \tag{7}$$

$$(1\text{-}F)\frac{V_1}{\gamma_1}\frac{dP}{dt}+F\frac{V_2}{\gamma_2}\frac{dP}{dt}=Q\frac{dF}{dt} \tag{8}$$

The mass burning rate of explosives is a general function of pressure

$$f=BP^n \tag{9}$$

Where $f$ is mass combustion rate, unit $g/(cm^2\cdot s)$ ; $B$ and $n$ are empirical parameters as a function of pressure.

The relationship between $dF/dt$ and mass combustion rate is as follows

$$\frac{dF}{dt}=\frac{1}{V}\frac{dV}{dt}==\frac{AV_1 f}{v_1} \tag{10}$$

$v_1$ is the unburned volume and $A$ is the burning surface area. Continue to bring in

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$$\frac{dP}{dt}=\frac{QABP^nV_1}{\left[\left(1\text{-}F\right)\frac{V_1}{\gamma_1}+F\frac{V_2}{\gamma_2}\right]v_1} \tag{11}$$

Assumptions $V_1/\gamma_1=V_2/\gamma_2$; Second, the change of combustion area per unit volume with time is similar to that of pressure. Is simplified to

$$\frac{dP}{dt}=\frac{\gamma_1QABP^n}{v_1}=\alpha P^n \tag{12}$$

Where $\alpha=\gamma_1QAB/v_1$. Integrate the above formula to obtain

$$\alpha t=\frac{n\text{-}1}{P_0^{n\text{-}1}} \tag{13}$$

For n=3

$$P_0^2t=\frac{1}{\alpha} \tag{14}$$

This is the initiation condition of RDX based energetic materials, which is related to the shock wave pressure and shock wave action time.

Walker and Walsey studied the explosion shock characteristics of energetic materials such as PBX-9404 according to the thermal explosion theory, and obtained that the critical initiation criteria of traditional heterogeneous explosives are $p^2t=C$ [16], $p$- pressure, $t$- shock wave action time.

Chen Xingwang et al. [17] in the study of shell charge impact initiation under shock wave and fragment impact, combined with the initiation criterion of explosive under strong shock wave load, and according to the ignition and growth reaction characteristics of charge, the value of $n$ and $C$ are determined by the least square method, $C$=1.24*$10^{12}$ , $n$=2.12, which $p$ is the shock wave pressure loaded on the charge to be fired and $t$ is the duration of shock wave action.

H.Cheung Et al. [18] sorted out the experimental data of the explosive reaction of PBX-9404 and HMX-filled explosives, put forward the theoretical basis of the initiation of condensed explosives, and proved the correctness of $p^2t=C$ critical initiation criterion. According to the relationship between initiation pressure and loading time, the value range of the constant is 2.0*$10^{12}$~8.0*$10^{12}$.

## 3.2. Analysis of safety distance of martyrdom explosion

According to the above shock wave initiation mechanism, the critical conditions of shock wave initiation are sorted out as follows: direct initiation. When the shock wave contacts the propellant to be fired, the pressure exerted on the propellant to be fired exceeds the critical initiation pressure, and it can be judged that it produces martyrdom explosion; For delayed initiation, if the pressure applied to the propellant to be fired is lower than the critical initiation pressure, it shall meet the critical initiation criterion of $p^2t=C$, in which the value range of $C$ is 2.0*$10^{12}$~8.0*$10^{12}$. The higher the content of HMX (or RDX), the smaller the pressure required for the critical initiation of composite propellant [19]. Combined with the material ratio of propellant, 3.0*$10^{12}$~4.5*$10^{12}$ is taken as the critical initiation threshold of NEPE propellant in this paper.

With the decrease of pressure, the product of initiation time and pressure square increases. Therefore, in this paper, the initiation standard of pressure continuously lower than 6.0*$10^7$Pa is determined as $C$=7.0*$10^{12}$.

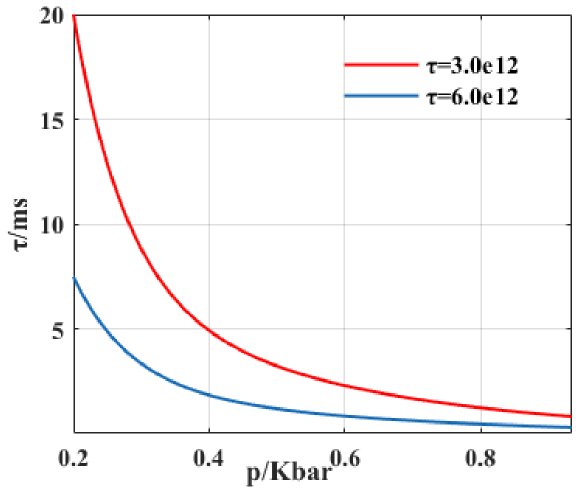


Figure 2: Critical initiation basis

For the range where the shell fragments near the explosive engine can be directly damaged, the above critical initiation conditions of delayed initiation are used to explore the critical martyrdom distance; For the range where shell fragments cannot reach directly, such as near the wall, when discussing whether the pressurization near the wall caused by reflection will cause martyrdom explosion, because the engine shell at the wall is intact, the critical condition of direct initiation of strong shock wave is used to determine the damage effect, that is, the initiation pressure is about 1.8 GPa.

## 4. Numerical simulation results and analysis

In this chapter, the flow field simulation of single high-energy propellant charge engine explosion is carried out, the variation law of pressure field is analyzed, and the safe initiation threshold is finally determined.

### 4.1. Simulation results and analysis of model I Acknowledgements

In order to observe the change law of pressure field, combined with the purpose of simulation, the section shown in Figure 3 is selected from model I. Section A is perpendicular to the Y-axis and at the same height as the engine axis.

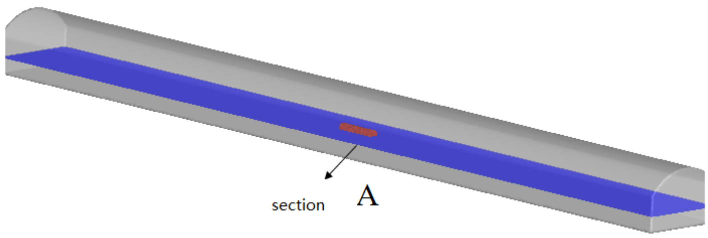


Figure 3: Schematic diagram of section A

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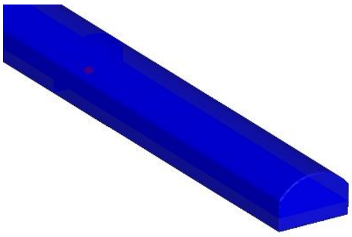
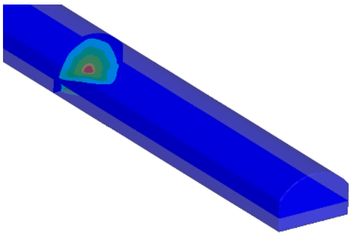
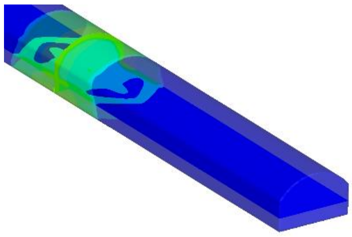
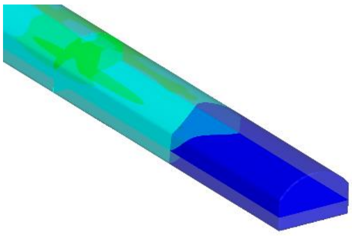
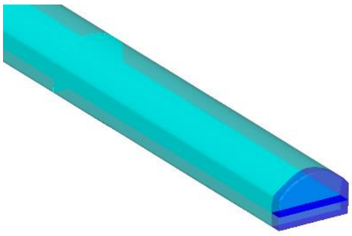

(a) t=0ms


(b) t=0.93ms


(c) t=3.73ms


(d) t=10.4ms


(e) t=21.2ms

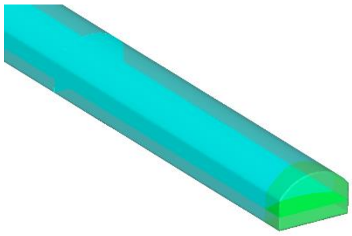
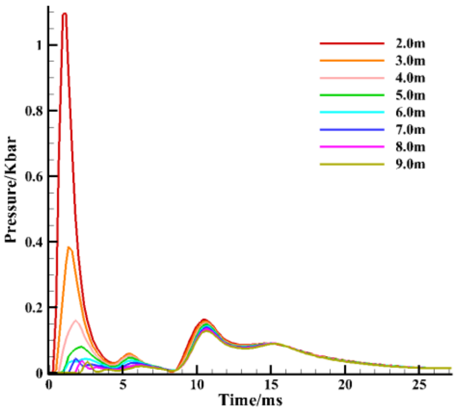
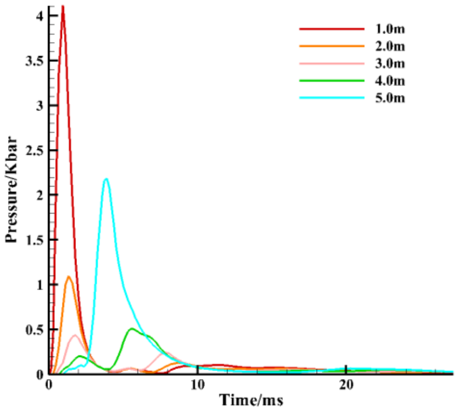

(f) t=27.2ms

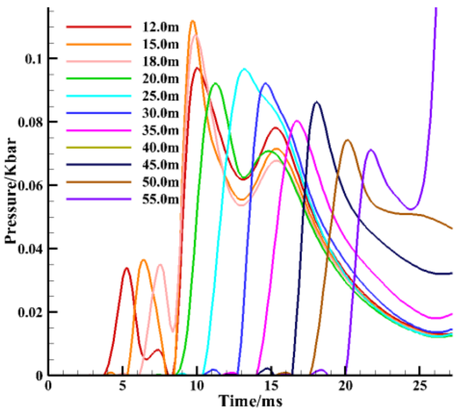
Figure 4: Pressure field change



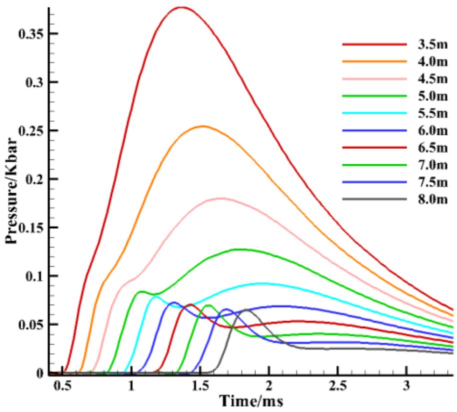
(a) Axial



(b) Radial



(c) Axial



(d) Axial

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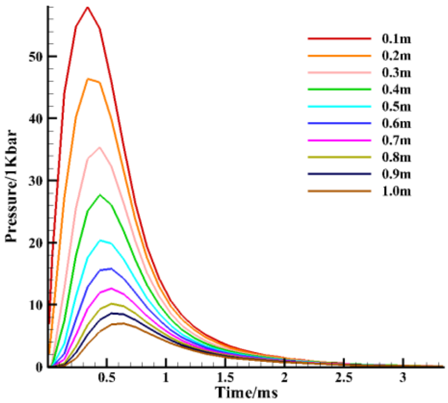
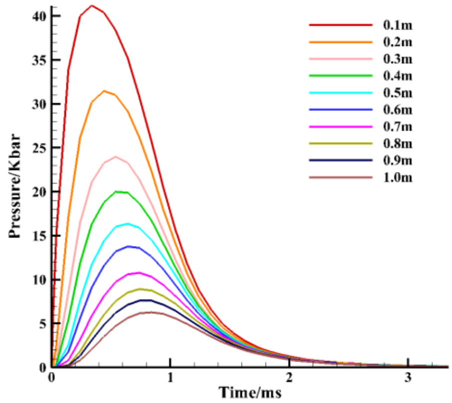
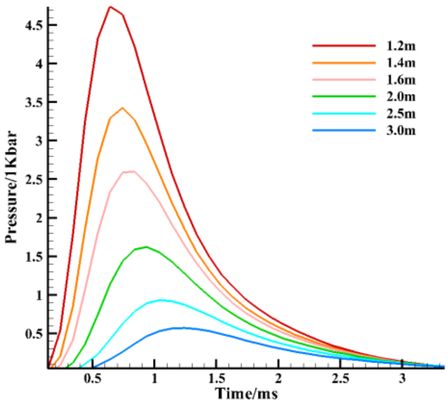


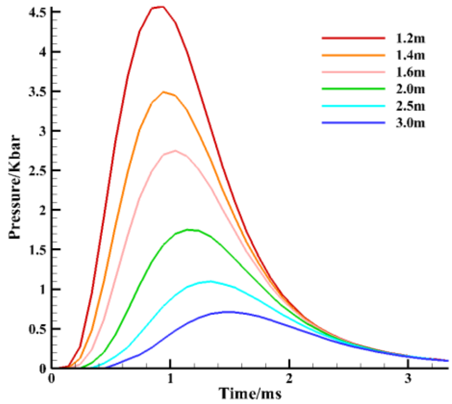

(e) Axial




(f) Radial




(g) Axial



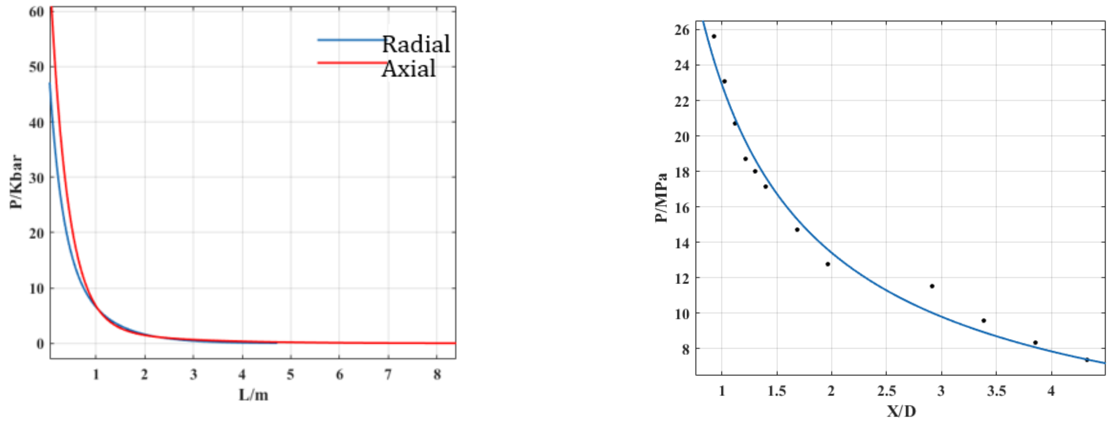

(h) Radial

Figure 5: Pressure versus time curves of axial and radial observation points

Figure 4 shows the variation of pressure field with time on section a. The length diameter ratio of the cylindrical charge of the two-stage engine is close to 1, so the cross section of the shock wave surface is roughly rhombic. Before and after 1.0ms, the shock wave is reflected on the side wall. The pressure variation data with time at several axial and radial observation points are extracted below (see Figure 5).

Figure 5 (a, b, c) and Figure 5 (d, e, f, g, h) show the pressure variation with time at each observation point in the axial and radial directions within 27.0ms and 3.6ms after explosion, respectively. The former is to reflect the pressure change law of the whole space; The latter is the pressure change before and after the first overpressure peak in the near region of the explosive engine.

According to the pressure change of each observation point near the engine, there are dangerous areas up to 1.0 and lasting more than 1.0ms within 2.0m from the engine shaft and radial direction and 0.5m from the wall. The secondary overpressure in the axial direction shall not exceed 0.2 and the duration shall not exceed 5ms, which is not enough to cause the engine to burst. The pressure 10m away from the explosion source is not higher than 0.1, so there is no risk of martyrdom explosion. The variation of the first overpressure peak with distance is fitted with MATLAB, as shown in Figure 6 (a).




(a) Radial and axial first overpressure peak (b) Peak axial overpressure

Figure 6: Relationship curve between radial and axial overpressure peak and distance

The fitting formula is

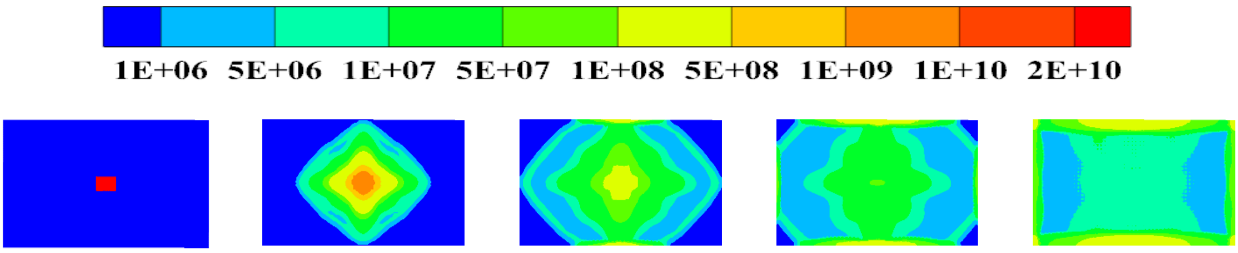
$$P=72.7e^{-2.76x}+4.0e^{-0.6x}$$
$$P=32.7e^{-3.85x}+21.3e^{-1.3x} \tag{15}$$

Where, $P$ is the peak value of overpressure; $x$ is the distance from the engine surface.

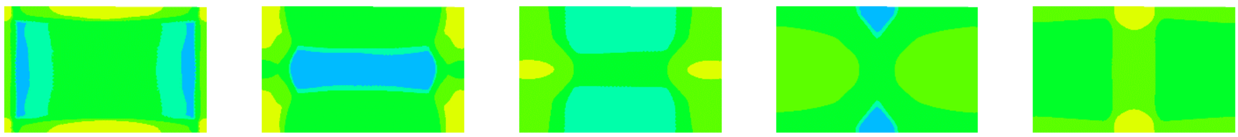
The fitting result of axial overpressure peak is

$$P=12.25\left(\frac{X}{10.6}\right)^{-0.32} \tag{16}$$

## 4.2. Simulation results and analysis of model II Acknowledgements




(a) t=0.0ms (b) t=1.04ms (c) t=1.94ms (d) t=2.64ms (e) t=3.64ms



(f) t=4.04ms (g) t=6.05ms (h) t=8.34ms (i) t=12.3ms (j) t=15.3ms

Figure 7: Pressure field at different times of section A of model II

The engine is 9.0m away from the front and rear walls, and the shock wave has reached the front and rear walls in about 2.0ms, and the reflection pressurization process begins. Combined with the change of pressure field (see Figure 7), only the data of observation points within 12.0ms after explosion are used. The change of pressure with time is shown in Figure 8.

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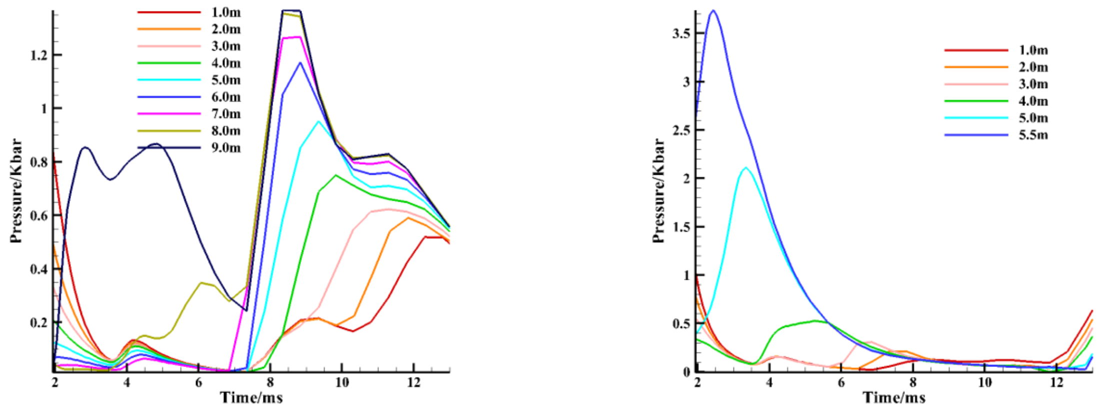



(a) Axial (b) Radial

Figure 8: Overpressure time history curve of axial and radial observation points

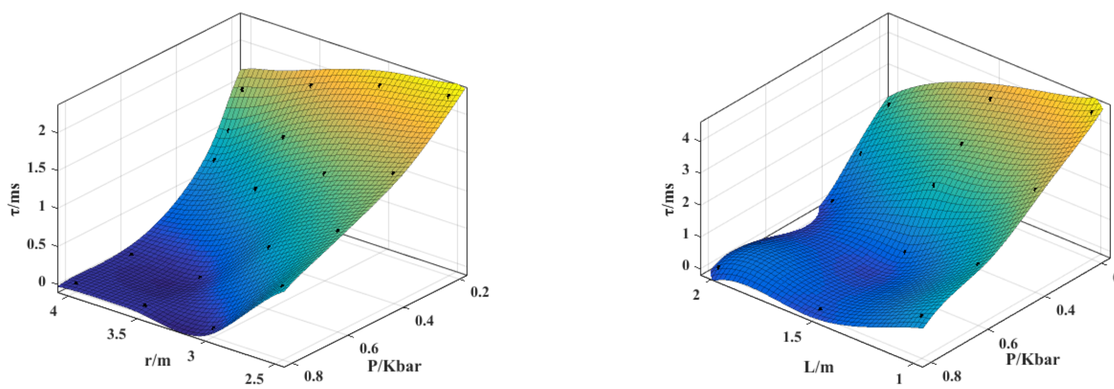
From the overpressure time history curve, the radial direction is consistent with the results of model I, and it can be determined that the risk area is at least 0.5m near the wall; In the axial direction, it can be roughly judged that there is a risk of delayed initiation within 3.0m from the wall.

## 4.3. Damage effect analysis

Summarizing the above known results: when the engine in the middle of the storage warehouse explodes, there is an initiation risk within 2.0m of the shaft and radial direction near the engine; There is a martyrdom risk area higher than 1.0 within 0.5m radially from the wall. When the engine at the bottom of the storage depot (9.0m from the bottom) explodes, there is an explosion risk within 3.0m near the axial upper wall.

Combined with the above analysis, the existing unknown areas of damage effect include: model I axial interval of 2.0m ~ 10.0m and radial interval of 2.0m ~ 5.0m. The damage effect caused by the pressure rise caused by the wall reflected wave within 6.0m away from the engine in the axial direction of model 2; The radial case is consistent with the model.

The pressure duration data of each observation point is extracted by MATLAB and plotted as shown in Figure 9 and Figure 10.




(a) First overpressure (b) Wall reflection overpressure

Figure 9: Relationship between radial upward distance, pressure and duration of model I

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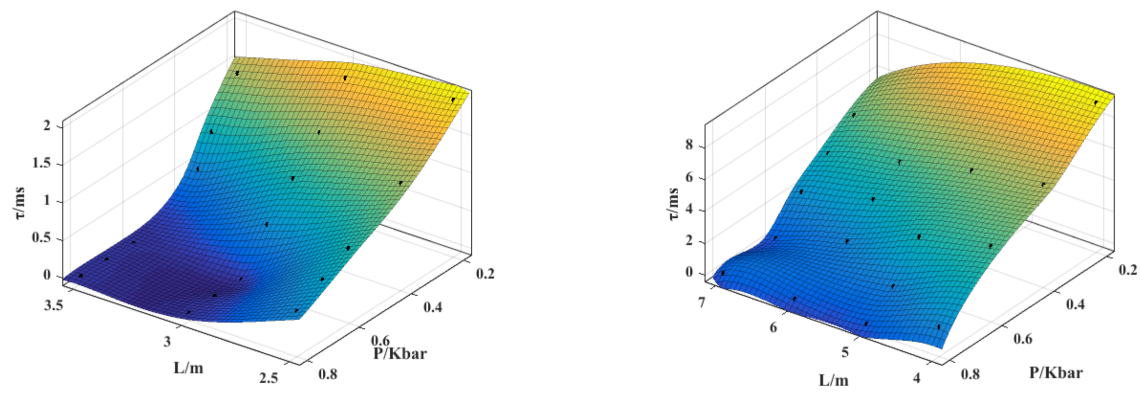


(a) First overpressure (Model I) (b) Wall reflection overpressure (Model II)

Figure 10: The relationship between axial distance, pressure and duration of model I and II.

Through MATLAB programming and combined with the critical initiation conditions, it is obtained that the axial critical detonation distance of the shock wave causing the first overpressure peak to NEPE propellant charge is 2.5 ~ 2.8m, and the radial critical detonation distance is 2.8m ~ 3.0m.

In the high-energy engine storage, the wall reflection causes the risk of delayed explosion within 1.5m near the radial wall; After the explosion of the engine close to the front (after) wall of the warehouse, the continuous medium and high pressure within 5.0m away from the wall may cause the damaged engine to ignite and explode in this area.

According to the wall reflection characteristics, it is estimated that when the incident pressure is greater than 1.5kbar, the reflection pressure will exceed 1.8gpa, which will cause local engine explosion. Combined with the first overpressure law, the peak overpressure of shaft and radial within 2.0m from the engine surface will exceed 2.0kbar. Therefore, for the high-energy propellant charge engine, the safe distance between the engines on both sides and the wall is more than 2.0m; The safe distance between the bottom engine and the bottom wall is more than 2.0m.

Based on the above analysis, this section puts forward the following suggestions for the construction of storage engineering:

For the storage engineering of high-energy propellant charge engine, it is suggested that the radial distance between engines should be greater than 2.8m and the axial distance can be about 2.5m. The engines on the two most sides shall be kept 2.0m away from the side wall. For the last row of engines, a distance of about 2.0m is reserved from the bottom.

## 5. Conclusion

In this paper, the explosion simulation of high-energy propellant charge engine in confined space is carried out. The variation law of pressure field is analyzed from three typical positions of radial, axial and wall, and the corresponding damage range is obtained. Combined with the damage effect, the corresponding suggestions are given from the perspective of storage engineering.

In the high-energy propellant charge engine storage, the distance between the front and rear of the engine placed coaxially shall be greater than 2.5m, and the distance between the engines placed radially in parallel shall be about 2.8m. The distance between the engines on both sides and the wall shall be 2.0m, and the distance between the bottom engine and the bottom of the storage warehouse shall be 2.0m. On the whole, the safety distance of martyrdom required in the radial direction is greater than that in the axial direction, and the difference between them is related to the length diameter ratio of the engine. The greater the aspect ratio, the greater the difference.

At present, the storage distance of engines in a single depot is to be determined, and the maximum storage capacity of a single depot is also unknown. By means of numerical simulation, this paper explores the storage safety distance to avoid missile martyrdom explosion, which provides a theoretical basis for the storage distance. In the next step, the maximum storage capacity of a single silo can be discussed and the maximum equivalent charge density of the silo can be calculated.

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