The Effect of Charge Density on Temperature and Stress of Propellant

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Abstract. In order to determine the effect of charge density on the internal temperature and stress in the propellant, based on the Visco-Scram model and the JWL equation of state, the influence of different charge densities on the internal temperature and stress distribution of the charge is analyzed by using the finite volume method. The result indicates that the maximum charge temperature decreases with the increase of charge density, the maximum value of stress increases with the increase of charge density, but the change of the charges are not significant, which shows that the influence of the charge density on the temperature and stress has a less impact, which provides a reference for the influence of the charge density on the launch safety.

1. Introduction
The safety of explosive charge under launch conditions has restricted the application of high explosives in large caliber grenades. The early bombing of explosive charge is a complex process with many factors. A large number of experiments and research results show that the quality of charging is the main reason affecting the safety of explosive launch, that is, the main factors that lead to charge chamber are the bottom gap, crack, bubble and shrinkage of the charge [1]. The explosive is in the process of launching and loading, as a result of overload of the drug column produced a sharp compression, shrinkage, bubble, crack and other defects at the same time produce adiabatic compression, resulting in explosives within the hot spot caused by early bombing, that is, follow the hot spot initiation mechanism, cracks, delamination in the rapid compression process may form a relative displacement, resulting in friction.

The research of explosive charge launch safety has been in the stage of development [2-6]. American scholars have first established the gun pressure simulator with propellant, and systematically studied the safety qualification condition of charge to the bottom clearance requirement. The scholars of Nanjing University of Sciences and Technology have established the chamber pressure test simulator and the test method; and the scholars of the North and South universities have studied the influence of the explosive charge defects on the performance of explosives. Xi'an Modern Chemical Research Institute studied the constitutive relation and structure response of explosive charge in launching process. These
studies are mainly from two aspects of experiment and numerical simulation. Due to the limitation of the existing experimental conditions, it is difficult to understand the deformation mechanism of explosives under microscopic level, and the solution is only to establish various approximate constitutive models to explain the deformation law of explosives. The “Visco-Scram model”, which was established by Bennett and Haberman [7], is a representative meso-damage model for the damage of energetic materials, and was based on the evolution and expansion mechanism of crack. It was characterized by coupling the generalized viscoelastic body on the crack body, and described the viscoelastic mechanical response of the explosive. And the micro-crack body is used to describe the damage evolution process. In this paper, the viscoelastic crack constitutive model is proposed, based on the finite volume method, the change of the temperature and stress of the explosive under the action of the bottom pressure are simulated; the influence of the density of the explosive on the distribution of the temperature and the stress in the explosive are discussed, which has a certain significance for the safety evaluation of explosives.

2. Visco-Scram Model
The “Visco-Scram Model” is suitable for the research and analysis of the dynamic damage under similar stress states such as impact problems. The “Visco-Scram Model” constitutive model is composed of two bodies: one is a generalized viscoelastic body which is formed by a plurality of viscoelastic bodies in parallel, and one is defined by the SCRAM model as a crack body. The specific derivation process of the computational model is shown in the references [8-10], where only a brief calculation formula is given.

The relation between the deviatoric stress rate \( \dot{S}_{ij} \) and the deviatoric strain rate \( \dot{e}_{ij} \) of viscoelastic statistical crack model is:

\[
\dot{S}_{ij} = \frac{2G\dot{e}_{ij} - \sum_{n=1}^{N} \frac{S_{ij}^{(n)}}{\tau^{(n)}} - 3\left(\frac{c}{a}\right)^{3} \frac{\dot{e}_{ij}}{a}}{1 + \left(\frac{c}{a}\right)^{3}}
\]

where, \( S_{ij} \) is the deviatoric stress, \( G \) is the shear moduli, \( S_{ij}^{(n)} \) and \( \tau^{(n)} \) are the deviatoric stress and relaxation time of the \( n \)th component, \( c \) is the average crack radius, and \( a \) is the initial flaw size. The deviatoric stress rate of single Maxwell model is:

\[
\dot{S}_{ij}^{(n)} = 2G^{(n)}\dot{e}_{ij} - \frac{S_{ij}^{(n)}}{\tau^{(n)}} - \frac{G^{(n)}}{G} \left[ 3\left(\frac{c}{a}\right)^{3} \frac{\dot{e}_{ij}}{a} - \frac{S_{ij}}{a} \right]
\]

Where, \( G^{(n)} \) is the shear moduli for the \( n \)th component.

3. Macroscopic volume heating model of viscoelastic statistical crack model
In the viscoelastic statistical crack model, macroscopic volume heating includes a mechanical term describing the variation of viscosity, crack damage and adiabatic volume, and a chemical thermal decomposition term. The chemical decomposition is described by Arrhenius first-level reaction kinetics. For macroscopic continuum, ignoring the whole heat conduction term, the time dependent temperature rate equation is as follows:

\[
\dot{T} = -\gamma T \dot{e}_{ii} + \frac{I}{\rho C_{V}} \left( W_{n} + W_{s} \right) + \frac{\Delta H}{C_{V}} Z \exp \left( -\frac{E}{RT} \right)
\]
Where, $T$ is the temperature, $\gamma$ is the Greisen coefficient, $C_r$ is the specific heat of fixed volume, $\dot{W}_v$ is the viscous power, $\dot{W}_c$ is the crack damage power, and $\Delta H, E, Z$ is the unit mass decomposition heat, activation energy and reference factor of thermal decomposition reaction of energetic materials.

4. Equation of State

The equation of state is used to describe the relationship between the pressure, volume and temperature of the material. Different equations of state apply to different problems. The state equation of the explosive is generally adopted by shock state equation or JWL state equation. The JWL equation of state is adopted in this paper.

$$P = A(1 - \frac{\rho}{R_1 V})e^{-\frac{\rho}{R_1 V}} + B(1 - \frac{\rho}{R_2 V})e^{-\frac{\rho}{R_2 V}} + \frac{\rho E_a}{V}$$  \hspace{1cm} (4)

where, $p$ is the pressure, $E_a$ is the unit initial volume internal energy, $V$ is the relative volume, and $A, B, R_1, R_2, W$ are material parameters, the values are shown in Table 1.

Table 1. Material Parameters

| $A$ / Mbar | $B$ / Mbar | $R_1$ | $R_2$ | $W$  |
|-----------|-----------|-------|-------|------|
| 7.781×10^3 | -5.031×10^{-2} | 11.3  | 1.13  | 0.8938 |

5. Numerical Simulation

The calculation model of the explosive is shown in the figure:

![Figure 1. Model of explosive](image)

The numerical model has a total length of 56.7cm, a maximum radius of 6.3cm. By using composite B explosive for numerical simulation, because there is no correlation parameter of the viscoelastic statistical crack model of composite B explosive, the relevant parameters of PBX9501 explosive are referenced in the calculation. The viscoelastic parameters, statistical crack parameters and thermodynamic parameters of composite B explosive are given in the following table.

Table 2. Viscoelasticity parameters

| $G^{(0)}$ /Pa | $G^{(2)}$ /Pa | $G^{(3)}$ /Pa | $G^{(4)}$ /Pa | $G^{(5)}$ /Pa |
|----------------|----------------|----------------|----------------|----------------|
| 9.440×10^6    | 1.738×10^6     | 5.212×10^6     | 9.085×10^6     | 6.875×10^6     |

Table 3. Crack parameters of explosive

| $\nu$ | $m$ | $c_o$ /m | $a$ /m | $v_{\text{max}}$ / (m·s$^{-1}$) | $K_o$ / (Pa·m$^{3/2}$) |
|------|-----|----------|-------|-------------------------------|----------------------|
| 0.3  | 10  | 0.00003  | 0.001 | 300                           | 5×10^5               |
Table 4. Thermodynamics parameters of explosive

| $k$ (W/m·K) | $C_f$ (J·kg$^{-1}$·K$^{-1}$) | $\rho_f$ (kg/m$^3$) | $\Delta H_f$ (J/kg) | $z_f$ (m·s$^{-1}$) | $(E/R)_f$ (K) |
|--------------|------------------------|-------------------|-------------------|-------------------|----------------|
| 0.5          | 1200                   | 1717              | $5.5 \times 10^6$ | $5 \times 10^6$   | $2.652 \times 10^4$ |

The simulated bottom pressure curve is shown in the figure 2.

**Figure 2.** Pressure of bottom of projectile

By using the finite volume method and the “Visco-Scram” constitutive model and the JWL state equation, the internal stress and temperature variation of the explosive under simulated projectile bottom pressure is calculated. The following calculation results (Fig.3- Fig.8) are the variation curves of the stress and temperature with time in the explosive.

**Figure 3.** Temperature-time curve at the bottom of explosive

**Figure 4.** Temperature-time curve at the middle of explosive
From the results, it can be seen that under the action of the projectile bottom pressure, the whole temperature of the explosive is constantly rising and the stress is changing, and the change trend of the stress is consistent with that of the applied pressure, which shows that the calculation result is credible.

When the charge is uniform, the stress and temperature changes inside the explosive density of 1.56 g/cm³, 1.66 g/cm³, 1.76 g/cm³ and 1.86 g/cm³ are calculated, and the influence of the variation of explosive density on the temperature and stress of the explosive is analyzed, and the results are as follows:
As shown in Fig. 9, the stress on the bottom of the explosive increases with the density, but the increase is smaller. And as shown in Fig. 10, the maximum charge temperature decreases with the increase of density, but the change is also smaller. This is because that, under the launching process, whether the charge density is greater, the modulus of elasticity is much greater, and the compressibility is smaller, so the heat converted from the elastic-plastic deformation and plastic work is small, and the temperature of the charge is reduced.

The calculation results show that the stress and temperature have no significant change with the increase of density. This is because that, the charge in the launching process, mainly by the role of inertia force, the total quality of the charge does not increase significantly when the charge density varies from 1.56g/cm$^3$ to 1.86g/cm$^3$, so the charge density is different when the inertia force of the state did not change significantly, Therefore, there is no significant change in the maximum stress and temperature of the charge.

6. Conclusion

1) The variation of temperature and stress inside the explosive is studied by using finite volume method, which is combined with the viscoelastic statistical crack constitutive model and the JWL state equation. The results of the analysis show that under the action of the projectile bottom pressure, the variation of the internal stress of the explosive is consistent with the pressure of the bottom, which can indicate the calculation result is correct. As the base pressure is applied to the bottom of the explosive, the temperature increases at the bottom of the explosive is more obvious, while the temperature of the center and the front of the explosive is relatively slow.

2) The influence of the variation of explosive density on the temperature and stress distribution of the explosive is analyzed. The calculated results show that the maximum charge temperature decreases with the increase of density, and the maximum load of the charge increases with the increase of density, but the changes are not significant, which can provide reference for the influence of charge density on the emission safety of explosive during the launching process.

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