Numerical simulation and experimental study on slow cook-off response characteristics of composite B

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Abstract. The response characteristics of composite B explosives (Shellless and shelled) under slow heating strips were numerically simulated using a zero-order reaction kinetics model. And the slow cook-off experiment was carried out on shell explosives and shellless explosives respectively. Comparing the experimental results with the calculated results, the key parameters such as melting process, temperature field evolution, ignition time, ignition temperature and ignition area of the slow cook-off test of the cast-casting charge were obtained. The results show that when the casting explosive is heated slowly, it is a heat conduction process before melting, the internal temperature gradient is large, the temperature of the liquid explosive tends to be uniform after melting, and the upper layer temperature is slightly higher than the lower layer temperature; When the temperature rises to a certain value, the explosive decomposes to generate a large amount of gas, and can be discharged from the pressure relief hole of the casing; Eventually, a high temperature region is formed in the middle of the top layer of the liquid explosive, and the ignition reacts violently.

1. Introduction

Ensuring the safety of ammunition during operation, storage, and transportation is an important problem facing the military industry. The design of insensitive ammunition for thermal stimulation such as slow cook-off and fast cook-off has become an important requirement for current ammunition designs. The response characteristics of energetic materials under thermal stimulation, such as ignition time and ignition position, have always been of concern. Researchers have been committed to related research on the thermal reaction process of explosives through theoretical analysis, experimental measurement and simulation calculation.

The thermal explosion theory was pioneered by N.N.Semenov and D.A. Frank-Kamenetskii as early as the 1940s. It was proposed to use a single-step reaction kinetic model to describe the thermal decomposition reaction of explosives through mathematical analysis of heat maps, calculate the critical temperature and the explosion delay in a homogeneous system [1]. However, b the theoretical calculation of explosive thermal decomposition is limited by the solution method, it cannot be solved for the charge under irregular structure and nonlinear heating conditions, and it is difficult to generalize it in practical engineering applications.

With the development of computer and experimental technology, combustion experiments cook-off test
and numerical calculations have now become an important means of thermal analysis of explosives. Wen-feng Li [2] established a three-dimensional non-steady-state heat conduction model of the AP / HTPB composite propellant, and performed numerical calculations for different heating rate conditions. The results show that the heating rate increases, the delay time decreases, and the ignition temperature increases. Krawietz [3] carried out slow cook-off experiments of RDX and mixed explosives of RDX and TNT under unrestricted conditions by using flasks, and obtained the heating curve and self-heating temperature of two kinds of explosives, which are melt-casting and pouring. It was found that both explosives had obvious self-heating process during slow cook-off. Erdogan Aydemir [4] developed a slow roasting experimental device for ordinary ammunition. The slow roasting experiment was carried out on the shelled charge containing PBXN-110. The internal temperature of the explosive was measured, and the ignition time, ignition temperature, and ignition position were obtained. The reaction kinetic parameters of explosives were obtained by TGA test. Daniel O. Asante [5] used CFD simulation software to perform numerical calculations on fast-baking and slow-baking M107 grenades loaded with TNT explosives, and obtained results such as the melting time, melting zone, and internal pressure increasing exponentially with the reaction rate.

The above research mainly obtains the response characteristics such as the temperature rise curve, ignition temperature and ignition time of the thermal decomposition of energetic materials through experiments and numerical simulations. The characteristics of phase transition and internal heat transfer and reaction of molten cast explosives need to be further investigated.

In this paper, the thermal response characteristics of explosive B were obtained through slow roasting experiments, and the FLUENT software embedded UDF self-defined function" method was used to perform numerical simulations on unconstrained explosives and shell-bound explosives. The calculated results are compared with the experimental results, and the melting temperature, ignition time, ignition temperature and ignition position of the charge are obtained. It can provide a theoretical reference for the design of insensitive warhead.

2. Theoretical model
After the charge is heated, the heat of the external environment is transferred to the inside of the explosive through the shell in the form of heat conduction. After the explosive is melted, the interior continues to heat up in the form of convective heat transfer. After the autothermal decomposition reaction occurs, the chemical energy of the explosive is converted into Thermal energy and heat continue to accumulate, and the temperature of the explosive gradually increases, which promotes the increase of the rate of autothermal decomposition and releases more heat, which eventually causes the explosive to ignite.

The thermal decomposition model of the slow roasting process of the compose B is as follows. First, the slow cook-off process is reasonably simplified and assumed:

1. The compose B is uniform, isotropic and equal in density, ignoring the influence of the interface between the air area and the explosive.
2. Physical properties such as density, specific heat capacity, thermal conductivity and chemical reaction kinetic parameters do not change with increasing temperature.
3. The rate of autothermal decomposition of explosives follows Arrhenius's law.

The dynamic relationship between heat conduction, heat accumulation, and heat generation is described using a single-step zero-order kinetic model. The two components are thermally decomposed separately.
The sum of the heat releases of the two components is the total reaction heat of the explosive.

The RDX thermal decomposition process is described by a three-step continuous chemical reaction [6], and the process can be expressed as:

\[ \text{A} \xrightarrow{R_1} \text{B} \xrightarrow{R_2} 2\text{C} \xrightarrow{R_3} \text{D} \]

Where A = RDX, B = H2C, C = CH2O + N2O, D is the final product.

The reaction rate equation of each step is expressed as:

\[ \frac{dC_n}{dt} = -k_i \]  

Where \( C_n \) is the concentration of different substances, \( k_i \) is the reaction rate constant for each step, and the chemical reaction at each step follows the Arrhenius rate equation:

\[ k_i = Z_i \exp \left( \frac{-E_i}{RT} \right) \]  

This article uses the mass fraction of a substance to describe the rate of a chemical reaction. The three-step chemical reaction of RDX thermal decomposition is described as follows:

Reaction 1

\[ \text{A} \rightarrow \text{B} \quad R_1 = Z_1 \exp \left( \frac{-E_1}{RT} \right) \rho_A \]  

Reaction 2

\[ \text{B} \rightarrow 2\text{C} \quad R_2 = Z_2 \exp \left( \frac{-E_1}{RT} \right) \rho_B \]  

Reaction 3

\[ \text{C} \rightarrow \text{D} \quad R_3 = Z_2 \exp \left( \frac{-E_1}{RT} \right) \rho_C^2 \]  

For each step of the reaction, the rate of heat generation can be expressed as:

\[ S_i = mQ_i k_i = Q_i Z_i \exp \left( \frac{-E_i}{RT} \right) \rho_n^x \]  

Where \( Q_i \) is the heat of reaction, and \( m \) is the mass of the reactant.

Therefore, the heat generated per unit time of the RDX thermal decomposition process is:

\[ S(\text{RDX}) = Q_1 R_1 + Q_2 R_2 + Q_3 R_3 \]  

The thermal decomposition of TNT can be described by a one-step chemical reaction, and its equation is as follows [7]:

\[ \text{C}_7\text{H}_5\text{N}_3\text{O}_6 \rightarrow 3.5\text{CO} + 3.5\text{C} + 2.5\text{H}_2\text{O} + 1.5\text{N}_2 \quad R_4 = Z_4 \exp \left( \frac{-E_4}{RT} \right) \rho \]  

The heat generated per unit time of the TNT thermal decomposition process is:

\[ S(\text{TNT}) = Q_{\text{TNT}} R_4 \]  

The mass fraction equation for each substance is as follows:

\[ \rho \frac{d\rho_1}{dt} = R_1 \]  

\[ \rho \frac{d\rho_2}{dt} = R_2 \]
\[ \rho \frac{d\omega_c}{dt} = R_3 \]  
\[ \rho \frac{d\omega_{NT}}{dt} = R_4 \]  

In the Cartesian coordinate system, the energy conservation equation of the solid explosive burning process is:

\[ \rho c_p \frac{dT}{dt} = \lambda \left[ \frac{\partial}{\partial x} \left( \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{\partial T}{\partial y} \right) \right] + S \]  

Where \( \omega_i \) is the mass fraction of each component, the left side of the above formula is the internal energy increment of the microelement, the first two terms on the right are the net heat entering the microelement from the \( x \) and \( y \) directions, and \( S \) is the source term of the thermal decomposition reaction of the explosive \([8]\). The total heat generated during the thermal decomposition of composite B per unit time is:

\[ S(\text{composite B}) = Q_1 R_1 + Q_2 R_2 + Q_3 R_3 + Q_4 R_4 \]  

This article adopts linear heating. The thermal boundary conditions of the shell are as follows:

\[ T_s = T_0 + kt \]  

Where, \( T_s \) is the temperature of the shell, \( k \) is the heating rate, and \( T_0 \) is the initial temperature.

The boundary conditions of the adiabatic surface are as follows:

\[ -\lambda_a \nabla T_a = 0 \]  

Where \( \lambda_a \) is the thermal conductivity of the adiabatic boundary surface, and \( T_a \) is the temperature of the adiabatic boundary surface;

This article ignores the thermal resistance of the interface between the shell and the explosive, and considers that the temperature and heat flow at the interface are continuous:

\[ T_1 = T_2 \]  
\[ \lambda_1 \nabla T_1 = \lambda_2 \nabla T_2 \]  

Where, \( T_1, T_2 \) and \( \lambda_1, \lambda_2 \) are the temperature and thermal conductivity of the two materials, respectively.

3. Experiment and calculation model settings

In order to carry out a comparative analysis of calculation results and experimental results and optimize the calculation model, the experimental bomb was designed for slow roasting experiments. The wall thickness of the experimental bomb was 10mm, the material was 45 # steel, and it was filled with B explosive (TNT and RDX mass ratio 40/60). A thermocouple is installed on the surface and inside the explosive, and its structure is shown in figure 1(a). Because the experimental projectile is a centrally symmetric structure, this paper uses a two-dimensional axisymmetric model for calculation. Use the ICEM software to perform modeling, set 4 observation points at different positions of the model, and observe the changes in temperature. The calculation model is shown in figure 1(b).

Electrical heating was used to slowly heat the experimental bomb with a heating rate of 1°C/min and heating until a violent reaction occurred. Because the heating jacket is in close contact with the experimental bomb, the thermal resistance of the contact surface can be ignored. Therefore, transient temperature boundary conditions are directly added to the shell surface of the calculation model during numerical simulation.
4. Results and discussion
This chapter mainly compares and analyzes the numerical calculation results and experimental results. Since the casting charge will melt when the temperature is not high, the first part simulates and experimentally studies the melting process of the shellless charge. In the second part, slow cook-off test and numerical calculations are performed on the charge with shell to obtain its ignition temperature, ignition time, ignition area and other characteristics.

4.1. Melting of shellless explosives
Put a Φ40 mm × 50 mm pellet in a transparent glass beaker, place it in the oven to heat up slowly at a rate of 1°C/min, and measure the temperature of the explosive with a K-type thermocouple. The layout is shown in figure 2(a); the calculation model uses a two-dimensional axisymmetric model, the calculation area around the explosive is air, and convection heat transfer and a temperature boundary condition of 1°C/min are used. The state is shown in figure 2(b).

![Figure 1. Experimental and computational model shells.](image)

![Figure 2. Experiment and calculation state diagram.](image)

The experimental results are shown in figures 3(a)–3(c). When the temperature rises to 97°C, the explosive starts to melt from the surface. Under the action of gravity, the molten explosive flows to the bottom of the cup.
It can be seen that with the increase of the heating time, more and more explosives are melted into the bottom of the beaker, and the solid pellets become smaller. The solid explosives are completely melted after about 30 minutes. The boundary conditions of the numerical calculation are the same as the experimental heating setting. The change process is represented by the volume fraction of the liquid phase in the calculation unit. The calculated melting process is shown in figure 3(d)~figure 3(f).

![Figure 3](image)

**Figure 3.** Comparison of experiments and calculations of the melting process.

It can be seen from the figure above that the melting occurred first at the corner of the outer surface. With the increase of time, the solid-liquid coexistence zone continuously moved from the surface of the grain to the center. The time from melting to completion of the phase change was 27 minutes. The experimental measurement of the temperature change of the explosive during the melting process and the temperature change obtained from the numerical calculation of measurement point 1 are shown in figures 4, and the consistency is good. The calculated and experimental temperature rise curves show an obvious temperature plateau at 97°C. This is due to the phase change endothermic process. When melting, the heat must transfer heat to the unmelted explosive, which causes the temperature to rise slowly, almost at fluctuations around the plateau.
4.2. Slow roasting process with shell explosives

Both experiments and calculations were performed at a heating rate of 1°C/min. The temperature change curve at the axis of the explosive was measured, and the response time and ignition temperature of the charge were obtained. The state change, temperature field distribution, and ignition position inside the shelled charge cannot be obtained through experiments, and can only be obtained through numerical simulation. The temperature field distribution at different times of the slow roasting process of constrained charge is shown in figure 5.

![Temperature rise curve of melting process calculation and experiment.](image)

**Figure 4.** Temperature rise curve of melting process calculation and experiment.

![Cloud diagram of temperature field distribution at different times.](image)

**Figure 5.** Cloud diagram of temperature field distribution at different times.

It can be seen from figures 5 that when the explosive is not melted, it is a heat conduction process from the outside to the inside, the outer layer temperature is high, the center temperature is low, and the internal temperature gradient of the charge is large. When heated for 4860s, the temperature at the center of the
explosive is 339k, and the temperature at the corners is 372k. At this time, the explosive starts to melt, and the molten paste-like area continues to expand toward the center. Its temperature distribution is shown in figure 5(b); When heated for 6531s, the explosive in the shell has completely melted, the liquid explosive has flowed under the action of gravity, the temperature of the upper layer is higher than the temperature of the lower layer, the flow of the explosive improves the heat transfer efficiency, the internal temperature difference is reduced, and the maximum temperature difference is about 6k. The liquid temperature distribution is shown in figure 5(c), and the temperature rise curve of explosives calculated and experimentally measured is shown in figure 6.

![Figure 6](image)

**Figure 6.** Temperature rise curve obtained from experiments and calculations.

It can be obtained from figures 6 that the experimental results agree well with the calculated results, and both have obvious temperature platforms and accelerated reaction stages. Because the measurement method of the thermocouple moving with the melting interface is used in the experiment, and the fixed-point measurement method is used in the calculation, the phase change platform of the temperature rise curve measured by the experiment is more obvious. After heating for 12582s, the temperature rose to 197°C. The temperature of the explosive had already exceeded the temperature of the shell. A high-temperature region was formed at the top middle position with a temperature of 475 k. The temperature distribution is shown in figure 5(e). At this time, the heating rate becomes significantly faster and increases exponentially. Explosives undergo rapid thermal decomposition under high temperature, releasing a large amount of heat, and the released heat cannot be lost in time. The accumulated heat further promotes the thermal decomposition of the explosives, forming a self-heating vicious cycle. After a brief acceleration reaction, the ignition and combustion of the explosive are caused. The temperature distribution at the ignition time is shown in figure 5(f). At this time, the explosive ignited from the high-temperature area, and quickly spread to the charge, and a violent reaction occurred.

The slow cook-off experiment with shell explosives has carried out a comparison experiment with vent holes and no vent holes. The experimental results show that when there are vent holes, a small amount of gas is discharged from the vent holes when the charge is heated to a certain value. Before the temperature rises to 163°C, the gas discharge volume does not increase significantly, and the discharged gas diffuses
freely, but after the charging temperature rises to 163 °C, the discharge volume increases rapidly, and the discharge rate increases. A large amount of gas is discharged, and the phenomenon is shown in figures 7. After a short acceleration reaction, the charge has a violent reaction, and the response temperature is 163 °C.

![Figure 7. Vent process during slow cook-off.](image)

The experimental wreck with vent holes is shown in figure 8(b). The shell ruptured outwards and the end caps bulged outward. This is because the pressure inside the shell was too large and the pressure was not released in time. As a result, the shell was broken into large pieces, and it can be judged that a deflagration reaction has occurred. When there is no vent hole, when the charging temperature rises to 171 °C, a violent reaction occurs. The debris after the experiment is shown in figure 8(a). It can be seen that the shell was exploded into fragments and an explosive reaction occurred.

![Figure 8. Wreckage of the shell after the experiment.](image)

5. Conclusion

(1) Using the calculation method of zero-order multi-step reaction, the numerical simulation results of slow roasting of the molten casting charge agree well with the experimental results. First, the surface layer melts to the center to become a liquid, and then the overall temperature rises. The upper layer temperature is slightly higher than the lower layer temperature. Finally, a high-temperature ignition region is formed in the middle of the upper layer.
(2) When the shelled explosive is slowly roasted, gas will be generated after the temperature rises to a certain value, and it can be smoothly discharged from the reserved hole. The slow-baking response of hermetically confined explosives is more severe than that of non-hermetically constrained explosives.

Reference

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