Numerical Simulation Research on Slow cook-off of Warhead of DNAN-based Melt-cast Explosive

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Abstract. RBOE explosive is a new type of DNAN-based insensitive melt-cast explosive with good thermal safety. In order to study the response characteristics of RBOE explosives under slow cook-off conditions, this study carried out a numerical simulation study of slow cook-off for the φ35mm×116mm RBOE cylindrical warhead. According to the thermal decomposition characteristics of each component of the explosive, the thermal reaction model of the RBOE explosive was established. Numerical simulation of RBOE warhead cook-off was carried out at a heating rate of 1K/min; the internal temperature rise curve, phase change cloud diagram and ignition cloud diagram of the warhead were obtained, and the thermal response characteristics of the RBOE explosive were analyzed.

1. Introduction
RBOE is a new type of DNAN-based insensitive melt-cast explosive (component mass ratio is 54wt% HMX, 20wt% NTO, 18wt% DNAN and 8wt% AL powder) [1]. There are few reports on the numerical simulation study of the explosive's cook-off. In order to study the cook-off characteristics of RBOE explosives, a theoretical model of RBOE explosive cook-off was established on the basis of the thermal reaction mechanism of the components in the mixed explosive. Based on the φ35mm × 116mm RBOE cylindrical warhead, a finite element model was established. Numerical simulation of RBOE warhead cook-off was carried out at a heating rate of 1K/min, and the response characteristics of the warhead under thermal stimulation were analyzed, which provides theoretical and data support for the thermal safety evaluation of RBOE warhead.

2. Establishment of theoretical model of RBOE warhead cook-off
2.1. Model assumptions
A numerical calculation model is established based on the thermal reaction mechanism of each component of RBOE explosives, and the following simplified assumptions are made:

(1) The heat transfer method in the slow cook-off process only considers heat conduction and convection heat transfer, ignoring the influence of radiant heat transfer on the temperature field.

(2) Ignoring the chemical reaction between the components in the mixed explosive, the self-heating reaction of each elemental explosive follows the Arrhenius law.

(3) After the explosive is melted, it is an incompressible flow; the density is only related to the temperature, and the change of density with pressure is not considered.

(4) The physical parameters of the warhead take the average value that changes with temperature, except for the explosive density.
(5) For the entire cook-off process before the response, it is assumed that the system never exchanges material with the outside world, and the mass, momentum and energy in the entire system are always conserved.

2.2. Cook-off model of RBOE explosive

RBOE is a mixed explosive made of 54wt% HMX, 20wt% NTO, 18wt% DNAN and 8wt% Al powder [1]. The numerical simulation of the cook-off process of the mixed explosive is mainly to accurately describe the thermal decomposition reaction of the mixed explosive [2]. In this study, a single-step + multi-step thermal decomposition reaction kinetic model is used to describe the decomposition reaction of each component, and the sum of the heat generated by their decomposition is used as the total reaction heat of the explosive.

2.2.1. Description of the thermal decomposition reaction of each component

(1) The thermal decomposition process of HMX is described by Tarver et al. [3] with a four-step chemical reaction:

\[ \text{Reaction 1: } \beta \text{HMX} \rightarrow \delta \text{HMX} \]  
(HMX endotherms and undergoes crystal form transformation);

\[ \text{Reaction 2: } \delta \text{HMX} \rightarrow \text{solid intermediate product} \] (endothermic reaction);

\[ \text{Reaction 3: solid intermediate product} \rightarrow \text{gas intermediate product} \] (a slight exothermic reaction produces intermediate gas products such as \( \text{CH}_2\text{O}, \text{N}_2\text{O}, \text{HCN} \) and \( \text{HN}_2\text{O} \));

\[ \text{Reaction 4: Intermediate gas product} \rightarrow \text{The final gaseous reaction product} \] (secondary gas phase reaction produces gaseous products such as \( \text{CO}_2, \text{CO}, \text{N}_2 \) and \( \text{H}_2\text{O} \)).

(2) The thermal decomposition process of NTO is described by Kou et al. [4] with a one-step chemical reaction:

\[ \text{Reaction 5: } \text{NTO} \rightarrow \text{product} \] (exothermic reaction)

(3) The thermal decomposition process of DNAN is described with reference to the study of Chen Lang et al. [5] with a one-step chemical reaction:

\[ \text{Reaction 6: } \text{DNAN} \rightarrow \text{product} \] (exothermic reaction)

(4) This article believes that Al does not participate in the thermal decomposition reaction of explosives.

2.2.2. Thermal decomposition rate

From the above reaction process, it can be seen that except for HMX, other thermal decomposition reactions are single-step zero-order reactions. Therefore, the thermal decomposition process of NTO and DNAN is described by the traditional Frank-Kamenetskii model, and the thermal decomposition process of HMX is described by McGuire-Tarver model.

(1) HMX:

\[ r_1 = Z_1 \exp\left(\frac{-E_1}{RT}\right)\rho_a \]
\[ r_2 = Z_2 \exp\left(\frac{-E_2}{RT}\right)\rho_b \]
\[ r_3 = Z_3 \exp\left(\frac{-E_3}{RT}\right)\rho_c \]
\[ r_4 = Z_4 \exp\left(\frac{-E_4}{RT}\right)\rho_d^2 \]

(2) NTO:

\[ r_5 = Z_5 \exp\left(\frac{-E_5}{RT}\right)\rho_e \]

(3) DNAN:
In the process, \( r_i \) is the mass reaction rate, \( Z_i \) is the pre-factor, \( E_i \) is the activation energy of the reaction, \( i \) is the reaction number, \( i=1, 2, 3, 4, 5, 6 \). \( \rho_m \) is the density of the reactants in each step, \( m=a, b, c, d, e, f \). \( R \) is the universal gas constant, and \( T \) is the temperature of the reactant.

2.2.3. Thermal decomposition reaction heat
This article defines the reaction heat \( S \) generated by the thermal decomposition of RBOE as the sum of the heat absorbed and released by the decomposition of HMX, NTO and DNAN.

\[
S(\text{RBOE}) = 0.54S(\text{HMX}) + 0.2S(\text{NTO}) + 0.18S(\text{DNAN})
\]

\[
S(\text{HMX}) = r_1 Q_1 + r_2 Q_2 + r_3 Q_3 + r_4 Q_4
\]

\[
S(\text{NTO}) = r_5 Q_5
\]

\[
S(\text{DNAN}) = r_6 Q_6
\]

Among them, \( Q_i \) is the heat of formation in each step of the reaction.

2.2.4. Thermal conductivity and specific heat capacity of explosives
Both the thermal conductivity \( \lambda \) and the specific heat capacity \( c \) of the explosive are functions of temperature, which are assumed to be constants here. According to the superposition principle, the thermal conductivity and specific heat capacity of RBOE can be expressed as [6]:

\[
\lambda = 0.54\lambda_{\text{HMX}} + 0.2\lambda_{\text{NTO}} + 0.18\lambda_{\text{DNAN}} + 0.08\lambda_{\text{Al}}
\]

\[
c = 0.54c_{\text{HMX}} + 0.2c_{\text{NTO}} + 0.18c_{\text{DNAN}} + 0.08c_{\text{Al}}
\]

3. Numerical simulation of RBOE warhead cook-off

3.1. Finite element model of RBOE warhead
This study selects the \( \phi 35 \text{mm} \times 116 \text{mm} \) RBOE cylindrical warhead as the research object to carry out the numerical simulation study on the cook-off. Since the RBOE cylindrical warhead is an axisymmetric structure, a 1/2 model is established. The warhead structure diagram and the finite element model diagram are shown in Figure 1. The warhead is composed of an upper end cover, a case, explosives and a lower end cover. The case and other metal materials are all made of 45# steel. A hexahedral mesh is used when dividing the mesh, and the maximum size of the mesh element is 1mm. In the numerical simulation study of the warhead, the temperature boundary conditions were set on the outer surface of the warhead case, the upper end cover and the lower end cover: the heating rate was 1K/min, and the initial temperature was 293K.
3.2. Solution parameter settings
Based on literature [2,7-10] and some physical property tests, the physical property parameters and reaction kinetic parameters of explosives are obtained in this study, as shown in Table 1~Table 3.

Table 1. Physical properties of each component of RBOE

|        | Density /kg·m⁻³ | Specific heat capacity /J·kg⁻¹·K⁻¹ | Thermal conductivity /w·m⁻¹·K⁻¹ |
|--------|-----------------|-----------------------------------|---------------------------------|
| HMX (54wt%) | 1850            | 1004.62                           | 0.5258                          |
| NTO (20wt%)  | 1850            | 1088                              | 0.27                            |
| DNAN (18wt%) | 1450            | 1170                              | 0.2                             |
| Al (8wt%)    | 2719            | 870                               | 1.39                            |

Table 2. Warhead physical parameters

|        | Density /kg·m⁻³ | Specific heat capacity /J·kg⁻¹·K⁻¹ | Thermal conductivity /w·m⁻¹·K⁻¹ | Viscosity /Pa·s | Melting point/K |
|--------|-----------------|-----------------------------------|---------------------------------|-----------------|----------------|
| RBOE   | 1850            | 1040.2948                         | 0.4851                          | 0.015           | 460.8          |
| 45 #steel | 7850            | 460                               | 32.6                            | -               | -              |

Table 3. Reaction kinetic parameters of each component of RBOE

|        | i   | E/J·mol⁻¹ | Z/s·l | Q/J·kg⁻¹ |
|--------|-----|-----------|-------|---------|
| HMX (54wt%) | 1   | 203574    | 7.9909E20 | -42000  |
|         | 2   | 221340    | 1.4130E21 | -252000 |
|         | 3   | 186060    | 2.0681E16 | 558600  |
|         | 4   | 143220    | 1.5984E12 | 5615400 |
| NTO (18wt%) | 5   | 1.675E5   | 1.1E12 | 3631610 |
| DNAN (20wt%) | 6   | 1.72E5    | 1.2E11 | 4.96E6  |

The natural convection formed by the buoyancy force after the melting of cast explosives is a low-speed flow field. Therefore, Boussinesq approximation is adopted for explosives [11]. The density of explosives is only related to temperature without considering its relationship with pressure. It holds that the explosive fluid in the flow field is incompressible. The mathematical expression [12] is as follows:

$$\rho_f = \rho_0(1 - \alpha_v \Delta T)$$

Where: \( \rho_f \) is the explosive density; \( \rho_0 \) is the initial density of explosive; \( \alpha_v \) is the coefficient of thermal expansion, \( \alpha_v = 1.1 \times 10^{-3} \).

3.3. Analysis of simulation results
Figure 2 shows the temperature rise curve of the RBOE warhead case and the center point of the explosive, and the change curve of the liquid fraction of the explosive. From Figure 2, it can be seen that the RBOE explosive starts to melt in 4130s and ends at 5440s, and the mass fraction of the liquid phase reaches 1. In the process of explosive melting, the temperature difference between the center of the explosive and the case gradually increases due to the heat absorption of the explosive melting, and reaches the maximum at the end of the explosive melting. Due to the large temperature gradient, the explosives are completely melted, and the convective heat transfer intensity increases, resulting in an increase in the temperature of the explosives, and finally the temperature of the case tends to be the
same. The RBOE warhead had an ignition reaction at 9883s, and the case temperature was 466K at this time.

Figure 2. RBOE warhead temperature rise curve and liquid phase mass fraction change curve

Figure 3 is the cloud diagram of temperature distribution and liquid fraction distribution of rboe explosive before and after phase change. As can be seen from Fig. 3, the warhead temperature is concentric and symmetrically distributed before the explosive phase change. During the phase change process, the unmelted explosive is suspended under the warhead in a conical shape, and the temperature is distributed from high to low. After the phase transition, the internal temperature of the warhead also shows a trend of high and low. This further shows that after the explosive melts, convection occurs in the warhead due to the action of gravity and buoyancy.

(a) Before the phase change (3000s)  (b) Phase change (5200s)
Figure 3. Temperature cloud map and liquid phase mass fraction distribution cloud map before and after phase transition of explosive

Figure 4 shows the mass fraction distribution of each component of the RBOE explosive at different times and the temperature distribution inside the explosive at the time of ignition. At the moment of ignition of the explosive, $\beta$HMX has reacted completely, and solid intermediate products and gaseous intermediate products are successively formed. DNAN and NTO have good thermal stability, and there is basically no thermal decomposition reaction before the RBOE explosive is ignited. Due to the effect of convection, the ignition temperature of the warhead appears on the top of the warhead, and the ignition temperature of the explosive is about 492K.

Figure 4. The mass fraction distribution of each component of the explosive at different times and the cloud diagram of the temperature distribution at the moment of ignition of the explosive

4. Conclusion
In this study, a single-step + multi-step thermal decomposition reaction kinetic model is used to describe the decomposition reaction of each component of RBOE explosive, and a RBOE explosive cookoff model is established to predict the distribution of the mass fraction of each component of the explosive over time. Through numerical simulation, it is found that the final ignition position of the warhead appears on the top of the warhead due to the convection effect after the explosive is melted. This research can provide theoretical and data support for the thermal safety evaluation of the RBOE warhead.
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