Numerical Simulation of Deflagration to Detonation Transition in High-Energy Propellant

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Abstract. The deflagration to detonation transition model was established based on AUTODYN/ANSYS to simulate the process of DDT and provide a basis for the safety analysis of high-energy propellant. The process of DDT was numerically simulated by the ignition and growth reactive flow model and ALE method. The detonation pressure, detonation velocity, the run distance and time to detonation were calculated. The simulating results indicate that the detonation velocity is about 2899 m/s, the run distance to detonation is about 138.3 mm when the density of propellant is 1860 kg/m³. The numerical results are in a good agreement with the experimental results.

1. Introduction
Solid propellant is the power source of weapon and rocket engine propulsion systems [1]. With the development of these systems, a large number of high-energy explosives, such as RDX and HMX, are added into solid propellants, which increase the energy and thrust of propellants, while increasing the hazard of propellants greatly at the same time.

The phenomenon of deflagration to detonation transition (DDT) is one of the important criteria for evaluating the safety of energetic materials [2]. Because DDT is a very complex, highly non-linear and scale-crossing transition process, and solid propellant is a composite energetic material based on polymer and filled with metal powder and oxidant, so it is extremely difficult to study DDT of propellant [3]. In recent decades, many scholars have studied DDT of solid propellants by means of numerical simulation method. At present, two phase mixed continuous flow models, including BN model proposed by Baer and Nunziato[4] and PSK model proposed by Powers[5] are widely used in the numerical simulation of DDT. Butler[6] and X. R. Jia[7] simulated DDT of solid propellant using two-phase reactive flow model. However, the actual propellant has low porosity, so it is not suitable to use two-phase flow model to study its DDT behavior[8]. Meantime, the three-dimensional numerical simulation of DDT needs further research and improvement. G. C. Qin[9] and N. Qin[10] studied the effects of different conditions on DDT for several propellants by experiments. Compared with the experimental method, the numerical simulation method not only has less cost and higher security, but also can obtain more data. Therefore, it is more conducive to the analysis of DDT process. From the existing experimental and numerical simulation studies[11], the researches on DDT of propellants mainly focuses on the low and medium density conditions, so it is necessary to carry out the research on the high density conditions.
In this paper, a three-dimensional numerical simulation model of DDT for high-energy propellant is established according to the actual experiment. The ignition and growth reactive flow model is used to describe the reaction process of high density propellant, and DDT process is analyzed. The detonation parameters, the run distance and time are calculated. It would provide a basis for analyzing and evaluating the safety of high-energy propellants.

2. Experiment and Numerical Models
The research model of DDT is mainly based on DDT tube. Based on the DDT tube experiment, the numerical model was established to solve DDT problem. The high-energy propellant in the tube is mainly composed of hydroxyl-terminated polybutadiene (HTPB), ammonium perchlorate (AP), cyclotrimethylenetrinitramine (RDX) and aluminium (Al), and its density is 1860kg/m$^3$.

2.1. Experiment of DDT
The experimental device is shown in Figure 1. The high-energy propellant is loaded into a slightness steel tube (DDT tube), and the igniter made from black powder and RDX is placed at the end of the propellant column. The igniter ignites the ignition powder. Then, the propellant is ignited and combust, and transit to detonation under certain conditions. The length of the DDT tube is 400mm, and the outer diameter and inner diameter of the shell are 28 mm and 10 mm. In order to fix the experimental device, the end caps are fixed on the thick steel plate and fastened by bolts. In order to measure the propagation velocity of detonation wave, some electrical pins are set along the axis of the tube wall. When the detonation wave reaches the positions of pins, the pins conduct electricity, and the signal reception device is triggered. The validation plate is placed under the experimental device, and DDT is judged by observing the deformation of the tube and validation plate.

![Figure 1. The experimental device photo.](image)

The DDT phenomenon of high-energy propellant was observed by the DDT tube experiment. By analyzing the fragments of tube and the indentation of validation plate as shown in Figure 2, the run distance to detonation was obtained about 135mm, and the stable detonation velocity is about 2940m/s measured by the electrical pins.

![Figure 2. Experimental apparatus results photo of DDT.](image)
2.2. Physical Model and Calculating Models

The physical model of DDT tube in this paper is shown in Figure 3 composed by end caps, shell, igniter and propellant. Compared with the experimental device, the validation plate and bolts are simplified.

![Figure 3. Physical model of the DDT tube.](image)

ANSYS/AUTODYN is an explicit non-linear dynamic analysis software, which can analyze the dynamic characteristics of solids, fluids and gases. It is widely used in the field of explosion research. The calculating model is established based on the physical model shown in Figure 3. Because of the symmetry of the physical model, the 1/4 three-dimensional model is established as shown in Figure 4. The calculation model is composed of DDT tube, high-energy propellant and end caps, and their sizes are the same as the experimental model sizes. The igniter is simulated by applying the ignition boundary on the propellant end surface. Automatic contact is defined between parts of the model.

![Figure 4. The calculating model.](image)

2.3. Physical Model and Calculating Models

The governing equations involved in the numerical simulation of DDT include conservation equations and material models, and material models include equations of state and strength models. The partial differential forms of the governing equations for the conservation of mass, momentum and energy are shown in equations (1)-(3).

\[
\frac{\partial \rho / \partial t}{\partial \rho / \partial t} + \rho \nabla \cdot (\mathbf{u} + \mathbf{e}) = 0
\]  
\[\rho (\partial \mathbf{u} / \partial t + \mathbf{u} \cdot \nabla \mathbf{u}) = \nabla \cdot \mathbf{\sigma}
\]
\[ \rho (\partial \varepsilon / \partial t + \mathbf{u} \cdot \nabla \varepsilon) = \sigma \cdot \psi \]  

where \( \rho \) is density, \( \mathbf{u} \) is the particle velocity, \( \varepsilon \) is internal energy, \( t \) is time, \( \sigma \) is stress tensor, \( \psi \) is strain rate tensor.

The materials include shell, end caps and high-energy propellant in this model. The materials of shell and end caps are 45\(^8\) steel and stainless steel. The shock equation of state and Johnson-Cook strength model were used in the material models as shown in equations (4)-(6). Some parameters of them used in calculation were listed in Table 1.

\[ u_s = c_0 + \varepsilon u_p \]  

\[ \sigma = (A_0 + B_0 \varepsilon^0)(1 + C_0 \ln \dot{\varepsilon}) (1 - T_i^m) \]  

\[ T_i^m = (T_i - T_0) / (T_m - T_0) \]

In equations (4)-(6), \( u_s \) is stress wave velocity in solid medium and \( u_p \) is particle velocity of wave front. \( c_0 \) is sound velocity of the medium. \( \sigma \) is strain stress. \( \varepsilon \) is effective plastic strain. \( \dot{\varepsilon} = \dot{\varepsilon} / \dot{\varepsilon}_0 \) is dimensionless strain rate. \( T_i \) is reference temperature. \( T_m \) is material melting point. \( S, A_i, B_i, n, C_i, m \) are constants.

### Table 1. The parameters of 45\(^8\) steel and stainless steel.

| Materials         | Density /kg·m\(^{-3}\) | \( c_0 \)/cm·μs\(^{-1}\) | \( s \) | Gruneisen coefficient | Shear Modulus /GPa | Yield Stress /GPa |
|-------------------|--------------------------|---------------------------|-------|-----------------------|-------------------|------------------|
| 45\(^8\) steel    | 7900                      | 0.457                     | 1.49  | 2.17                  | 81.8              | 0.35             |
| Stainless steel   | 7750                      | 0.457                     | 1.49  | 2.17                  | 81.8              | 1.54             |

It is very complex to establish the propellant material model. Not only the state and strength of propellant but also the process of DDT should be described. Ignition and growth reactive flow model has been widely used in shock ignition and DDT of explosives and propellants, which was used as the equation of state model of propellant materials. The model includes JWJ equations describing the state of unreacted propellants and products, and Lee-Tarver model describing the reaction rate [12] as shown equations (7)-(8). The first item on the right-hand side of equation (8) is the ignition term representing the creation of hot spots. The second and third terms are the growth and completion terms. The second item of equation (8) represents the process with a lower reaction rate before the formation of the detonation. The third item of equation (8) represents the detonation transition process with rapid reaction. The parameters of ignition and growth reactive flow model was listed in Table 2[13].

\[ p_i = A_i \left( \frac{1 - \omega}{R_{\nu}} \right) e^{\lambda \tau} + B_i \left( \frac{1 - \omega}{R_{\nu}} \right) e^{-\lambda \tau} + \frac{\omega y e}{\bar{\nu}} \]  

\[ \frac{dF}{dt} = I \left[ (1 - F)^i \right] \left[ \rho / \rho_0 \right] - a + G_i (1 - F)^i F^i P^i \]  

where \( F \) is pressure, \( i \) is 0 for unreacted propellant. \( i \) is 1 for reaction products. \( \bar{\nu} \) is relative volume. \( A_i, B_i, R_i, R_2 \) are respectively constants. \( \omega \) is Gruneisen coefficient. \( F \) is the degree of reaction. \( \rho \) and \( \rho_0 \) are current density and initial density respectively. \( I, G_1, G_2, a, b, c, d, e, g, x, y \) and \( z \) are respectively constants.

### Table 2. The parameters of ignition and growth reactive flow model for high-energy propellant.

| \( I \)   | \( b \)   | \( a \) | \( x \) | \( G_1 \) | \( c \) | \( d \) | \( y \) | \( G_2 \) | \( e \) | \( g \) | \( z \) |
|---------|----------|--------|-------|--------|-------|-------|-------|--------|-------|-------|-------|
| 7.4×10\(^{11}\) | 0.667    | 0      | 20    | 7      | 0.667 | 0.111 | 1.5   | 800    | 0.333 | 1     | 2     |
3. Simulation Results And Discussions
Based on the above calculation model, the appropriate mesh size was obtained by calculation, and the results of relevant parameters were obtained, and the DDT process of high-energy propellant was calculated and analyzed.

3.1. Verification of Grid Independence
The numerical simulation regarding grid independence is carried out in order to increase the accuracy of calculation. The sizes of grids in calculations are 5mm, 2mm, 1mm, 0.5mm and 0.25mm respectively. Figure 6 shows the curves of velocity vs time calculated from different grid sizes. From the figure, it can be seen that the curves of velocity vs time are similar for different grid sizes, but the velocity values at the same time calculated by different grid sizes are different. When the grid sizes are 0.25mm and 5mm, the maximum deviation of velocity values is about 500m/s. It means that the difference of grid sizes could cause calculation deviation. The deviation under different grid sizes are shown in the Table 3. As the grid sizes decrease, the number of grids increase, and the calculation deviation decreases, but the calculation time increases. When the grid size is 0.5 mm, the deviation is 0.35%. The calculation time increases obviously, and the calculation speed is very slow when the grid size is 0.25 mm. Considering the calculation accuracy and cost, the grid size with 0.5mm is the most suitable determination to calculate the model.

![Figure 6. Variation of velocity values with different grid sizes.](image)

| Grid Size /mm | 5   | 2   | 1   | 0.5 | 0.25 |
|---------------|-----|-----|-----|-----|------|
| Deviation     | 14.8% | 5.2% | 3.9% | 0.35% | -    |

3.2. Simulation Results of DDT Parameters
The numerical simulation had been studied according to the experiment, and the results were compared with the above experimental results. The reaction degree(F) of different reaction periods is different. It is an important parameter to describe DDT of propellant which can be obtained by calculation. When \( F=0 \), the propellant doesn’t react and the propellant reacts completely when \( F=1 \). In order to analyze the change of the reaction degree during the DDT process of propellant and determine the run distance to detonation more accurately, the curves of the reaction degree-time at different positions were shown in Figure 7. It can be seen that the reaction degree only reaches 40% when the distance is 18.4mm (Gauge#10), and the reaction is complete at 108mm (Gauge#55), but it still needs some reaction time, so the detonation doesn’t occur yet. When the distance is 138.3mm (Gauge#70), F increases vertically to 1, and the reaction is complete quickly. The detonation occurs at this position, and the reaction time to the position is about 42.6μs. The phenomenon lasts until the whole column finishes the reaction. The
stable detonation occurs. Therefore, the run distance and time to detonation of high-energy propellant are about 138.3mm and 42.7μs under this condition. Figure 8 shows the peak values of pressure and velocity vs distance along the propellant column. It can be seen that the pressure and velocity linearly increase at first, and they suddenly rise at 118mm. When the detonation wave propagates to 138 mm after 42.7μs, the detonation pressure and velocity reach stable values of 35.6GPa and 2899m/s, respectively. Compared with the experimental results, the deviation of detonation velocity is about 1.4%, and the deviation of the run distance to detonation is about 2.4%. Therefore, the model is very effective to calculate DDT of high-energy propellant.

3.3. DDT Process of High-Energy Propellant
The DDT process of propellant was studied by observing the reaction process and analyzing the changes of parameters such as pressure and velocity in propellant. Figure 9 shows the pressure nephogram at different times. As seen in Figure 9, the high-energy propellant is ignited and burned under the action of ignition energy at the boundary. As the reaction proceeds, the pressure increases, producing a large number of gas products and leading to ignition of more propellant and accelerating the reaction. The reaction is more and more intense, and the accelerated deflagration can eventually lead to shock compression of the unreacted propellant and finally transit to detonation. The width of the high-pressure reaction zone decreases with the increase of the reaction pressure, especially when the detonation occurs, the high-pressure reaction zone becomes very thin. Because when the detonation occurs, the pressure in the reaction zone is very high, and the reaction completes quickly and continue to react forward. Meanwhile, with increase of reaction time, pressure in the tube gradually increases beyond the allowable stress of the tube, the deformation of the tube occurs.

The pressure and velocity at different positions of the propellant varies with time as shown in Fig. 10. It can be seen from the curves that the pressure at the beginning is low and the reaction velocity is
subsonic, showing combustion characteristics. As the increase of compressional wave strength, a strong shock wave forms, and the pressure and velocity rise sharply, showing the detonation characteristics. DDT occurs when the accelerating subsonic deflagration wave transmits to a high order detonation wave. The increase of pressure in the tube is not only due to the gas product released by the reaction, but also the restriction of the shell. Meantime, the reaction rate increases with the pressure that makes the velocity increase.

![Image](a) $t=4\mu s$  
![Image](b) $t=16\mu s$  
![Image](c) $t=32\mu s$  
![Image](d) $t=42\mu s$  
![Image](e) $t=44\mu s$  
![Image](f) $t=60\mu s$

**Figure 9.** Pressure nephogram of propellant at different times

![Image](a) Time/μs  
![Image](b) Pressure/Mbar  

**Figure 10.** Curves of pressure and velocity vs time at different positions

4. **Conclusions**
According to the state of high density charge, the calculating model of DDT in high-energy propellant is established, and the process of DDT is analyzed. The results show that DDT could occur when the high-energy propellant ignited under strong confinement. The ignition and growth reactive flow model can describe the reaction process of propellant very well, and the ALE method can be used to solve the DDT problem. The detonation velocity and pressure are 2899m/s and 35.6GPa, and the run distance and time are about 138.3mm and 42.7μs, respectively. The numerical results are in a reasonable agreement with the experimental results. When the high-energy propellant transits from deflagration to detonation, a large amount of energy would be released, so it needs to pay attention to avoid DDT caused by accidental ignition of propellants.

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