Research paper

Numerical simulation of pyrotechnic device based on propellant deflagration model

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Abstract

A Propellant Deflagration Model (PDM) was developed to understand the physics and predict the functional performance of pyrotechnic devices. The model is based on the Lee-Tarver reaction rate model, and could consider the combination of combustion process and the unsteady gas dynamics in the performance of devices. The closed vessel test was used for fitting the PDM parameters of SL17 (64%Nitrocellulose, 34%Nitroglycerin), and the validity of the model and parameters is assessed for firing tests of catapults. The results of calculation are in good agreement with the test results. The model can be used to quickly explore and assess the effects of geometric, structural, and energetic material design modifications on the power producing capability and performance of pyrotechnic devices in different environments.

Keywords: pyrotechnic device, propellant burn, deflagration model, closed vessel

1. Introduction

Pyrotechnic devices are mechanical devices that are powered by energy released from chemical reactions in energetic materials. Their ability to rapidly deliver high pressures renders them the tool of choice to perform such functions as pulling pins, exploding bolts, and cutting cables. In order to better design these devices, it is necessary to understand the interaction between the combustion process and the operation of the device[1]. However, it is not easy to understand the details such as the burning of pyrotechnic charge and the destruction of components in the firing tests due to its high-speed transient process. For this reason, the computational modeling of pyrotechnic device is valuable to be established to facilitate interpretation of experimental results and assist in the design of new and modified devices. For decades, a great deal of research has been carried out on computational modeling related to the performance of several types of pyrotechnic devices. Ng developed one of the earliest models for explosively actuated devices called MAVIS[2], in which mass and energy release due to the combustion process are not explicitly modeled, but rather an empirically determined equation of state is used to describe the pressure that drives piston motion. Similarly, the work of Emery and Jones, et al[3), 4)], describes the work required to move a piston within an explosively actuated valve. Afterwards some researchers considered the thermochemistry of pyrotechnic device. Their models include the time-dependent mass and energy release of pyrotechnic charge into gas and condensed phase products, in which the thermodynamic quantities are spatially homogeneous at any time interval. This assumption allows the model to consist of a system of ordinary differential equations with respect to time[5)-12)]. All the models mentioned above that do incorporate combustion assume that acoustic time scales are much smaller than the devices operation time. The work of Lee[13] explored the effects of unsteady gas dynamics within a closed vessel and determined that the quasi-equilibrium assumption becomes invalid as the device operation time approaches the gas dynamic wave propagation timescale. However, Lee's model does not include the mass and energy production from charge combustion, but rather imposes a high pressure discontinuity as an initial condition to simulate combustion. Therefore, the previous models have not considered the combination of combustion process and the unsteady gas dynamics in the prediction and analysis of the performance of pyrotechnic devices.

The goal of the present work is to formulate a comprehensive, but simple, mathematical model that describes the burning rate of propellant and the heterogeneous gas distribution spatially, which can be used to quickly explore and assess the effects of geometric, structural, and energetic material design modifications on the power producing capability and performance of pyrotechnic devices in different environments.

The outline of this paper is as follows. A mathematical model named Propellant Deflagration Model is described in Section 2. The experiments used to derive the major performance parameters for the model are summarized in Section 3. The verification of the model is introduced by the calculation of performance of a catapult in Section 4. In the Section 5, the calculation results of the PDM are discussed by fitting parameters of the model and comparing the velocity-time traces.

2. Propellant Deflagration Model (PDM)

A mathematical model was developed to simulate the performance of pyrotechnic device. Understanding the physics of propellant burning in the pyrotechnic device is key to predict its performance. Therefore, the model should include the burning rate of propellant which can completely describe the variation of burning with pressure in the expansion chamber. The classic combustion process of propellant is shown in Figure 1. Propellant deflagration from the left would produce a plane combustion wave spread to the right. The combustion wave would gradually transfer into the unburned propellant, and then the propellant starts the chemical reaction until the gas reaction product is formed. For this process, there is a relatively wide reaction zone between the unburned propellant and reaction product, in which gasification and reaction of propellant are occurred. The combustion wave ignites the unreacted propellant by heat conduction and diffusion, and the unreacted propellant coming into the reaction zone reacts controlled by the chemical reaction rate. The propellant burned completely left into the product zone finally. In this case, the reaction zone width can be determined by macroscopic combustion wave velocity (start of burning) and microscopic reaction rate (end of burning). Based on the above analysis, the Propellant Deflagration Model in this paper would be comprised of unreacted state equation, macro combustion equation, micro reaction rate equation and reaction product equation. The combustion wave velocity is controlled by macro combustion equation, and the reaction of propellant is controlled by micro reaction rate equation. As the reaction converts the unreacted propellant to the reaction product, these unreacted state equation and reaction product equations are used to calculate the mixture of unreacted propellant and reaction product defined by the fraction reacted Ψ ($\Psi=0$ implies no reaction, $\Psi=1$ implies complete reaction). The temperatures and pressures are assumed to be equal during reaction. Therefore, this model could describe the propellant combustion process phenomenologically.

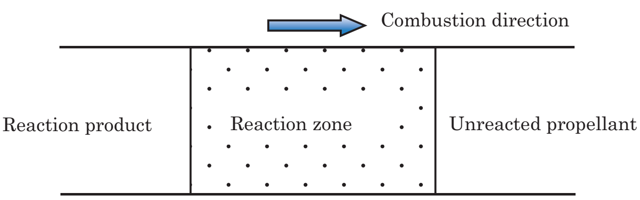

Figure 1 Scheme of classic propellant burn.

Macroscopic combustion equation is mainly to establish the relation between combustion velocity u (in m·s^{-1}) and pressure P (in Pa), which is derived from the geometrical combustion model of propellant:

$$u = BP^{n} \tag{1}$$

Microscopic reaction rate equation is mainly to build the relation between reaction fraction Ψ and ressure P, which is similar to Lee-Tarver reaction rate model of explosives[14]:

$$\frac{d\Psi}{dt} = A\,(1-\Psi)^{R1}\Psi^{R2}P^{n} \tag{2}$$

Unreacted propellant equation is established by perfect gas state equation, which is used to describe the pressure variation of unreacted propellant under low pressure.

$$P = \rho RT \tag{3}$$

Reaction product equation is mainly established by Van Der Waals gas state equation, which is used to describe the pressure variation of reaction product under high pressure.

$$P = \frac{\Psi\omega RT}{(V-(1-\Psi)\,\omega/\rho_s - \Psi\omega\alpha)} \tag{4}$$

In these equations, u is macroscopic combustion velocity, P is gas pressure (in Pa), ω is the amount of propellant (in kg), Ψ is reaction degree, R is gas constant, T is gas temperature (in K), V is relative volume (in kg·m^{-3}), ρ_s is propellant density(in kg·m^{-3}), α is co-volume, A, B, R_1, R_2, n is constant, which are inherent properties of the propellant. The above four equations could completely describe the process from propellant deflagration to reaction product by chemical reaction.

Finally, the PDM model is embed into the Explicit Dynamic Software(MSC Dytran). In each step of calculation, the PDM model is used to calculate the combustion rate of propellant and the production of gas, then Dytran could be used to calculate the process of gas expansion in the chamber. According to the pressure calculated around the charge, the PDM could calculate the burning rate of propellant and production of gas again in the next step. This iterative calculation continues until the burning of the propellant is finished.

3. Input parameters fitting of PDM

Propellant deflagration model involves several parameters, some of which have not physical meaning. Therefore, it is the premise to determine the model parameters for accurate description of combustion characteristics. The gas pressure is the key parameter to show the burning performance of propellant. Therefore, the closed vessel test is used as the standard experiment to catch the pressure-time trace of different propellants. In the fitting process of parameters, the combustion of propellant in the vessel is simulated by PDM and Dytran with the initial input parameters, and the calculated pressure and experimental pressure are repeated fitting by the Optimization Software Isight to obtain the optimized PDM parameters.

Figure 2 is the schematic diagram of a typical closed vessel test. The test device is composed of the igniter, prime charge, closed vessel and piezoelectric sensors. When the igniter receives the electrical signal, the propellant is initiated by the igniter, the combustion of propellant produces a high-temperature and high-pressure gas, the pressure-time trace curve is recorded by the piezoelectric sensor. In this experiment, the volume of closed vessel is 10 ml, the igniter is specified to produce (10 ± 4) MPa in 10 ml vessel, and the prime charge is a Double-Base propellant named SL17.

The finite model of closed vessel is constructed with axisymmetric elements to determine the input parameters of PDM of SL17, as shown in Figure 3. The model is simplified to only include air domain and prime charge. The igniter is defined as an energy source. In the calculation, the energy source injects a certain pressure into the vessel, when the pressure reaches a certain value, the propellant SL17 is ignited. The combustion of propellant leads to the pressure in vessel increasing gradually until the propellant burns out.

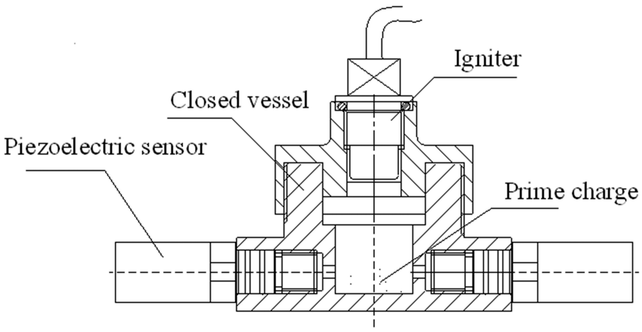

Figure 2 Geometry of closed vessel test.

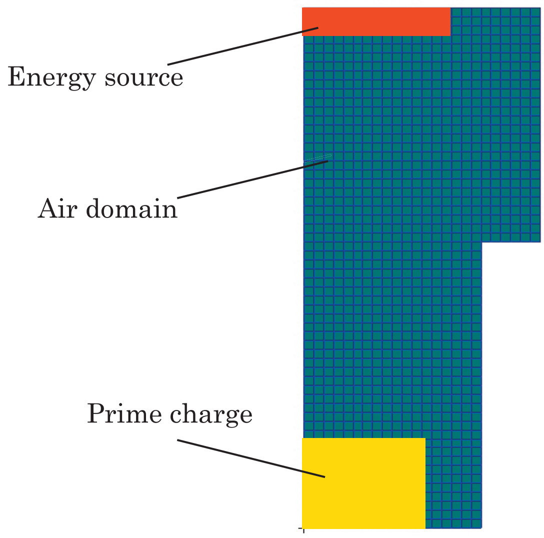

Figure 3 Numerical model of closed vessel.

4. Validation of PDM

In order to verify the accuracy of PDM and its parameters, the calculation of working process of a catapult is developed. The ejection speed of inner barrel in calculation is compared with experimental result to verify the accuracy of the model.

Figure 4 is the scheme of the catapult. The catapult is mainly composed of the outer barrel, inner barrel, piston, rod, shear pin, prime charge and igniter. When the igniter receives an electric signal to release the energy, the prime charge is initiated and produces a high-pressure gas. When the chamber pressure reaches a certain value, the piston actuates the rod to cut the shear pin and impact the inner barrel, eventually the inner barrel flies out of the outer barrel. According to the physical model, the calculated model of catapult is established and simplified in Figure 5. The igniter is still simplified as the energy source, and the shear pin is assumed as a binding force between the rod and inner barrel. The materials of the inner barrel, outer barrel, piston and rod are stainless steel described by elasto-plastic material model, the prime charge is 100 mg SL17 described by PDM. The force between the rod and inner barrel sets to 2000N.

5. Calculation results and discussion

5.1 Parameters of SL17

The fitting process of SL17 parameters is as follows: firstly, the combustion process is calculated by the input of a set of parameters of SL17, and the calculated pressure-time trace is compared with the closed-vessel experiment.

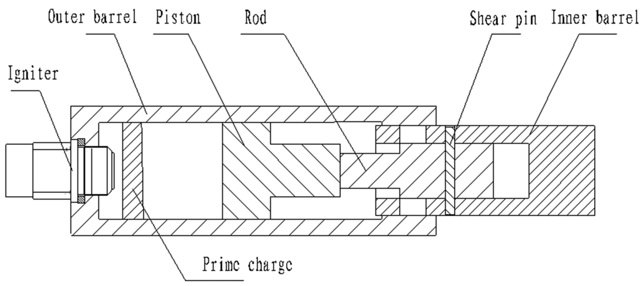

Figure 4 Geometry of the catapult.

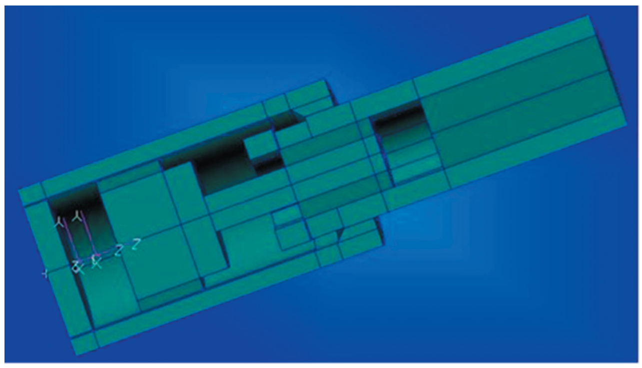

Figure 5 Numerical model of the catapult.

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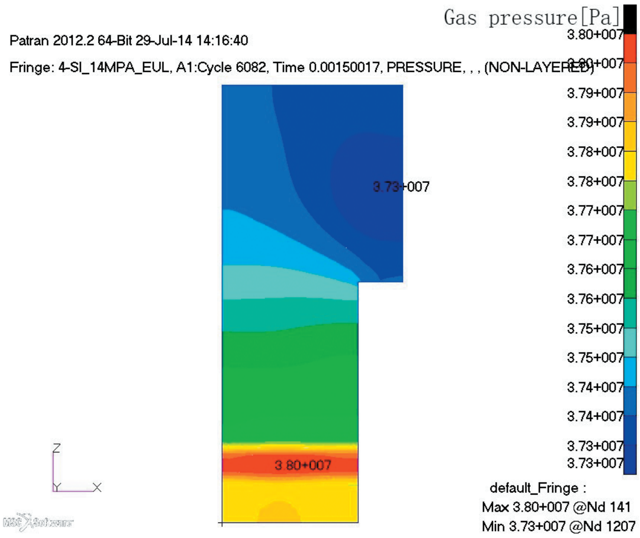

Figure 6 The calculation pressure contour.

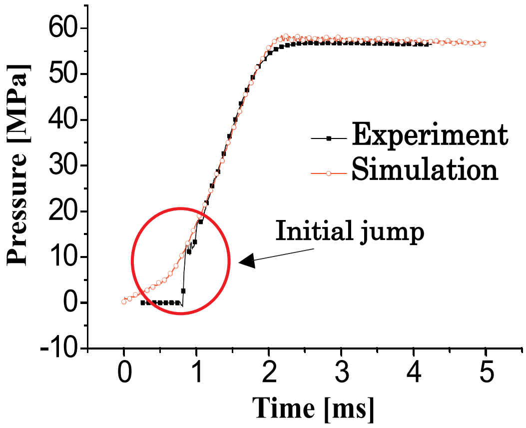

Figure 7 Comparison between calculation and test curve.

Then the parameters are adjusted according to the difference, and input the code to calculate again until the simulated pressure agree well with the experimental pressure. Finally, the determined parameters would be used to describe the reaction of SL17.

Figure 6 is the calculated pressure contour of closed vessel. At 1.5 ms, the maximum pressure in the vessel is 38 MPa, and the minimum pressure is 37.3 MPa, which show that the pressure in the chamber is almost uniform, and the gas has enough time to diffuse during the combustion. Therefore, it could be considered that the pressure distribution in the vessel is quasi-equilibrium. Taking a position to monitor the pressure in the vessel, as shown in Figure 7, the result is used to compared with experimental result. At 2.2 ms, the gas pressure reaches up to 55 MPa, then the pressure remains constant, which shows that the propellant burns completely. In the experimental pressure -time trace, the pressure curve can be divided into two periods, the initial pressure jump is the energy output of igniter, and the subsequent slow pressure increase is the gas output of propellant combustion. From the comparison between test and calculation, it has some differences in the initial period of two curves, but they are in good agreement during propellant combustion period. This is because that there is some difference in output characteristics between real igniter and energy source,

Table 1 Model parameters of SL17.

ρ_s[kg·m^{-3}]	B	A	R_1	R_2	n	α
0.8e3	1200	20	0.48	0.48	0.1	0.9e−3

and the output rate of energy source is lower than that of igniter. Overall, the calculated results on propellant combustion are in good agreement with the experimental results, which show that the model could describe the combustion characteristics of propellant wonderfully. Finally, the fitted model parameters of SL17 are obtained, as show in Table 1.

5.2 Catapult simulation

The fitting parameters of SL17 are applied to catapult calculation to predict its performance. Figure 8 is the working process of the catapult. At 0.17 ms, the propellant starts to burn, and the pressure in the chamber is up to 5 MPa. The force that gas pushing piston is still lower than that to cut the shear pin, so the piston is still motionless. When the force is bigger than the force of shear pin, the pin would be cut off, and the piston begins to push the rod to move forward. At 0.62 ms, the piston and rod assembly impacts the inner barrel, and the maximum pressure in the chamber is about 11 MPa, then the assembly of piston, rod and inner barrel are accelerated together. At 1.29 ms, the piston stops moving by the impact of outer barrel, and the inner barrel and rod assembly continue to move forward by inertia, and the maximum pressure in the chamber drops to 9.2 MPa. At 1.34 ms, the inner barrel and the rod assembly separate from catapult in a speed, and the pressure drops to 9 MPa. The above results show that the calculation can reflect the ejection process of catapult completely. When the chamber is small, the pressure in the chamber is uniform. While the chamber increases bigger, the gas pressure starts to show a heterogeneous distribution. The maximum pressure is 2 MPa higher than the minimum, and the pressure around the propellant is higher than the back of rod.

Figure 9 is the calculation velocity-time trace of the inner barrel. The inner barrel speed is stepped up gradually. At 0.6 ms, the piston and rod assembly impacts the inner barrel, which causes the inner barrel velocity increasing rapidly to 17 m·s^{-1}. Then the velocity-time curve appears as a platform, which is caused by the separation between assembly and the inner barrel after impact at 0.9 ms, the piston and rod assembly catches up with the inner barrel and impact again by the gas driving in the chamber, the velocity of inner barrel is further increased to 25 m·s^{-1}. Then, the speed stays constant again, and the assembly separates from the inner barrel again. Overall, after four times of collision, the piston stops in the outer barrel, and the inner barrel and rod assembly flies out of the outer barrel in the velocity of 35 m·s^{-1}.

Figure10 is the test velocity-time trace of the inner barrel. The test curve is relatively smooth, which is caused by the sampling frequency of measurement being only 4000 Hz, while the time of inner barrel from static to maximum speed is about 1 ms, therefore, this test could

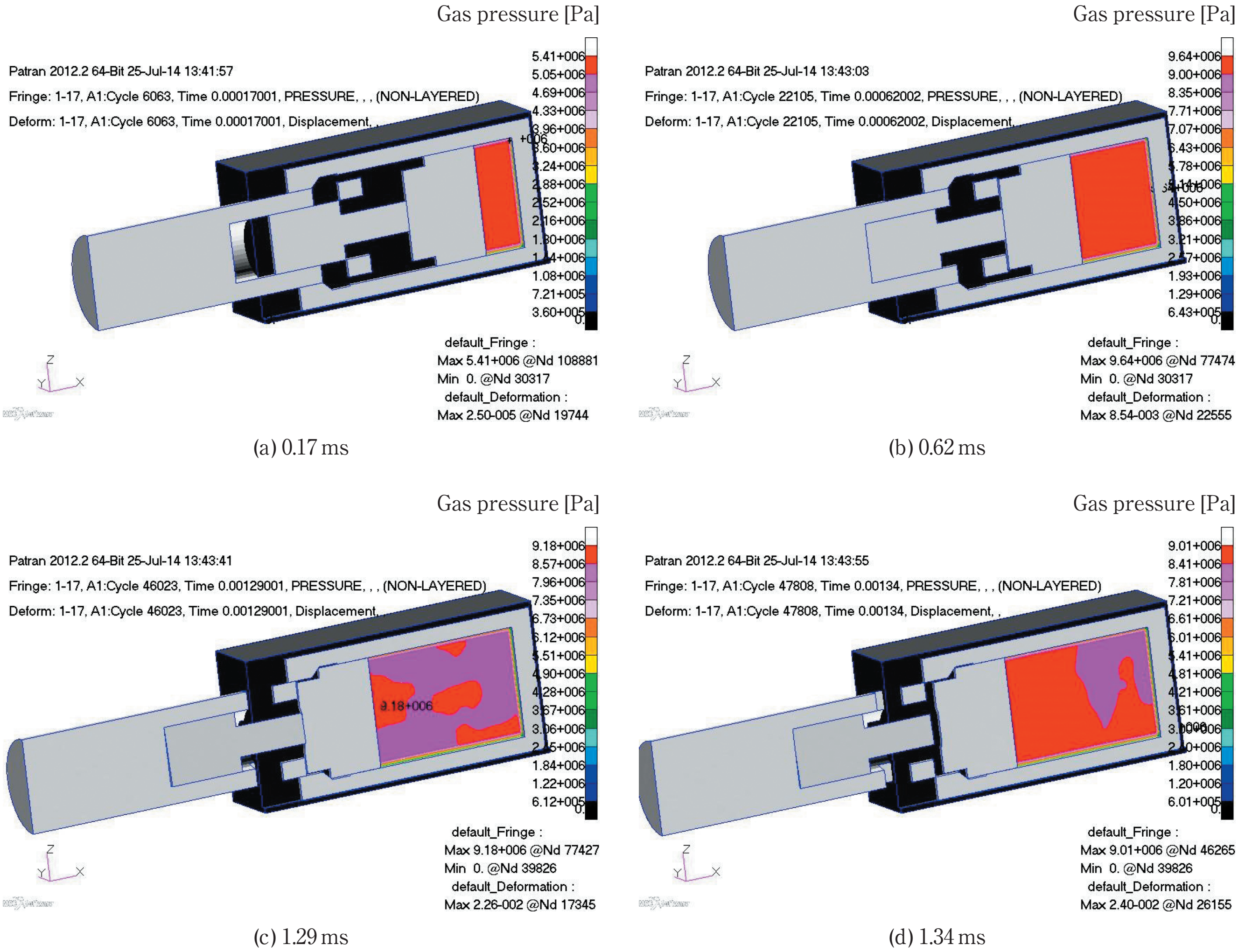

Figure 8 The movement process of catapult at different moments.

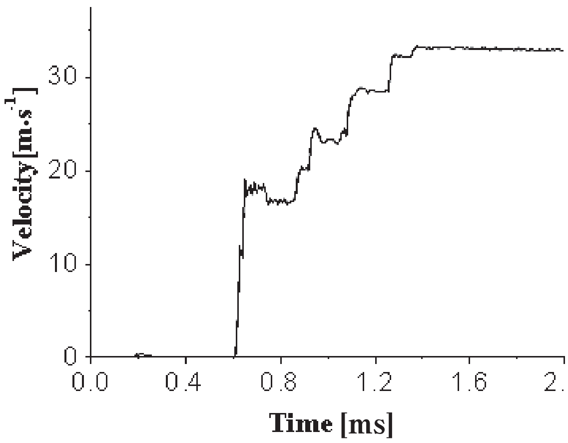

Figure 9 Calculation velocity-time curve.

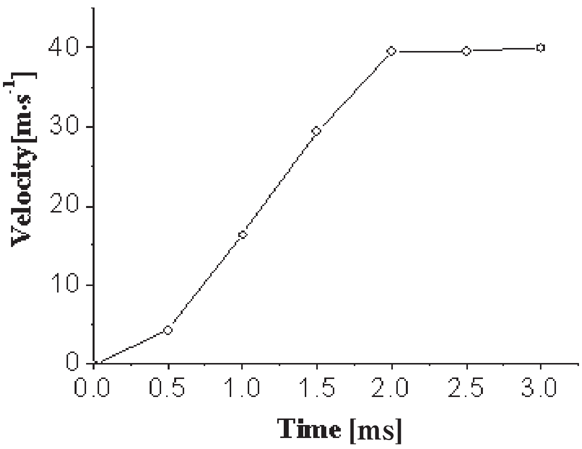

Figure 10 Test velocity-time curve.

not reflect the details of the inner barrel acceleration process. Finally, the maximum velocity of test is 40 $m \cdot s^{-1}$, and that of calculation is 35 $m \cdot s^{-1}$, between which the error is about 10%. Considering the simplification of the catapult and the difference on the output energy about igniter, it could be considered the calculation results agree well with the experimental results.

6. Conclusion

Based on the Lee-Tarver reaction rate model, a model of propellant combustion was developed to predict the performance of pyrotechnic devices. The PDM consists of unreacted state equation, macro burning equation, micro reaction rate equation and reaction product equation. The PDM parameters of SL17 are fitted by the closed vessel test, and then the working process of catapult is calculated to predict its performance by PDM.

The results show that the velocity-time trace of calculation is in good agreement with that of test with about 10% overall error. The PDM model makes it possible not only to predict the velocity of the inner barrel, but also to understand the very complicated catapult physics involving the pressure in the expansion chamber and impact process during acceleration. Since the numerical model verified with ballistic test results allows for various design changes, the development cost and time can be greatly reduced by minimizing the number of experimental tests required. Because of this advantage, the current PDM model can be applied to design one-shot devices used in aerospace and military applications.

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