Experiments and numerical simulations of plate gap model for high energetic materials

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Abstract. Experimental and numerical study for detonation propagation was conducted using the system in which the high energy materials and air gaps alternately stacked. The aim of this simulation is an extraction of information of the EOS for detonation product at arbitrary initial density from the numerical simulation with EOS at TMD (theoretical maximum density). In this report, we described the numerical procedure and an example of the calculation result. On the other hand, the experiment was designed for confirmation of the validity of our reactive flow simulation. The experimental system for this study consists of the pellet explosives and PMMA rings, PMMA pipe and booster explosive part. The pellets and the rings were alternately stacked in the PMMA pipe to make the system. The diameter of the pellet was 20 mm and the thicknesses were 10 or 5 mm. The thickness of the ring was varied to adjust the size of the air gaps between the pellets. The sample explosive was a composition A5 (RDX 98.8 wt%). The relationship between the bulk density which was estimated by the thicknesses of the pellets and the air gaps and the average detonation velocity was compared with the data for RDX. The slopes of those relationships differed mutually. Although the experimental results can be used for confirmation of the validity of the numerical procedure, it does not simulate the detonation wave in the powdered explosive. It may show the interesting process that consists of the shock wave in air, shock to detonation transition and steady detonation.

1. Introduction

In previous study, to determine the EOS surface for detonation products, we have used experimental data for the initial densities and corresponding detonation velocities, and the C-J isentropic line for theoretical maximum density (TMD). The conservation law, the thermodynamic definition of the Gruneisen parameter, and the Jones-Stanyukovich-Manson relation [1] were combined to formulate differential equations whose solution is the Gruneisen parameter as a function of the specific volume [2,3]. The proposed unified form of the EOS could be applied to the numerical simulation of detonation propagation for an arbitrary initial density without changing any parameters [4,5]. In contrast, we are trying to extract the state quantities from the simple simulation to obtain the EOS parameters for arbitrary initial density. Because the relationship between the initial density and detonation velocity is determined by the simulation itself, only the EOS information of TMD is necessary to simulate the propagation process of the detonation wave for an arbitrary initial density. The conceptual diagram of our simple simulation is shown in figure 1. The calculation field is constructed by the mesh of the micro meter order. The high energetic material and air blocks are alternately arranged to make the main part of the model. The bulk density of this part can be adjusted by changing the size of the blocks. Detonation is reproduced by high velocity impact problem. According to the C-J hypothesis, if the reaction rate is very high, the velocity of the detonation propagation does not depend to the reaction rate, only the EOS for detonation products is important. Therefore, we considered that our proposed simulation can reproduce the expansion process of the detonation products for arbitrary initial density case. However, because the results may depend to the block size of the high energetic materials and air gap, we have considered that both for qualitatively understanding of such block size effect and for confirming the validity of the numerical simulations, the experimental study is also necessary. Since the experiment with block of the micron size was difficult, relatively large size experiments were conducted.

In 1960s, to investigate the characteristic of the porous solid under the shock loading, the propagation process of the shock wave on the system where the pellets and the air gaps were arranged alternately were measured [6]. The model was called as the plate-gap model [7]. Because the configuration of main part of our experiment is similar to such model, here, our model is called as the plate gap model for high energetic materials. In this paper, as the sample high energetic materials for the experiments, the Composition A5 was used, and for the numerical simulations, PETN was used.

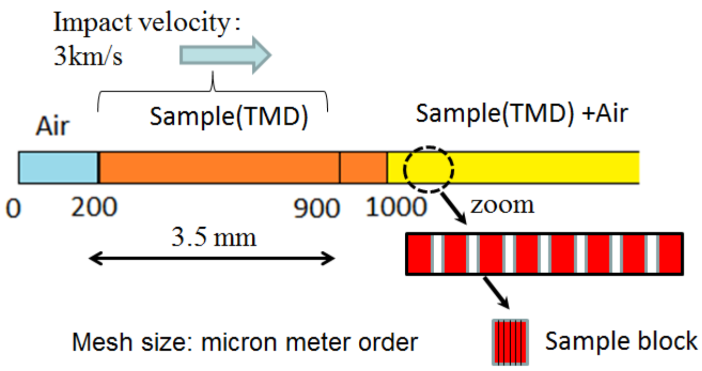


Figure 1. Conceptual diagram of pate-gap model for high energetic materials.

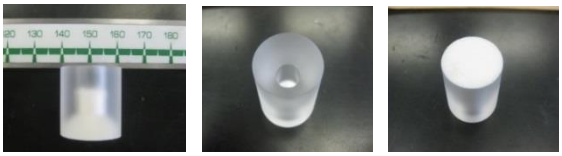
2. Experiment and numerical simulation

2.1. Experiment.

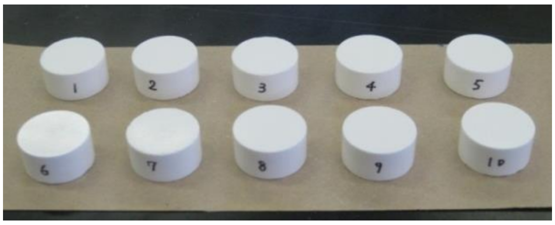
The basic elements for our experimental system are the pellet explosive, the PMMA spacer, and the two grams Composition C4 booster, and are shown in figure 2. The Composition C4 was filled in PMMA holder. The booster part, pellet explosive, and the spacer were put in the PMMA tube where a part of tube was cut. The experimental setup is shown in figure 3. Three pellets were arranged below the C4 booster to obtain the steady detonation in pellet explosives. Two PVDF gauges (Dynasen PVF2-11) are set to measure arrival time of the shock wave. One gauge was set directly between second and third pellet. To make the air gap under the third pellet, PMMA with the ring shape was alternately stacked between the pellets. The second gauge was put between the last pellet and cylindrical PMMA block. Using the arrival times and a distance between two gauges, the average detonation velocity was estimated. The relationship between the size of the air gaps and detonation velocity was investigated. The diameter of the pellet is 20 mm, and the thicknesses were 10 and 5 mm. The pellet made by composition A5 (RDX98.8 wt%) was used. The initial density of the sample pellet was 1.64 g/cc. The thickness of the spacer was varied from 0.5 to 4 mm.

2.2. Numerical simulation.

The governing equations are the conservation of mass, momentum, and energy. The advection equations of the volume fraction for each material are also employed to solve multi-materials flow with Eulerian coordinate system.



(a) Booster; composition C4(2g)



(b) Pellet; Composition-A5 (φ20×10mm)

(c) Spacer; PMMA ring 0.5～4 mm

Figure 2. Basic elements for our experimental set-up.

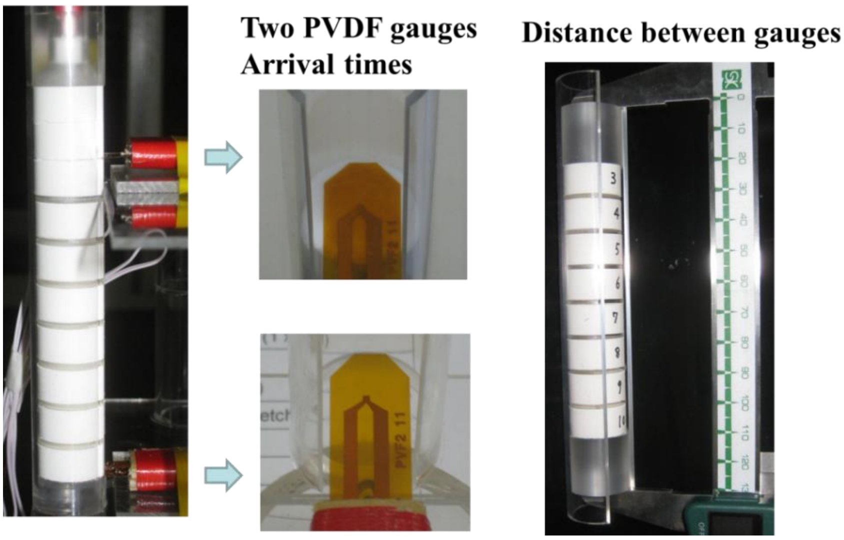


Figure 3. Experimental setup for plate gap model for high energetic materials.

The pressure at the multilaterals cell was calculated using following equation [8].

$$= \sum P^{\alpha} f^{\alpha} / K^{\alpha} \times \left(\sum f^{\alpha} / K^{\alpha} \right)^{-1}. \tag{1}$$

where superscript α denotes the component of the αth material, *f* is the volume fraction of the component. K^{α} is the bulk modulus of the αth component, *K* is the equivalent bulk modulus of all the components. Where the bulk modulus of each component is

$$K^{\alpha} = -v^{\alpha} \left(\frac{\partial P^{\alpha}}{\partial v^{\alpha}} \right)_S = \rho^{\alpha} \left(c^{\alpha} \right)^2. \tag{2}$$

Here, subscript s denotes the entropy, *v* is the specific volume, and *c* is the sound velocity.
The ignition and growth model was applied as burn model [9]. The pressure at the partially reacted state for high energetic material regarded as the simple mixture phase of the completely reacted state and non-reacted state. Linear relationship of the specific volume and that of the specific internal energy were used to calculation of the pressure on the partially reacted state [10]. The one dimensional numerical simulation as shown in figure 1 was conducted.

3. Experimental Results

The average detonation velocities obtained by the plate gap model for high energetic materials are plotted in figure 4. A horizontal corresponds to the bulk density of the system. The bulk density is defined by the multiplication of the pellet density and the ratio between two thicknesses. The ratio is total thickness of the pellets and sum of the total thickness of the pellets and gaps. Regardless of the difference of the thickness of the pellets, the linear relationship between measured detonation velocity and the value of the horizontal axis was confirmed. There is well known linear relationship between bulk density and the detonation velocity for the high explosive [11], so, in qualitatively experimental results are plausible. Because the sample consists of the RDX of the 98.8 wt%, the characteristics of the detonation phenomena both of this sample and RDX may be similar. The linear relationship for the RDX is plotted in figure 4 for comparison. Remarkable difference of the slope of the linear relationship can be confirmed. This experimental does not simulate the detonation wave in the powdered explosive. However, it can be used as the data to estimate the validity of the simulation method, and may show the interesting process that consists of the shock wave in air, shock to detonation transition and steady detonation.

4. Simulation result.

The mesh size was set 5 micro-meters. A PETN block consists of 10 meshes, and an air block is 4 meshes, so the bulk density is 1.264 g/cc. The detonation was generated by the impact of the 3.5 mm PETN with 3 km/s. The propagation process of the detonation wave obtained by numerical simulation is shown in figure 5 with pressure distributions. Although it is overdriven at an initial stage, it gradually approaches the steady state of the case of 1.264 g/cc PETN.

5. Summary

The plate gap model for high energetic materials has been proposed. This model constructs EOS for detonation products at an arbitrary initial density using the numerical simulation with EOS information at TMD case. Experiments for this model were also conducted. Since the experiment with block of the micron size was difficult, relatively large size pellets were employed. The bulk density was defined by the pellet density, thickness and thickness of the air gap. The linear relationship between bulk density and average velocity was confirmed. However, the slope of the linear relationship obtained by this experiment differs from that of the linear relationship between initial density and detonation velocity.

Although this experiment does not simulate the detonation wave in the powdered explosive, it may show the interesting process that consists of the shock wave in air, shock to detonation transition and steady detonation. On the other hand, the result of the numerical simulation with micron order mesh approaches general relationship between initial density and detonation velocity.

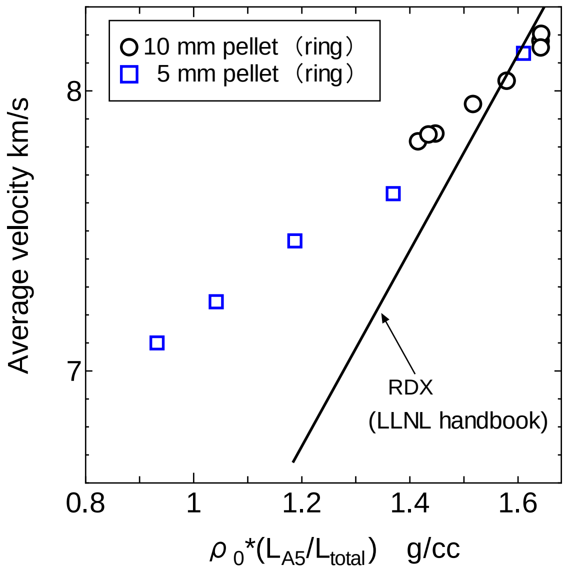


Figure 4. The relationship between the average velocity and the bulk density of the experimental system of the plate gap model for high energetic.

The solid line for RDX from LLNL Handbook (Reference 11)

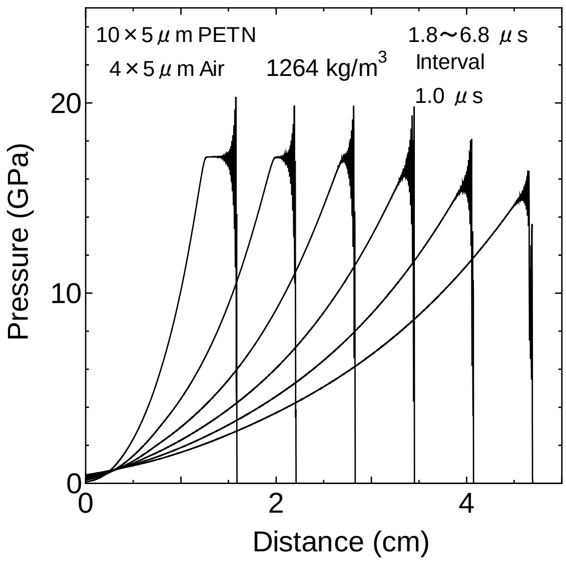


Figure 5. The pressure distributions obtained by numerical simulation of the plate gap model for high energetic.

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