Study on aluminum particle/oxygen and air two-phase detonation

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1 Introduction

Aluminum is an important chemical material which is used in many places and occasions. The recent use of aluminum material, for example, a thrust additivity for solid rocket engine, which is a positive use. Because of such possibility of aluminum as an energetic material, there may be an accident during a use of aluminum. Many researchers have being working on such accidental problem of Aluminum, which has a high exothermic energy. We know many numerical analyses and less experimental ones.

Table 1 Review of alminum/O2 or air two-phase detonation studies

Year	Authors	E:Exp. N:Num.	Temperature (K)	Pressure (MPa)	Particle size (μm)	Detonation Velocity (m/s)	Cell size (cm)	remarks
1968	Strauss [2]	E	T0=298	Pg0 = 0.1 Pmax = 3.2	5	1680	-	Dtube=2.64 (cm) DDT distance>60 cm
2002	Veyssiere Ingignoli [3]	E	T0=298	Pg0=0.1 Pmax=12.5	3.5, 13.0	1880 (Dp=30) 1886 (Dp=100)	0.8-2.65	Tube length= 4.15 m
2003	Carrel Thomas Brown [4]	E	T0=298	Pg0 = 0.1	15	1877-2000	-	Ignite by 2H2+O2+3Ar
2003	Benkieiwcz Hayashi [5]	N	T0=300 Tignit = 1350	P0 = 0.1 Pgmax = 0.5	1, 2.5	DCJ=1735 ug=1500 up=1280	λ=1.1(Dp=1μ) λ=1.4(Dp=2.5)	Euler-Euler
2005	Fedorov Khmel [6]	N	T0=300	P0 = 0.1 Pgmax = 5.2	1-12	u=1560	D0=10μm→λ=27	2-Equs. System Al/O2
2006	Benkiewicz Hayashi [7]	N	T0=300 Tgmax=3500 Tpmax=3000	P0 = 0.1 Pgmax=5.2 PCJ=2.29	2.5-7.5	DCJ=1657	λ≈6cm	Euler-Euler Al/O2
2006	Zhang, Murray, Gerrard [8]	E	T0=300	0.1→Pmax=4.5 (no det.) 0.15→Pmax=3.76 (det)	0.1, 2.0	Du=1599 →detonat.	-	Tube length=9.6m, Dtube=8cm
2008	Fedorov Khmel [9]	N	T0=300	P0 = 0.1	1, 2	Du=1560	λ1μm=0.7 λ2μm=4.4	Al/O2
2012	Hosoda Hayashi Yamada [10]	N	T0=300	P0 = 0.1	0.1~80	Du=1400-1890	λ=0.2~200mm	Comparing with other λs.
2009	Zhang, Gerrard, Rypley [11]	E	T0=298	P0 = 0.1	0.1, 1.6-3.3	Du=1600-1700	-	Al/Air Dtube=8cm
2020	Zhang, Wen, Liu, Zhang, Jiang [12]	N	T0=300	P0 = 2.5	0.1,2.0	Dumax= 1611-1699 (Dp=2.0μm)	λ=10.5(Dp=2μm)	E-L method
2020	Khmel, Lavruk [13]	N	T0=300	P0 = 16.5	1, 0.05	-	-	Dtube =5cm

In the present study, aluminum particle/O_2 and air detonation are investigated numerically and are compared with experiments. First of all, some of experimental and numerical works are reviewed to see what are known from such passed studies. Then, this study will show the numerical work on aluminum/O_2 and air two-phase detonation. We have been working on two-phase detonation numerically for more than 20 years and from the starting, we used the Euler-Euler two-phase system because the Euler-Euler method should work on the large system. Some researcher use the Eulerian-Lagrangian method. Both have an advantage and disadvantage.

Table 1 shows some review of aluminum/O_2 and air studies. This table work is based on the review work by Fedorov and Khmel [1] in 2019. I added some and skipped some from their picked-up works. As they picked an older study of Strauss (1968), I did also picked it as one of the old experimental works. He had an excellent experimental work at such old year by his deep thinking. Then, Table 1 consists of both experimental and numerical works for the data of detonation temperature, pressure, aluminum particle size, velocity, cell size, and some remarks.

2 Numerical Method

2.1 Governing equations and their integration

The present two-phase numerical system of governing equations consists of the two-dimensional method compressible Euler equations for both gas and solid particle physics, which is called the continuous model, while thier diffusion, heat conduction, and viscous terms are neglected. The gas-phase convection terms are integrated by the Harten-Yee type TVD scheme, while the solid-phase convection terms are integrated by the MUSCL Hancock TVD scheme. The source terms are calculated by the time-splitting method and the time integration is performed by the 2nd-order Strang-type fractional step method. For the grid system, AMR (adaptive mesh refinement) system and moving grid system are applied for the calculation to keep a best grid resolution. The data in Table 1 include the aluminum size from nano to micro meters to understand what detonation features are from the data.

2.2 Aluminum particle combustion

Aluminum particles and oxygen are uniformly mixed and the aluminum sublimate quickly to be gasified, then gaseous aluminum is reacted with oxygen. The chemical reaction between gasified aluminum and oxygen is modeled by two step reaction mechanism.

when gaseous temperature becomes between 1350 K and 3500 K, aluminum reacts with oxygen as follows:

$$Al + \frac{3}{4}O_2 \Rightarrow \frac{1}{2}Al_2O_3$$

.

But when gaseous temperature becomes higher than 3500 K, aluminum becomes AlO instead of Al2O3 as follows:

$$Al + \frac{1}{2}O_2 \Rightarrow AlO \qquad Al_2O_3 \Rightarrow 2AlO + \frac{1}{2}O_2$$

The details of the aluminum combustion will be discuss at the presentation.

2.3 Numerical conditions

The initial condition for pressure and temperature is 0.1 MPa and 300 K, respectively. Seven particle diameters of 0.1 μm, 0.25 μm, 0.5 μm, 0.75 μm, 2.5 μm, 5.0 μm and 10.0 μm are used for the initial Aluminum size.

The boundary conditions are such that the upper and bottom wall are adiabatic and left and right boundary are free boundary.

Two cases of two-dimensional sizes are applied for the present calculation: (1) 3.75 m (length) x .25 m (width) and (2) 1.875 m (length) x 0.125 m (width). After some grid study, it is found that the coarse grids do not give a good answer for detonation. Since an AMR (Adaptive Mesh Refinement) method is applied for the present calculation, the starter grid size of (1) is 2.6 mm and that of (2) is 1.3 mm. The step grid, which is the minimum size of the step grid is .650 mm for (1) and .325 mm for (2).

A moving computational grid system is applied in the present analysis. The moving speed is 800 m/s, which is picked up empirically.

3 Results and Discussion

We can discuss about (1) effect of aluminum particle diameter on detonation velocity, (2) effect of aluminum particle concentration on detonation velocity, and (3) detonation cell size to aluminum particle diameter, and so on. But due to page size, detonation cell size problem will be briefly discuss here.

3.1 Detonation cell size vs. Aluminum particle diameter

Detonation cell size is one of the measures to forsee dangerous situation. For example, the larger cell size detonation may not siriously occur in the smaller tube because the triple shock waves cannot hit each other or walls before it will get the stronger energy energy, then flame will be dying off. But, if tube diameter is large enough and tube length is long enough comparing with detonation cell size and flame can keep to get more than DDT distance, then it is going to be detonation.

Figure 1 shows the relation between aluminum particle diameter and detonation cell size. When looking at Fig. 1, we can recognize two straight lines which cross at the aluminum diameter of near 0.5 μm. Before talking about the reason of this branch haooning, let me talk a bit about those two lines. They comes from the following relation:

$$\lambda = \lambda_0 \left(\frac{d}{d_0}\right)^{\theta}$$

where λ is the cell size; λ_0 is the transverse size of detonation cell [6], d is the alminum particle diameter; d_0 is the initial aluminum particle diameter, and θ is the fractorial. This style of equation is seen for the d^2-law of flame. Fedorov and Khmel discuss this provlem using a similality from the d^2-law. As can be seen from Fig.1, the fractorial θ is dependent on the

detonation cell size. In the present study, at the smaller cell size than about 6 μm, θ is 1.6 for the aluminum-O2 detonation.

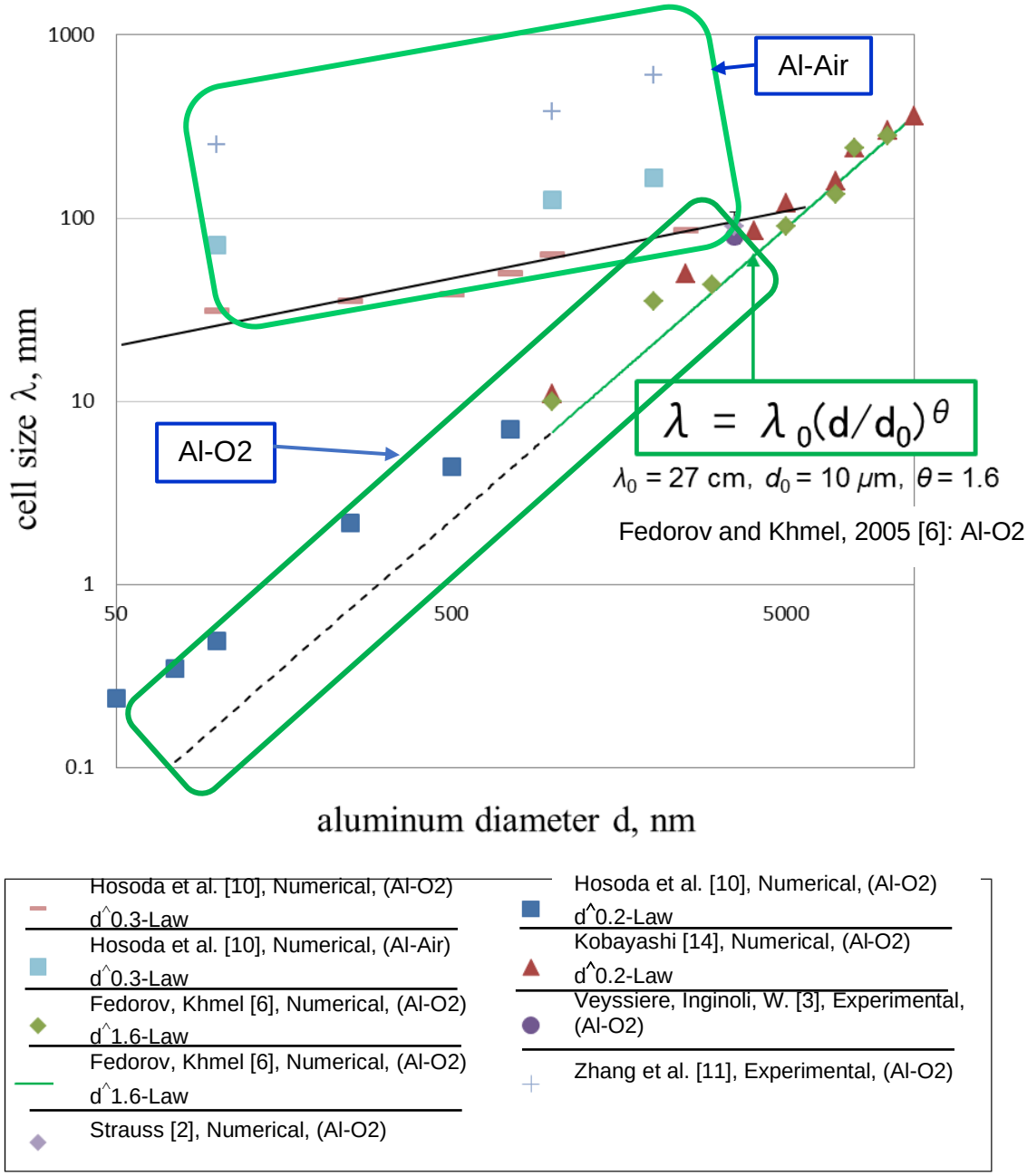

Fig. 1 Cell size vs. aluminum particle diameter. Several other study cases are compared to see the validity of the present numerical system and the aluminum particle size effect on detonation cell size for rather smaller aluminum size.

4. Conclusions

The review and numerical analyses of aluminum partcle/O_2 and air are performed using two-phase detonation. So far, the followings are figured out presently:

(1) From the review of the passed studies, there must need a futher work on the aluminum/O_2 and air detonation. This should be said to all other heterogeneous detonations' problem. For example, it is the fractorial θ. The fractorial θ must be strongly related with the energy the material has.

(2) When we compare with the oxizer, our results of aluminum/air has a close results of Zhang [12]. Then, does air provides the different slope from that of O_2?

(3) In any way, detonation cell size becomes smaller as aluminum particle becomes smaller. First of all, this is because the energy pervolume becomes larger, then aluminum detonation becomes stronger.

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