

Detonation in Gas-Fuel Droplet Systems

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Abstract

The detonation in decane+O₂ two phase system is numerically modeled by using two-phase fluid model. The development process of detonation in such two-phase system after ignition by different energy is modeled and the parameters of the detonation are obtained. The effect of saturation vapor pressure of the fuel in different temperature is also modeled. The results show that the fuel vapor pressure in two-phase system influences the parameters of detonation wave distinctly.

Introduction

The gas-fuel droplet system formed accidentally may detonate by ignition. Great damage would occur. So it is very important to study such two-phase detonation. With the development of computational fluid mechanics, two-phase fluid model was used to study the detonation of fuel-spray system. Numerical modeling became an important means to solve such problem. Mitrofanov and Eidelman [1,2] used multiphase model to investigate the detonation in gas-fuel spray system. The gas-fuel droplet interaction was considered in these models. The interphase mass and momentum transfer was considered behind the leading shock wave. The droplet was stripped and evaporated by the gas flow. The energy release model was simplified.

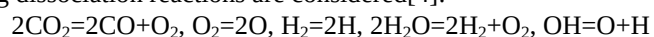
In this paper, the concentration of the fuel vapor and product is considered and the energy release is described by one-step chemical reaction rate of the fuel with oxygen and some dissociation reactions are also considered. The interphase exchange including phase change and convective transfer is considered.

Analysis Model

The ignition and growth of the detonation in gas-fuel droplet systems is a complex process. It contains phase transition, mixture, chemical reaction. When shock wave enters the gas-fuel droplet system, the fuel droplets accelerate, deform, atomize and evaporate behind the leading shock wave. Interphase mass, momentum transfer occur as a result of the thermal and mechanical influence of a gas flow behind the leading shock wave on the droplets. The shedding and evaporation of the droplets and diffusion of vapors into the oxident develop a combustible mixture behind the leading shock wave. The energy is released in mixture. If the energy released from the reaction zone can transfer the energy to the leading shock wave and compensate the energy depleting of the leading shock wave motion, the self-sustained detonation is developed. It is usually concerned with the structure and parameters of the detonation. In this paper, two-phase model is used to solve these problems by numerical modeling.

The medium is composed of oxygen or air as gas and liquid fuel droplet as fluid. Two phases have their own state variables such as density, velocity, internal energy. Each phase obeys conservation laws, but there is interphase exchange terms of mass, momentum, energy in balance equation. The assumption about the medium properties are following: the temperature and pressure of all the gases in mixture are the same; the droplets dispersed in gas behave as a continuous medium. They are spherical in size and keep same shape in the processing of shattering and evaporation; The volume occupied by the droplets is negligible and the collision between the droplets can be neglected. The shattering and atomization of the droplets immediately evaporate into vapors. The chemical reaction only occur in gases. The energy released from chemical reaction is absorbed by gaseous phase.

In this paper the fuel is n-decane. The chemical heat release is described by Westbrook's one-step reaction rate[3]. Also the following dissociation reactions are considered[4]:



the equilibrium concentration of the chemical species is solved. The equation of state of gaseous phase is the ideal gas.

The second order accurate MacCormack finite difference equation is used along with FCT-techniques[5-7] for above equations. A program is designed to solve the development of detonation in two-phase systems. The point explosion of initiation energy of 10MJ is numerical modeled to examine the program and compared with the analytical solution. In the range of 1m,the maximum error of the pressure of shock wave is 1.3 percent. The error of motion of shock wave is less than 0.6 percent.

Results and Discussion

Two-phase detonation with different ignition energy

The ignition condition is high temperature and high velocity gas with different energy which is released in the center of the gas-fuel spray system. The cylindrical radius of the system is 2m.The gas phase is pure oxygen while the liquid fuel is n-decane. The density of decane is 730kg/m^3 .The diameter of droplets is 400μ .Initial gas pressure is $P_0=0.1013\text{Mpa}$,density of oxygen is 1.31kg/m^3 .Initial temperature is 298K and equivalence ratio is 0.32.

Ignition energy is 1.1,1.7,4.4,7.2MJ/m separately. Figure 1 represents the pressure of the gas phase vs coordinate r as the ignition energy is 4.4MJ/m.The time is from $100\mu\text{s}$ to $1100\mu\text{s}$ and the interval of every curve is $100\mu\text{s}$. The curves from top to bottom in figure2 and figure 3 represent the velocity of detonation and pressure in the condition of different initial ignition energy from large to small. The ignition energy influences the velocity and pressure of detonation wave. As the ignition energy is 7.2MJ,the detonation velocity decreases in the computing limit. As the ignition energy is 1.1 and 1.7MJ/m,the ignition is lower that its influence is not so strong. Figure 2 shows that the velocity of detonation decreases first then increases. It shows that detonation velocity do not tend stable even as it moves near 2m.This result is accorded with the method of detonation of shock dynamics(DSD). In DSD the detonation velocity is related to the detonation curvature. The detonation velocity is slower as the curvature is higher. The wider of the detonation wave is, the more of the detonation velocity is influenced by its curvature. From the result by numerical modeling here the width of detonation wave in gas-fuel droplet system is more than ten centimeters. As the radius of detonation wave is larger, its curvature is smaller, then its velocity is faster. The CJ surface of detonation wave can be determined, which is defined as the surface with $u_1+c_1=D$, c_1 is the equilibrium sound speed. The width of detonation wave is defined as the distance between leading shock wave and CJ surface, the detonation wave width is about 20cm.Most part of the fuel droplet is shattered and evaporated ahead of CJ surface. Although the remaining droplet is still stripped and evaporated then release energy, but the energy released behind the CJ surface can not be transferred to the leading shock wave. The evaporation efficiency of droplets is defined as the ratio of evaporated volume droplet from shock front to CJ surface to initial volume of droplet. Table 1 shows that the gas phase parameters both of leading shock wave and CJ surface of two-phase detonation in 1.4m.R is droplet radius and its unit is $\bullet\text{m}$. D is the average detonation velocity which from 1m to 1.4m/s. P, $\bullet$,u,T are pressure,density,velocityand temperature .L denotes width of the detonation and $\bullet$ is the evaporation efficiency of droplet.

Table 1.parameters of the two-phase detonation

E_0 MJ/m	D m/s	P_{sh} Mpa	ρ_{sh} kg/m ³	u_{sh} m/s	T_{sh} K	P_{cj} Mpa	ρ_{cj} kg/m ³	u_{cj} m/s	T_{cj} K	$\bullet$	L cm
1.1	1429	2.42	5.93	1138	1472	1.27	1.55	422	2993	0.822	16.8
1.7	1465	2.48	5.95	1164	1516	1.36	1.56	438	3116	0.867	18.8
4.4	1577	2.90	6.36	1259	1648	1.50	1.61	517	3276	0.913	20.5
7.2	1676	2.99	6.41	1313	1734	1.66	1.61	569	3457	0.982	24.2

The results shows that all of the parameters increase with the increasing of the igniting energy.

Two-phase detonation with different fuel vapor pressure

The diameter of fuel droplets is also 400μ .Initial gas pressure is $P_0=0.1013\text{Mpa}$.Initial temperature is from 20°C to 58°C . The system is fuel droplets and its vapor with oxygen. The vapor pressure in the decane mixture is the fuel saturation vapor pressure. Equivalence ratio is 0.39.The ignition energy is $6.5\times 10^{-3}\text{MJ/m}$ at 50°C , 58°C and 0.166MJ/m at 20°C , 40°C .

The higher the initial temperature is, the higher the fuel vapor pressure is. Because the atomization and evaporation of fuel droplet by the gas flow behind the leading shock wave is much slower than the chemical reaction of fuel vapor with oxygen, the energy released by fuel vapor is more rapid by fuel droplet. The

parameters of leading shock wave is dependent on the concentration of fuel vapor. The fuel vapor behind the leading shock wave react with oxygen. The product forms and chemical energy is released. The temperature of the leading shock is higher as the vapor pressure is higher due to the more energy released by fuel vapor behind the leading shock wave. The energy raise the gas temperature. The rising of temperature lower the gas density. With the increasing of vapor pressure the density and pressure of leading shock wave decrease. The higher of the fuel vapor is, the higher the temperature of leading shock wave is . The tendency of the density and pressure in CJ surface are not same as tendency in the leading shock wave. Although the gas temperature in leading shock is very different, that in CJ surface is almost same. Besides at 58°C the width of detonation wave is quite similar.

Table 2.parameters of the two-phase detonation with fuel vapor

T °C	D m/s	P _{sh} Mpa	ρ _{sh} kg/m ³	u _{sh} m/s	T _{sh} K	P _{cj} Mpa	ρ _{cj} kg/m ³	u _{cj} m/s	T _{cj} K	•	L cm
20	1529	2.67	5.59	1179	1723	1.57	1.65	470	3302	0.850	20.5
40	1640	2.52	3.93	1121	2294	1.56	1.61	521	3347	0.840	22.5
50	1680	2.37	3.15	1030	2630	1.65	1.70	591	3351	0.752	19.8
58	1801	2.34	2.64	963	3052	1.85	1.95	729	3327	0.488	11.8

Figure 4 represents the pressure of gas phase vs coordinate r at 40°C. Figure 5 represents the pressure of leading shock front vs radius of shock wave in the condition of different initial temperature. The pressure of two curves rise from low two high is 50°C,58°C. At 58°C pressure tends stable in the range of computation. At 50°C the pressure of detonation exceeds that at 58°C near 2m.The pressure of two curves decrease first then increases is 20°C,40°C. At 20°C the pressure of detonation exceeds that at 40°C.

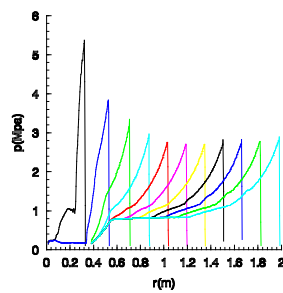


Figure 1 the pressure of gas phase vs coordinate r

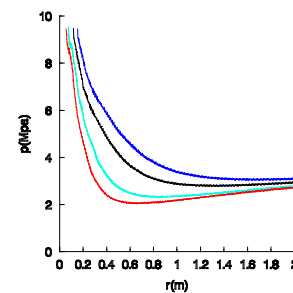


Figure 3 pressure of detonation vs its radius

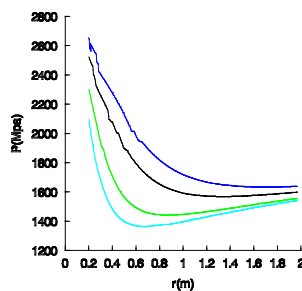


Figure 2 velocity of detonation vs its radius

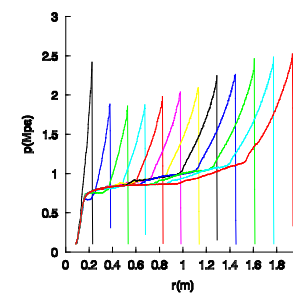


Figure 4 the pressure of gas phase vs coordinate r at 40°C

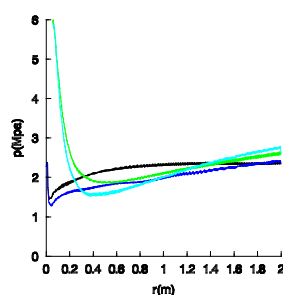


Figure 5 pressure of detonation vs its radius

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