Numerical Modeling of Detonation Limit of Fuel Concentration in Gas-Fuel Droplet Systems

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1 Introduction

The gas-fuel droplet system formed accidentally may detonate by ignition and 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 such as Mitrofanov [1],Eidelman and Burcat[2,3]. The interphase mass and momentum transfer was considered behind the leading shock wave. The droplet was stripped and evaporated by the gas flow but the energy released in the model was simplified.

In this paper, the concentration of the species of gas phase is considered. The energy release is described with a three-step chemical reaction rate and some dissociation reactions are considered. The development of detonation in gas-fuel droplet system is numerical simulated and the detonation limit of fuel concentration in decane spray systems is obtained.

2 Analysis Model

The ignition and growth of the detonation in gas-fuel systems is a complex process. It contains phase transition, mixture, chemical reaction. When shock wave enters the gas-fuel 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 a 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. In this paper, two-phase model is used to simulate the ignition and growth of detonation in gas-fuel droplet systems.

The medium is composed of oxygen or air as gas and decane 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 conservation equation. The assumption about the medium properties are following: the temperature and pressure of all the species of gas in mixture are 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. The collision between the droplets is neglected; The shattering and atomization of the droplets immediately evaporate into vapors; The chemical reaction only occur in gases and the energy released from chemical reaction is absorbed by gaseous phase.

The two-phase model is described by the following equation.

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Mass conservation

$$\frac{\partial}{\partial t}(\alpha_1\rho_1)+\frac{1}{r^\alpha}\frac{\partial}{\partial r}\left(r^\alpha\alpha_1\rho_1u_1\right)=I_d \tag{1}$$

$$\frac{\partial}{\partial t}(\alpha_2\rho_2)+\frac{1}{r^\alpha}\frac{\partial}{\partial r}\left(r^\alpha\alpha_2\rho_2u_2\right)=I_d \tag{2}$$

Momentum conservation

$$\frac{\partial}{\partial t}(\alpha_1\rho_1u_1)+\frac{1}{r^\alpha}\frac{\partial}{\partial r}\left(r^\alpha\alpha_1\rho_1u_1^2\right)=-\alpha_1\frac{\partial p}{\partial r}-F_d+I_du_2 \tag{3}$$

$$\frac{\partial}{\partial t}(\alpha_2\rho_2u_2)+\frac{1}{r^\alpha}\frac{\partial}{\partial r}\left(r^\alpha\alpha_2\rho_2u_2^2\right)=-\alpha_2\frac{\partial p}{\partial r}+F_d-I_du_2 \tag{4}$$

Energy conservation

$$\frac{\partial}{\partial t}\left[\alpha_1\rho_1\left(e_1+0.5u_1^2\right)\right]+\frac{1}{r^\alpha}\frac{\partial}{\partial r}\left[\alpha_1\rho_1u_1\left(e_1+0.5u_1^2+\frac{p}{\rho_1}\right)\right]=-Q_d+Q_c-F_du_2+I_d\left(e_2+\frac{p}{\rho_2}+0.5u_2^2\right)-LI_d \tag{5}$$

$$\frac{\partial}{\partial t}\left[\alpha_2\rho_2\left(e_2+0.5u_2^2\right)\right]+\frac{1}{r^\alpha}\frac{\partial}{\partial r}\left[\alpha_2\rho_2u_2\left(e_2+0.5u_2^2+\frac{p}{\rho_2}\right)\right]=Q_d+F_du_2-I_d\left(e_2+\frac{p}{\rho_2}+0.5u_2^2\right) \tag{6}$$

α =0,1,2 denotes slab, cylindrical, spherical coordinate. Subscripts 1,2 denote gas and liquid. ρ ,u, p, e are density, velocity, pressure and specific internal energy respectively. α_1 and α_2 volume fraction of gas and fuel droplets and have relation $\alpha_1+\alpha_2=1$.I_d is the mass increase per unit volume in gaseous phase due to the evaporation and shattering from the fuel droplets.F_d is the interphase force acting on the particles by the gas flow.Q_d is the energy exchange by convective heat transfer.Q_c is the chemical heat release term. L is the heat of evaporation of fuel.

The gaseous phase is a mixture of chemical gases. The concentration of each component phase is Y_j (1,2,⋯,N), where j=1 corresponds to fuel vapor, j=2 oxident, j=3 nitrogen, j=4 carbon dioxide, j=5 water vapor, j=6 carbon monoxide, j=7 hydrogen. The mass equation for species j is

$$\frac{\partial\left(\rho_1\alpha_1Y_j\right)}{\partial t}+\frac{1}{r^\alpha}\frac{\partial}{\partial r}\left(r^\alpha\rho_1\alpha_1Y_ju_1\right)=\dot{\rho}_j^{\,c}+I_d\delta_{j1} \tag{7}$$

The equation of state of gaseous phase is

$$p=\rho_1RT_1\sum_{j=1}^{N}\frac{Y_j}{W_j} \tag{8}$$

W_j is the molecular weight. The rate of droplet's shattering[4] is

$$I_d=-n\rho_2 4\pi R^2\frac{dR}{dt} \tag{9}$$

$$\frac{dR}{dt}=-\frac{1}{2}\sqrt{3\pi}\left(\frac{\rho_1\mu_1}{\rho_2\mu_2}\right)^{\frac{1}{6}}\left(\frac{\mu_2}{\rho_2}\right)^{\frac{1}{2}}\left(u_1-u_2\right)^{\frac{1}{2}}R^{-\frac{1}{2}} \tag{10}$$

R is the radius of liquid droplet. μ is the dynamic viscosity. n is the fuel particle number in unit volume. Nu is the Nusselt number of the gas.

$$Nu=2+0.6\,\mathrm{Re}^{\frac{1}{2}}\,\mathrm{Pr}^{\frac{1}{3}} \tag{11}$$

Re is Renolds number. Drag force on the particles by gas flow

$$F_d=nf_d \tag{12}$$

$$f_d=\frac{3\rho_1C_D}{8\rho_2R}\left|u_1-u_2\right|\left(u_1-u_2\right) \tag{13}$$

$$C_D = \begin{cases} 27\,\mathrm{Re}^{-0.84}, \mathrm{Re} < 80 \\ 0.27\,\mathrm{Re}^{0.21}, 80 \le \mathrm{Re} < 10^4 \\ 2, \mathrm{Re} \ge 10^4 \end{cases} \quad (14)$$

The convective heat transfer from gaseous phase

$$Q_d = 4\pi R^2 n q_d \quad (15)$$

$$q_d = \lambda_1 Nu_d (T_1 - T_2)/(2R) \quad (16)$$

λ_1 is the heat transfer coefficient of gas. Chemical reaction rate is the following:

$$\dot{\rho}_j^c = W_j \sum_r (b_{jr} - a_{jr})\omega_r \quad (17)$$

and the chemical heat release term in the energy equation is

$$Q_c = \sum_r Q_r \omega_r \quad (18)$$

$$Q_r = \sum_j (a_{jr} - b_{jr})(\Delta h_f^0)_j \quad (19)$$

The chemical reaction occuring in the system are symbolized by $\sum_j a_{jr} x_j \leftrightarrow \sum_j b_{jr} x_j$ .The stoichiometric coefficients must satisfy $\sum_j (a_{jr} - b_{jr}) W_j = 0$. $(\Delta h_f^0)_j$ is the heat of formation of species j at absolute zero.

In this paper the fuel is decane. The model of chemical reaction mechanisms is a three-step described by the following[5,6]:

$C_{10}H_{22}+10.5O_2=10CO+11H_2O$ (r1) $2CO+O_2 \leftrightarrow 2CO_2$ (r2) $2H_2+O_2 \leftrightarrow 2H_2O$ (r3)

The second order accurate MacCormack finite difference equation is used along with FCT-techniques[7-8] for above equations.

3 Calculation results

Detonation in oxygen-decane droplet systems ignited by different ignition energy is numerically simulated and compared with experimental results. In experiment, two-phase mixtures are ignited by high explosive in the center of cylindrical equipment. In calcultion the ignition condition is high temperature and high velocity gas with different energy. The gas phase is pure oxygen while the liquid fuel is decane. The density of decane is 730kg/m^3.The diameter of droplets is 400μ. Initial gas pressure is p_0=0.1013MPa. Initial temperature is 20°C and equivalance ratio Φ is 0.32.

Ignition energy is 1.1, 1.7, 4.4, 7.2MJ/m separately.Table 1 lists average detonation velocity between 0.89-1.07m by calculation and experiment[9].

Table 1.parameters of the two-phase detonation velocity

E_0 (MJ/m)	D_{cal}(m/s)	D_{exp} (m/s)
1.1	1399	1430
1.7	1455	1493
4.4	1523	1541
7.2	1589	1582

The parameters in the table 3 shows the influence of ingnition energy. It shows that the detonation velocity increases with the increasing of the igniting energy between 0.89-1.07m. It means that detonation does not tends stable in that places. The result is agreement with experimental ones quite well.

Then the detonation concentration limit in air-fuel systems is determined by calculation. The diameter of fuel droplets is 100μ.Initial gas pressure is p_0=0.1013MPa.Initial temperature is 20°C. Detonation wave is spherical symmetric. Ignition energy is 1MJ. The detonation in air-decane droplet systems is numerical simulated with

different concentration of fuel droplets. Table 2 lists the parameters of different equvalence ratio of fuel droplet below 1.

Table 2 detonation parameters in two-phase systems

ϕ	D m/s	P_{sh} Mpa	P_{cj} Mpa	ρ_{cj} kg/m^3	u_{cj} m/s	T_{cj} K	Y_{CO}/Y_{CO2}	Y_{H2}/Y_{H2O}	γ
1.0	1692	2.77	1.68	2.01	679	2826	0.035/0.145	0.29e-4/0.89e-1	1.224
0.9	1656	2.64	1.59	1.95	645	2769	0.022/0.150	0.24e-4/0.85e-1	1.232
0.8	1616	2.53	1.48	1.95	643	2616	0.82e-2/0.148	0.11e-4/0.73e-1	1.235

Fig. 1 is the pressure of leading shock wave of detonation as Φ=0.79,0.8. As Φ=0.8, pressure of leading shock wave tends to stable after it arrives at r=1.3m. The detonation is developed in this two-phase system. As Φ=0.79, pressure of leading shock wave attenuates rapidly at r=1m which means detonation fails. It can be concluded that the lower limit of detonability of fuel concentration is Φ=0.8.Fig. 2 is pressure of the flow field from 100-1100μs at inteval of 100μs as Φ=0.8. Fig. 3a is the distribution of concentration of gas components at t=1000μs. Fig. 3b is the temperature distribution.

Table 3 is the parameters of spherical detonation wave in two-phase systems with fuel concentration ϕ>1. Figure 4 is the pressure of leading shock waves as ϕ＝2.0,3.0,3.1.As ϕ＝3.0, pressure of leading shock of detonation decreases first and then tends stable which means detonation waves developed. But as ϕ＝3.1, pressure of leading shock waves attenuates at 1m and it fails. It is concluded that the detonation upper limit of fuel concentration is ϕ=3.0.

Table 3 detonation parameters in two-phase systems with ϕ>1

ϕ	D/m/s	p_{sh}/MPa	p_{cj}/MPa	ρ_{cj}/kg/m^3	u_{cj}/m/s	T_{cj}/K
1.0	1732	3.00	1.73	2.05	720	2891
2.0	1745	3.11	1.87	2.22	720	2770
3.0	1693	2.84	1.73	2.17	704	2574

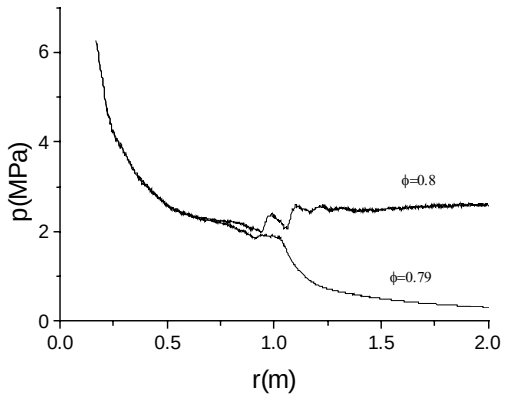


Fig.1 The pressure of leading shock wave vs shock position as ϕ =0.8,0.79

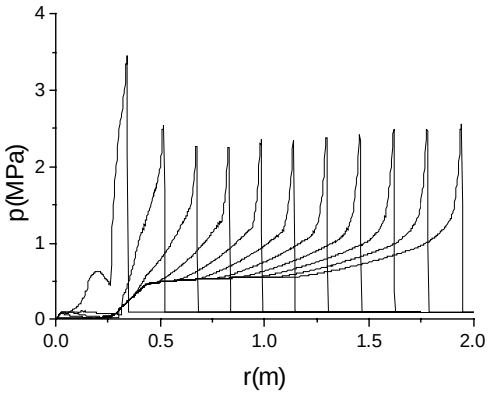
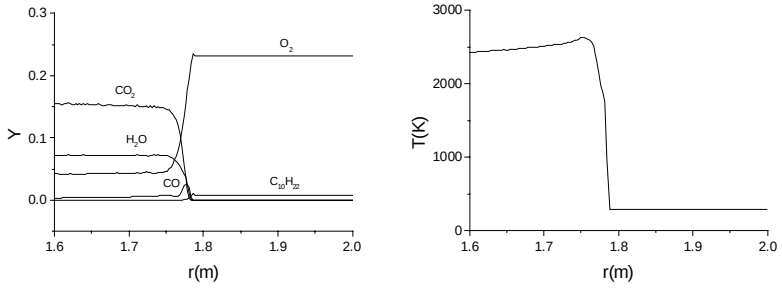


Fig. 2 pressure in flow field at different time as ϕ =0.8



3a 3b

Fig3a mass concentration of components at t=1000μs.3b Distribution of temperature

4 Conclusion

A model of two phase reacting flows is developed and detonation in gas-fuel droplet system is numerical modeled. The ignition and development of detonation and the parameters of detonation in gas-decane droplet sysytem is obtained. The result of detonation velocity is well agreement with the result of experiments. With this model, detonation limit of fuel concentration of two-phase systems is determined. If ignition energy is 1MJ and the diameter of fuel droplets is 100μ while initial gas pressure is p_0=0.1013MPa and initial temperature is 20°C. The lower limit of detonability of fuel concentration of the two-phase system is Φ=0.8 and upper limit of detonation is Φ=3.0.

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