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激波点燃粉尘的数值模拟研究

许厚谦
(南京理工大学 南京 210014)
于 强 H Grönig
(德国亚琛理工学院)

摘要 建立了用于模拟入射激波后可燃粉尘颗粒点火的一维非定常两相化学反应流模型,该模型考虑了气固两相间的相互作用、粉尘颗粒的加速、加热和化学反应。粉尘颗粒着火前的化学反应用发生在颗粒外表面和内孔表面的非均相反应描述,颗粒内部的温度变化用一含有化学反应源项的非稳态热传导方程来描述,以颗粒外表面温度的突跃上升作为可燃粉尘颗粒点燃的着火条件。我们用该模型和PSIC方法,对由中等强度激波从纯气相传入煤粉-氧气混合物而引起的非定常两相流动现象,包括气固两相间的相互作用、粉尘颗粒的加速、加热以及点火过程进行了数值研究,计算了对应于不同载荷比、马赫数为4～5的入射激波后煤尘颗粒的点火延迟时间,分析了由于可燃粉尘颗粒的存在,入射激波及波后气固两相流动参数的变化规律。数值计算结果与实验数据符合较好。

文中建立的模型和所用的基于PSIC算法的数值方法,用最自然的方式描述气固两相流动,即用连续流模型(欧拉方程)描述输运相(气相)的流动,用轨道颗粒模型(拉格朗日方程)描述分散相(颗粒相)的运动。用这种方法模拟含尘介质中激波后颗粒的点火是很有效的,它可以清楚地确定哪一个颗粒群最先着火,它的初始位置以及在整个点火延迟时间内的运动轨迹、速度和温度变化规律。这是用双流体模型和欧拉方法难以做到的。本文是粉尘燃烧与爆轰数值研究的初步尝试,进一步选择合适的可燃粉尘颗粒燃烧模型,将计算扩展到反应区,就可以完整地模拟粉尘爆轰波的详细结构。

关键词 两相流 粉尘激波 计算流体动力学

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NUMERICAL INVESTIGATION OF SHOCK WAVE IGNITION OF DUST

Xu Houqian, Yu Qiang*, H Grönig

(*Nanjing University of Science and Technology, Nanjing, China* 210014)

(* *Shock Wave Laboratory, RWTH Aachen, Germany*)

ABSTRACT A one-dimensional unsteady two-phase flow model has been developed to simulate the ignition of dust particles behind incident shock waves. Heterogeneous reactions occurring on the particle surface and in the pores within the particle are used to model the chemistry. For different loading rates, the ignition delays of coal dust particles behind incident shock waves with Mach numbers between 4 and 5 are calculated using a numerical method based on the PSIC approach. The results agree well with experimental data.

KEY WORDS two-phase flow, dusty shock wave, CFD

1 INTRODUCTION

The ignition of dust particles is the first step in dust explosions which pose a serious safety hazard in industry, and the ignition delay has a major influence on detonability. Many investigators[1~8], therefore, have studied the ignition of dust particles behind incident shock waves in order to know the detailed structure of dust detonations and the detonability characteristics of dust-oxidizer mixtures. Theoretical models in some of these papers[3,5,6,7] are based on one-dimensional steady two-phase flow equations and the heat conduction equation including a reactive source term. In this paper, a one-dimensional unsteady two-phase flow model has been developed to study the ignition of dust particles behind incident shock waves. Numerical calculations of the two-phase supersonic flow field induced by the shock waves are made using a method based on the PSIC (particle-source-in-cell) approach[9]. As an example, the ignition delay of coal dust particles has been calculated. The results are in good agreement with experimental data.

2 PHYSICAL MODEL

The flow under study is shown schematically in Fig. 1. A planar shock wave which moves in the pure gas with a constant velocity propagates into a uniform suspension of combustible dust particles in an oxidizing gas. After the passage of the shock wave each dust particle is staying in an unsteady supersonic, high temperature and high pressure flow. The drag forces cause the particles to accelerate, and the convective heating causes a rapid increase in the particle surface temperature. With increasing particle temperature the rate at which the gaseous oxidizer and the particle react increases until the reaction heat release results in temperature runaway or ignition.

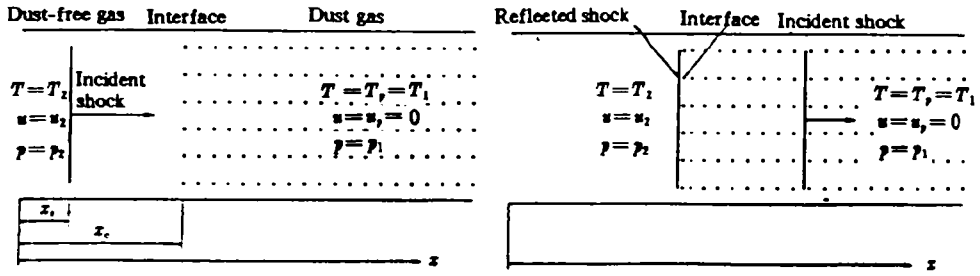


Fig. 1 Scheme of flow field considered

To simulate the non-equilibrium phenomena numerically, we employ a one-dimensional unsteady two-phase flow model in which the gas phase is described by a continuous model and the particle phase by a trajectory model respectively. The following basic assumptions are adopted:

• The gas phase is treated as a perfect gas. Its viscosity and heat conductivity are considered only when the particles interact with it;

• The particles are monodisperse, incompressible, spherical and of uniform diameter.

• The volume occupied by particles in the suspension and particle-particle interactions can be neglected.

• Ignition reactions occur only on the outside and pores surface of a particle. Gaseous products can be neglected before ignition.

• The devolatilization of particles is insignificant and negligible within the ignition delay time.

Based on the assumptions presented above, the governing equations for the gas phase can be written as follows(for the notation see the list of symbols at the end):

$$\frac{\partial U}{\partial t}+\frac{\partial G}{\partial x}=H \tag{1}$$

$$U=\begin{bmatrix}\rho\\ \rho u\\ \rho(C_v T+\frac{u^2}{2})\end{bmatrix},\quad G=\begin{bmatrix}\rho u\\ p+\rho u^2\\ pu+\rho u(C_v T+\frac{u^2}{2})\end{bmatrix},$$

$$H=\begin{bmatrix}0\\ F_p\\ Q_p+F_p u\end{bmatrix},\ F_p=\sum_k n_k f_k \tag{2}$$

$$f_k=\frac{1}{8}\pi d_k^2 C_{D,k}\rho|u_k-u|(u_k-u) \tag{3}$$

$$Q_p=\sum_k n_k q_k \tag{4}$$

$$q_k=\pi d_k Nu\cdot n_k\lambda(T_{p,k}-T_f) \tag{5}$$

and the equation of state is:

$$p = \rho RT \tag{6}$$

Each computational particle, called parcel and labeled by the subscript k, represent a number of real particles having approximately the same initial conditions, particle size, particle velocity and temperature. The Lagrangian equations of motion for the particles in parcel k are

$$\frac{dx_k}{dt} = u_k \tag{7}$$

$$m_k \frac{du_k}{dt} = -f_k \tag{8}$$

The temperature variation within a non-isothermal particle is governed by the unsteady heat conduction equation including a reactives source term,

$$\rho_p \frac{\partial(CT_p)}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}(k_c r^2 \frac{\partial T_p}{\partial r}) + S \tag{9}$$

where S is the reactive source term. Assuming a first-order reaction, as was also done by Ural et al. (1982), Sichel et al. (1985) and Lee et al. (1986)[3,5,6], this term is given by

$$S = P\rho_p S_i P_{O_2} \cdot A\exp(-\frac{E}{RT_p}) \tag{10}$$

The boundary condition is

$$k_c \frac{\partial T_p}{\partial r}|_{r=R} = h(t)[T_f(t) - T_p(R,t)] \tag{11}$$

Equations (1)～(11) along with relations for C_D and Nu represent the closed model. The ignition criterion states that the rate of rise of the surface temperature exceeds a critical value. The ignition delay is taken as the time between the shock passage and the particle surface temperature runaway.

3 NUMERICAL ALGORITHM

Our numerical algorithm is based on the PSIC technique. The detailed solution procedure within one time step is as follows:

a). At the first Eulerian step, the gas flow variables are computed using the particle variables calculated in the last time step;

b). At the second Lagrangian step, the gas variables of the first step are used to compute the particle variables;

c). a) and b) are repeated until convergence is achieved on the particle source terms.

To solve Eq. (1), we apply the operator-splitting technique to deal with the coupling effects between the gas phase and the particle phase, which can be represented with two operators in the following expression:

$$U_i^{n+1} = L_x(\frac{\Delta t}{2})L_p(\Delta t)L_x(\frac{\Delta t}{2})U_i^n \tag{12}$$

where L_x and L_p are two difference operators responded to following Eqs. (13) and (14) respectively:

$$\frac{\partial U}{\partial t} + \frac{\partial G}{\partial x} = 0 \tag{13}$$

$$\frac{\partial U}{\partial t} = H \tag{14}$$

The difference operator L_x is constructed by using piecewise-linear method[10] which can yield a sharp discontinuous solution with high resolution. The difference scheme for Eq. (13) can be written as

$$U_i^{n+1} = U_i^n + \frac{\Delta t}{\Delta x}(G_{i-1/2}^{n+1/2} - G_{i+1/2}^{n+1/2}) \tag{15}$$

with

$$G_{i\pm 1/2}^{n+1/2} = G_{i\pm 1/2}^n + \frac{1}{2}\left[\Delta x - \Delta t\left(\frac{\partial G}{\partial U}\right)_{i\pm 1/2}^n\right]\left(\frac{\partial G}{\partial x}\right)_{i\pm 1/2}^n \tag{16}$$

(see Ref. [10] for details)

Eq. (14) can be solved by using the forth-order Runge-Kutta method. The Lagrangian equations of particle motion (Eq. (7) and (8)) are integrated for a respresentative number of particle trajectories by Euler's predictor-corrector technique, and the unsteady heat conduction equation (9) is solved using the implicit finite difference scheme proposed by Patanka (1980)[11].

4 SAMPLE COMPUTATION

The model described above has been used to simulate the unsteady non-equilibrium two-phase flow induced by incident shock waves propagating in coal-oxygen mixtures. The ignition delay of coal dust particles, diameter of 53 μm, behind incident shock waves of Mach numbers between 4 and 5 are calculated and compared with experimental data (Sichel et al. 1985)[5].

Because the relative velocity between gas and particles ranges from supersonic to very low subsonic values, the empirical expression for the drag coefficient C_D in Eq. (3) presented by Walsh (1975)[12] was used in the computations and has the form

$$C_D = C_{D,C} + (C_{D,FM} - C_{D,C}) \cdot \exp(-ARe^N) \tag{17}$$

where $C_{D,C}$, $C_{D,FM}$, A and N are empirical functions of the particle Mach number.

The Nusselt number Nu in Eq. (5) and the film conductance $h(t)$ in Eq. (11) also vary over a wide range during particle acceleration. Thus, the empirical expression for h given by Fox et al. (1977)[2] was used to evaluated $h(t)$. Accordingly,

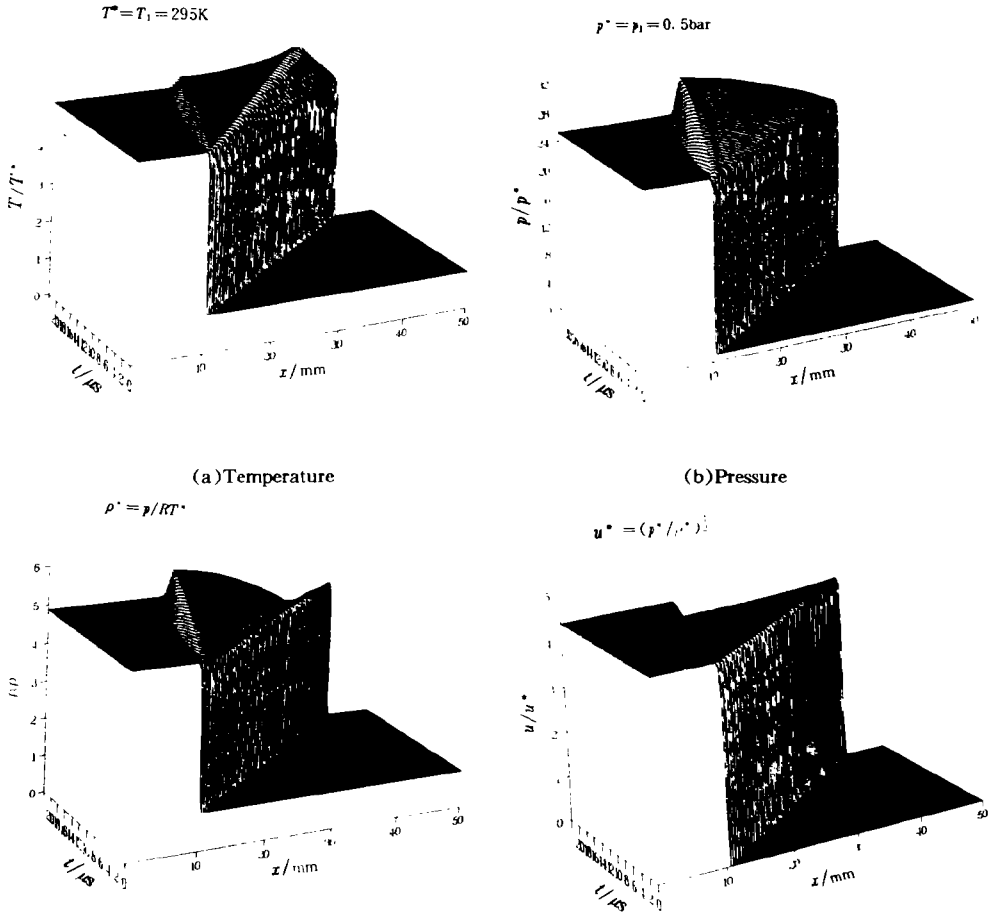
$$Nu = \frac{d_p h}{\lambda} = \frac{2\exp(-M)}{1 + 17M/Re} + 0.459Pr^{0.33} \cdot Re^{0.55} \cdot \frac{1 + 0.5\exp(-17M/Re)}{1.5} \tag{18}$$

The thermal properties of coal dust, i.e. the specific heat C and the thermal conductivity k_c in Eq. (9), are taken from Badzioch et al (1964)[13] in the empirical functions of the temperature. The internal surface area S_i and the kinetic data in Eq. (10) are taken from Gan et al. (1972)[14] and Field et al. (1967)[15], as it was also done by Sichel et al. (1985)[5], and shown as follows

$\rho_p=1.2$ g/cm^3; $S_1=4.26\times10^6$ cm^2/g; $Q=8559$ cal/g;
$E=35.7$ kcal/(g · mol); $A=8.71\times10^3$ g(cm^2 · s·atm).

5 NUMERICAL RESULTS AND DISCUSSION

Parts of numerical results are shown in Figs. 2～5 and discussed in detail below. Fig. 2 shows the gas temperature, pressure, density and velocity histories for different times. The unsteady characteristics of the incident shock wave, the reflected shock wave and the gas parameters can be seen clearly.



(a)Temperature (b)Pressure

(c)Density (d)Velocity

Fig. 2 Dimensionless gas temperature, pressure, density and velocity histories

$M_s=4.66$, $d_s=53$ μm, $\eta=1.0$, $p^*=1.013$ bar, $T^*=295$ K, $\rho=p^*/RT^*$, $u=\sqrt{RT^*}$

The temperature history, as shown in Fig. 2a, is, unlike the case of a pure gas where the shock fronts are sharp, here only sharp in the frontal part. The sharp portion is followed by a further increase toward a maximum value, and a temperature peak is formed after which the temper-

ature decreases gradually up to the value behind the reflected shock wave. The temperature peak value increases as the incident shock wave penetrates further into the dust suspension until the ignition of dust particles occurs.

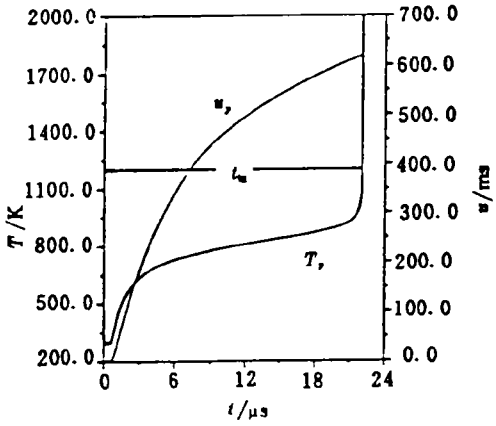


Fig. 3　Surface temperature and velocity histories of a 53 μm coal dust particle for the conditions specified in Fig. 2

The pressure history shown in Fig. 2b is slightly different from the temperature history. The maximum pressure is close to the reflected shock wave, while the temperature peak follows the incident shock wave. Thus, there is a valley in the gas density history, as shown in Fig. 2c, corresponding to the temperature crest.

The gas velocity is seen to rise sharply at the incident shock front. The sharp rise is followed by a gradual decrease up to the reflected shock wave.

The surface temperature and the velocity history of a 53μm coal dust particle are shown in Fig. 3. This particle belongs to the particle parcel in which ignition occurs first and has an initial location being 1.5 mm apart from the interface.

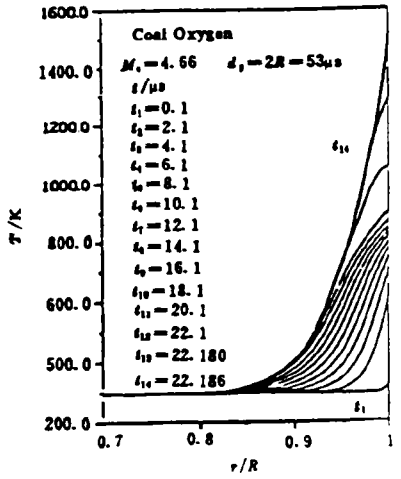


Fig. 4　Temperature distribution profiles inside a coal dust particle for the specified in Fig. 2

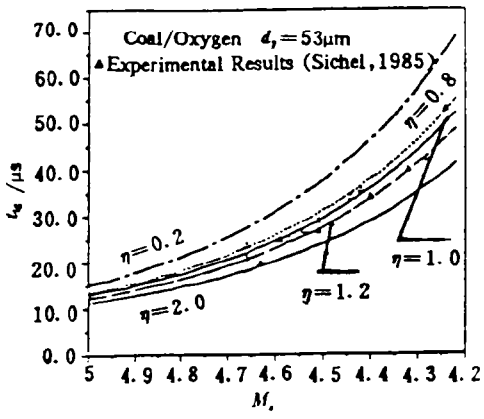


Fig. 5　Ignition delay versus incident shock Mach number for the conditions specified in Fig. 2

Fig. 4 shows time histories of the temperature distribution inside this particle. The heated region is confined almost entirely to the vicinity of the particle surface. From Figs. 3～4 it can be seen that the particle surface temperature rises rapidly at a rate of about 75 K per μs within the first 6 μs, then the rate decreases to about 11K per μs, after $t=20$ μs the rate increases sharply to about 175 K per μs due to the rapid increase in the reaction rate and the particle surface tempera-

ture runaway occurs after $t=22.18$ μs. The ignition of the particles has taken place in the flow field.

Fig. 5 gives the comparison of computed and measured ignition delays for the coal dust considered. The computed results are corresponding to five different loading rates. The experimental data are taken from Sichel et al. (1985)[5] in which the loading rate was not given because of the difficulty in measurement. It can be seen that the computed results are in good agreement with the experimental data in the loading rate range of 0.8～1.2.

6 CONCLUSIONS

A one-dimensional unsteady two-phase flow model which considers the temperature variation inside the particle and heterogeneous reactions occurring on the particle surface and in the pores within the particle has been developed to simulate the unsteady non-equilibrium flow field induced by an incident shock wave.

The ignition of coal dust particles dispersed in pure oxygen behind incident shock waves was studied numerically using this model. The ignition delays of coal dust were calculated which are in good agreement with experimental data.

The gas behaviour behind incident shock waves was discussed in detail which is unlike the case of a pure gas and has outstanding unsteady characteristics.

The present numerical method, based on the PSIC approach, was found to be a powerful method used for modelling the ignition of dust particles behind incident shock waves. It can be clearly seen which particle parcel ignites first, where the initial location of this parcel is and what track it takes within the whole ignition delay time.

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NOMENCLATURE

A=pre-exponential factor
C=specific heat of particle
C_D=drag coefficient
d_k=diameter of a dust particle in parcel k
C_v=specific heat of gas at constant volume
E=activation energy
F_p=drag force per unit mass
f_k=drag force of a particle in parcel k
h=film conductance
k_c=thermal conductivity of particle
M=Mach number
M_s=incident shock Mach number
m_k=mass of a particle in parcel k
n_k=number density of particle parcel k
Nu=Nusselt number
p=pressure
p_{O_2}=oxygen partial pressure
Pr=Prandtl number
Q=combustion heat per unit mass
q_k=rate of heat transfer between gas and a particle in parcel k
Q_p=heat conduction flux
R=gas constant, particle radius
$\bar{R}$=universal gas constant

Re=Reynolds number
r=radius within particle
S_i=internal surface area per unit mass
t=time
T=gas temperature
T_r=recovery temperature
T_p=temperature within particle
T_{ps}=particle surface temperautre
u=gas velocity
u_k=velocity of particle in parcel k
x=distance
x_k=position of particle parcel k
η=loading rate
λ=thermal conductivity
μ=viscosity constant
ρ=gas density
ρ_p=density of particle material

REFERENCES

1 Nettleton M A, Shock-wave Chemistry in Dusty Gases and Fogs. A Review, Comb. and Flame, 1977, 28: 3～16

2 Fox T W, Rockett C W, Nicholls J A. Shock Wave Ignition of Magnesium Powders. In: Proc of 11th Symp (Int.) on Shock Tubes and Waves. 1977. 262～268

3 Ural E A, Sichel M, Kauffman C W. Shock Wave Ignition of Pulverized Coal. In: Proc of 13th Symp (Int.) on Shock Tubes and Waves, 1982. 809～817

4 Boiko V M, Papyrin A N, Wolanski M, Wolanski P. Dynamics of Shock Waves, Explosions, and Detonations. New York, AIAA, 1984, 94: 293～301

5 Sichel M, Baek S W, Kauffman C W, Maker B, Nicholls J A. The Shock Wave Ignition of Dusts. AIAA J, 1985, 23: 1347～1380

6 Lee F P, Kauffman C W, Sichel M, Nicholls J A. Detonability of RDX Dust in Air/Oxgen Mixtures. AIAA J, 1986, 24: 1811～1816

7 Fan B C, Sichel M. A Comprehensive Model for the Structure of Dust Detonations. In: Proc 22th Symp (Int.) on Combustion. The Combustion Institute, 1988. 1741～1750

8 Geng J H, van de Ven A, Zhang F, Grönig H. Ignition Delay of the Cornstarch Dust Behind an Incident Shock Wave. Presented at 14th ICODERS, Coimbra, Portugal, 1993

9 Crowe C T, Sharma M P, Stock D E. The Particle-Source-in-cell Model for Gas-Droplet Flows. 1975, ASME paper 75-WA/HT-75

10 Sommerfeld M, Selzer M, Grönig H. Shock Wave Reflections in Dusty-gas. In: Proc of 15th Symp (Int.) on Shock Waves and Tubes, 1986. 683～689

11 Patankar S V. Numerical Heat Transfer and Fluid Flow. [s. l.]: Hemisphere Publishing Corporation, 1980

12 Walsh M J. Drag Coefficient Equations for Small Particles in High Speed Flow. AIAA J, 1975, 13: 1526～1527

13 Badzioch S, Gregory D R, Field M A. Thermal Conductivity and Thermal Diffusivity of Coal. Fuel, 1964, 43: 267～280

14 Gan H, Nandi S P, Walker P L. Nature of porosity in American Coals. Fuel, 1972, 51: 272～277

15 Field M A, Gill D W, Morgan B B, Hawksley P G W. Combustion of Pulverized Coal. Leatherhead: the British Coal Utilisation Research Association, 1967