Numerical Simulation of Multiphase Reactive Boundary Layer Flow By Mass Split Technique

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Abstract A model of multiphase reactive boundary layer flow induced by a shock is presented. Because of the particle reaction in the boundary layer, the source terms are involved in the governing equations. The mass split technique is developed to deal with the problem of the source terms. By above split technique, the set of equations can be transformed into similarity plane and the resolution of them becomes possible.

The BOX method is employed to solve the gas phase equations. The particle phase equations are solved by the forth-order Runge-Kutta method. To give a coupling of gas phase and solid phase equations, the method of Particle-Source-in-Cell (PSIC) is modified to match with the BOX method because the PSIC method is based on the SIMPLER scheme which is constructed on the cells but BOX scheme on the junctions. The results reveal the basic structure of the multiphase reactive boundary layer.

Key Words: boundary layer, multiphase reactive flow, dust combustion, numerical simulation, shock wave

Introduction

When a high temperature gas flow passes over a flat plate laden with dusts, a boundary layer flow of multiphase reaction between the dust particles and gas phase will be induced. It is related to the phenomenon of the interaction between a shock wave with a dust deposit and the explosion propagation of the dust deposits[1~2]. The formation mechanisms of the boundary layer were explained by previous researchers[1~4].Some of them give the contributions to the modeling of the boundary layer but the process dust combustion is rarely considered.

The problems of the reactive boundary layer are universal and important in the areas of the aeronautics and astronautics[5]. Within these reactive boundary layers, the chemical reactions occur often between different gas species or on the interface between gas and the surface of the condense wall. So the reactive boundary layer is called the gas reactive boundary layer or the interface reactive boundary layer. In the present reactive boundary layer, the chemical reactions take place between gas and suspend particles. It is considered as a reactive boundary layer of multiphase flow which must be described by the models of the multiphase flow and multiphase reaction such as particle combustion.

Based on the particle trajectory model for multiphase flow[6] and Prandtl's assumption of boundary layer[5], a comprehensive model of multiphase reactive boundary layer flow induced by a shock passing over a dust-laden surface is provided in the present work. Because of the multiphase reactions, the governing equations of the boundary layer involve source terms so that the similarity transformation can not be implemented directly. The mass split technique for solving the problem is developed in this work which will be explained in detail following. By the mass split, the equations of the model can transformed into the similarity plane by the similarity transformation similar to that of Leeds-Dorodnitzyn[7].

Numerical simulations are also conducted in the present work. The BOX method of implicit, second-order accuracy scheme is employed to solve the gas phase equations. The particle phase equations are solved by the forth-order Runge-Kutta method. To make a coupling of gas phase and solid phase equations, the method of Particle-Source-in Cell (PSIC)[8] is employed and modified. The numerical results by the present methods reveal the basic structure of the multiphase reactive boundary layers.

Mathematical Model

Governing Equations

Consider a plane shock wave passing over a flat plate laden with dusts in a constant velocity, u_s. If the coordinates are fixed on the shock front and the dusts are combustible, the flow behind the shock front is a steady multiphase reactive boundary layer flow. Assuming the dust suspension flow is a dilute system so that the volume fraction of particles and the interactions between particles can be neglected. Neglected the thermal motion of particles contributing to the pressure of the mixture system. The dusts are considered as spherical rigid particles of the same diameter. According to the particle trajectory model for the multiphase flow[6] and Prandtl's assumption of boundary layer[5], following governing equations can be derived.

Gas phase

$$\frac{\partial(\rho u)}{\partial x}+\frac{\partial(\rho v)}{\partial y}=\Gamma \tag{1}$$

$$\rho(u\frac{\partial Y_i}{\partial x}+v\frac{\partial Y_i}{\partial y})=\frac{\partial}{\partial y}(\rho D_{eff}\frac{\partial Y_i}{\partial y})+\Gamma_i \tag{2}$$

$$\rho(u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y})=-\frac{\partial p}{\partial x}+\frac{\partial}{\partial y}(\mu_{eff}\frac{\partial u}{\partial y})-V_x \tag{3}$$

$$\frac{\partial p}{\partial y}=-V_y \tag{4}$$

$$\rho(u\frac{\partial H}{\partial x}+v\frac{\partial H}{\partial y})=u_s\frac{\partial p}{\partial x}+\frac{\partial}{\partial y}[(\frac{\mu}{\Pr})_{eff}\frac{\partial H}{\partial y}]+\frac{\partial}{\partial y}[(\mu_{eff}-(\frac{\mu}{\Pr})_{eff})\frac{\partial(u_s-u)^2/2}{\partial y}]+S_Q \tag{5}$$

Particle phase

$$\frac{d\rho_p}{dt_p}=-\Gamma-\rho_p(\frac{\partial u_p}{\partial x}+\frac{\partial v_p}{\partial y}) \tag{6}$$

$$\frac{du_p}{dt_p}=\frac{1}{\rho_p}(V_x+(u_p-u)\Gamma) \tag{7}$$

$$\frac{dv_p}{dt_p}=\frac{1}{\rho_p}(V_y+(v_p-v)\Gamma) \tag{8}$$

$$\frac{dT_p}{dt_p}=\frac{1}{c\rho_p}(Q+S_{Qp}) \tag{9}$$

where u and v represent the velocity components in the x and y directions. T and ρdenote the temperature and the density of gas phase or particle phase. The parameter with a subscript p is that of the particle phase. H, p are the total enthalpy and pressure of gas. μ_{eff} and D_{eff} are the efficient viscosity and diffusivity of turbulence. Pr is Prandtl's number. c is the specific heat. $\Gamma$is the mass transfer between gas and particle phase. V_x ,V_y are the components of the momentum transfer between two phase in x , y direction. Q is the heat transfer. S_Q, S_{Qp} are the source terms which are determined by following.

$$S_Q=\Gamma(\beta Q_c+H_p-H)-Q-(u_s-u)V_x-v_pV_y \tag{10}$$

$$S_{Qp}=\Gamma((1-\beta)Q_c-(u_p-u)(u_p-u_s)-(v_p-v)v_p) \tag{11}$$

where Q_c andβrepresent the heat exhausted and the fraction of reaction heat contributing to the gas phase.

Boundary Conditions

The problem has three boundaries. (1) For the shock front, *x=0*. Replace the boundary at *x=0* with $x=\varepsilon$($\varepsilon$is infinitesimal) . The parameters of particle phase are zero and that of gas can be determined by Blasius' similar resolutions. (2)External boundary $y=\delta(x)$. The parameters of particle phase are zero and those of gas equal to those of free flow on the boundary. (3)Wall boundary *y=0*. For particle phase, $u_p=u_w$, $v_p=v_{pw}$, $t_p=t_{pw}$,$\rho_p=\rho_{pw}$. For gas, $u=u_s$, $\frac{\partial u}{\partial y}=-\frac{\tau_w}{\mu}$,$T=T_0$. τ_w can be given according to Mirels' theory[4].

Mass Split Technique and Similarity Transformation

Because of the particles combustion, the governing equations (1) to (9) involve source terms. As a result, the some of similarity transformations such as Leeds' transformation which is valid to solve the problems of ordinary boundary layer[5,7] can not be employed to solve the equations of the present boundary layer. Based on the view of the mass conservation, the gas can be split into two parts. One part is the intrinsic part which is from the initial gas phase and another part is the extrinsic part which is generated during the process of multiphase reaction. And the concepts of extrinsic gas density and intrinsic gas density can be defined as followed. The extrinsic gas density denoted by ρ_c is the gas density increment due to the multiphase reaction in the boundary layer and the intrinsic gas density represented by ρ_I equals to the gas density of the boundary layer flow presuming without any chemical reaction. Therefore, the general gas density $\rho=\rho_I+\rho_c$. Let $\varphi=\rho_c/\rho_I$, then $\rho=(1+\varphi)\rho_I$. So the mass equation (1) can be split into two mass equations, the extrinsic mass equation (12) and intrinsic mass equation (13).

$$\frac{\partial}{\partial x}(\rho_1 u)+\frac{\partial}{\partial y}(\rho_1 v)=0 \tag{12}$$

$$\rho_1 u\frac{\partial \varphi}{\partial x}+\rho_1 v\frac{\partial \varphi}{\partial y}=\Gamma \tag{13}$$

Based on the intrinsic mass equation (12), the flow function ψ is defined. With the transformation similar to that of Leeds-Dorodnitzyn[7]

$$\xi=\frac{x}{\lambda},\qquad \eta=\frac{1}{\sqrt{2\xi}}\int_0^{\bar{y}}\frac{\rho}{\rho_e}d\bar{y}$$

where $\lambda=u_s\tau, \bar{y}=\frac{y}{\lambda}\sqrt{R_{e\lambda}}, R_{e\lambda}=\frac{\rho_e u_e\lambda}{\mu_e}$. τ is the dynamic relaxation time of particle. The subscript *e* denotes free flow. In terms of the dimensionless function *f* and other dimensionless variables defined by

$$f=\frac{\psi}{\sqrt{2\xi\lambda}\sqrt{\rho_e u_e\mu_e}},\quad f'=\frac{\partial f}{\partial \eta}=\frac{u}{u_e},\quad v^*=\frac{v}{u_e}\sqrt{R_{e\lambda}},\quad \theta=\frac{H}{c_p T_e},\quad p^*=\frac{p}{\rho_e u_e},\quad \rho^*=\frac{\rho_1}{\rho_e},$$

the gas phase equations (1) to (5) and boundary conditions of gas phase can be written as

$$(bf'')'+mff''+m_1=2\xi m\left(f'\frac{\partial f'}{\partial \xi}-f''\frac{\partial f}{\partial \xi}\right) \tag{14}$$

$$\left(\frac{b}{\mathrm{Pr}}\theta'\right)'+m_2\theta'+m_3=2\xi m f'\frac{\partial \theta}{\partial \xi} \tag{15}$$

$$\left(\frac{b}{Sc}Y_i^{*\prime}\right)'+mfY_i^{*\prime}+w_i=2\xi m\left(f'\frac{\partial Y_i^*}{\partial \xi}-\frac{\partial f}{\partial \xi}Y_i^{*\prime}\right) \tag{16}$$

$$f\varphi'+m_4=2\xi\left(f'\frac{\partial \varphi}{\partial \xi}-\frac{\partial f}{\partial \xi}\varphi'\right) \tag{17}$$

$$-\sqrt{2\xi}\rho^* v^*=f+2\xi\frac{\partial f}{\partial \xi}-\eta f' \tag{18}$$

where

$$b=\rho^*\mu_{eff}^*,\qquad m=1+\varphi,\qquad m_1=\frac{1}{\rho^*}\left(\eta\frac{\partial p^*}{\partial \eta}-2\xi\frac{\partial p^*}{\partial \xi}-\frac{2\xi\lambda}{\rho_e u_e^2}V_x\right),\qquad m_2=(1+\varphi)\left(f+2\xi\frac{\partial f}{\partial \xi}\right)$$

$$m_3=\frac{2\xi\lambda}{c_p T_e}\left(1-\frac{1}{\mathrm{Pr}}\right)\left[b\left(f'-\frac{u_s}{u_e}\right)f''\right]'+\frac{u_s u_e}{\rho^* T_e}\left(2\xi\frac{\partial p^*}{\partial \xi}-\eta\frac{\partial p^*}{\partial \eta}\right)+\frac{2\xi\lambda S_Q}{\rho_e u_e T_e\rho^* c_p},\qquad m_4=\frac{2\xi\lambda}{\rho_e u_e\rho^*}\Gamma,\qquad w_i=\frac{2\xi\lambda}{\rho_e u_e\rho^*}\Gamma_i$$

and $\eta=0,\quad f'=\frac{u_s}{u_e},\quad f''=f_w'',\quad \theta=\theta_w,\quad Y_i^*=Y_{iw}^*,\quad \varphi=0$

$\eta=\eta_\infty,\quad f'=1,\qquad \theta=\theta_\infty,\quad Y_i^*=1,\quad \varphi=0$

Numerical Method—Modified Particle-Source-in-Cell Method

Equations (14) to (18) are similar to those of the nonreactive boundary layer mentioned by Cebeci and Smith[7] but equation (16) to (17) are added due to multiphase reactions. The effects of the multiphase reactions on gas flow are also implied in the parameters *m*, m_1, m_2, m_3, m_4 and w_i. The transfers between two phase cause difficulty to solve the equations numerically. The Particle-Source-in-Cell Method[8] can solve the coupling problems of gas phase with particle phase. When PSIC method is employed to solve the present problem it should be modified because the PSIC method is based on the calculation cell but the numerical scheme for resolving the equations of boundary layer are often based on the junctions.

The BOX method[7] is sifted to solve the gas equations (14) to (18). It involves four steps: (1) Reduce the governing equations to a system of first-order ones, (2) Write difference equations with central differences, (3) Linearize the resulting algebraic equations and write them in matrix-vector form, (4) Solve the linear system by the block tridiagonal elimination method. The difference is a implicit scheme of second-order accuracy. To obtain the source terms, the PSIC method is modified below. In terms of calculation junction (ξ_n,η_j) for gas equations, a cell $P_1P_2P_3P_4$ is reconstructed as shown in Fig 1. And the average values of particle sources in the cell are regarded as those in the junction (ξ_n,η_j) for gas equations. The particles in the flow can be divided into a lot of groups based on some properties such as the diameter of the particles. Perhaps some of the particle trajectories will cross the cell $P_1P_2P_3P_4$. The time duration of *i*th trajectory or *i*th group particles crossing through the cell is denoted by Δt_i. In this duration, the mass of

the ith group particles in the cell $m_i=n_i\Delta t_i\, m_{pi}$, where n_i is the number density of the ith group particles and m_{pi} is the mass of one particle. If the total number of particle trajectories crossing through the cell is k groups, the total mass of the particles in the cell can be determined, that is $m = \sum_{i=1}^{k} n_i \Delta t_i m_{pi}$. In terms of mass weighted average, the transfers between two phases F can be determined.

$$F = \frac{n_i \Delta t_i m_{pi} F_i}{n_i \Delta t_i m_{pi}}$$

where F_i represents the parameters of ith group particles which can be solved from equations (6) to (9) by fourth-order Runge-Kutta Method conveniently.

Results and Discussions

The turbulence of gas phase and particle phase are simulated by Cebeci-Smith turbulent model and random trajectory model respectively but the effects of turbulence on the multiphase combustion are not considered. The drag force, *Saffman* lifting force[6] and gravity are considered acting on the particles. Considering a shock Mach number Ms=4.2, cornstarch dusts have a mean diameter of 30μm. The typical results reveal the basic features of the multiphase reaction boundary layer. The general structure is shown in Fig 2. The solid curves draw outline of the three different zones which are induction zone, reaction zone and diffusion zone bordering with the free flow area. The dotted lines are the contours of the oxygen fraction in gas phase. It is shown that the oxygen concentration of gas phase in the reaction zone is the lowest among three zones. This case is due to the particle combustion in the reaction zone. In the induction zone, the particles are raised from the surface of the dust deposit and heated by shocked gas but the particle temperature is not high enough to ignition and combustion.

SUMMARY

A comprehensive model of multiphase reactive boundary layer and the mass split technique for solve the model equations involved source terms have been developed. By introducing the concepts of the intrinsic and extrinsic gas density, the mass equation is divided into the intrinsic mass equation and extrinsic mass equation. As a result, the equations are transformed by the Leeds-Dorodnitzyn' similarity transformation and given out the numerical solutions successfully. The Particle-Source-in-Cell method has been modified to couple the equation of gas and particle phase. The numerical results reveal the complicated structure of the multiphase reactive boundary layer.

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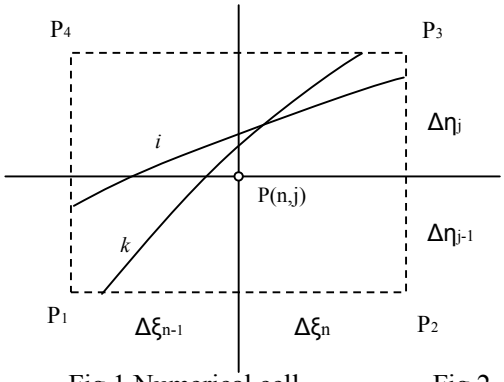

Fig.1 Numerical cell

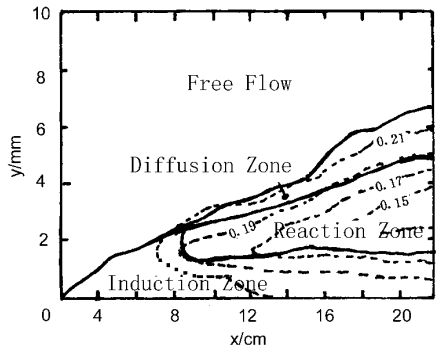

Fig.2 Structure of multiphase reactive boundary layer