Large Eddy Simulation of a Combusting Droplet

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abstract

Gas flow and flame structures surrounding a combusting ethanol droplet are studied by large eddy simulation (LES). The instantaneous flow and flame structures under different inlet velocities, droplet sizes and inlet temperatures are presented. The flame structures show three combustion regimes--fully enveloped, partially enveloped and wake flames, similar to the previous experimental results about 50 years ago by Zhou and by recent PLIF measurements.

Key words: large eddy simulation, combusting droplet, flame structure

Introduction

The theoretical and experimental studies of the evaporation and combustion of a single droplet can be tracked back to the years of 1950's to 1980's [1, 2, 3]. The classical stagnant film theory makes many simplification assumptions, including a spherical flame, a stagnant film, unity Lewis number, and infinitely fast chemical kinetics. These simplified theories provide valuable qualitative insight into the physics of droplet evaporation and combustion, but quantitatively these theoretical results were validated only by measured global characteristics, such as the so-called "evaporation constants". Dietrich et al.[4] studied the combustion of a decane droplet in microgravity. Mercier et al.[5] investigated the droplet combustion in counter-flow diffusion flames using planar laser-induced fluorescence (PLIF). PLIF measurements applied to OH radical and acetone were used to measure the spatial distribution of the fuel vapor concentration and the structure of the flame front around the droplet. Ogami et al.[6] studied single butanol droplet flame in constant and oscillatory flow fields under microgravity at elevated pressures using an experimental approach. Birouk et al.[7] studied the effect of isotropic turbulence on a droplet combustion experimentally. Imamura et al.[8] studied the single droplet combustion in electric fields. Ethanol, n-octane, and toluene were used as fuels, and the flame shape and the burning-rate constants were measured. From these studies it is seen that there are still lack of rigorous studies on the detailed flow field and flame structures surrounding a combusting droplet. In this paper, the gas flows and flame structures surrounding a combusting droplet under different ambient pressures, gas relative velocities, initial droplet sizes and gas temperatures are studied by LES. The fuel for all of these cases is ethanol. The simulation is a transient one with a single-step, finite-rate chemistry. The instantaneous results of combustion regimes will be compared with the experimental results reported by Zhou in the 60's of the last century and recent PLIF measurement results. The statistical results of the single-droplet evaporation and combustion will be compared with Zhou's analytical solution and the simplified spherical-flame solution.

Gas-Phase Governing Equations for LES of a Combusting Droplet

Neglecting the gravitational force, the filtered gas continuity, momentum, energy and species equations for the gas flow surrounding a combusting droplet can be given as:

$$\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x_i}\left(\rho \bar{u}_i\right)=0 \tag{1}$$

$$\frac{\partial}{\partial t}\left(\rho \bar{u}_i\right)+\frac{\partial}{\partial x_j}\left(\rho \bar{u}_i \bar{u}_j\right)=\frac{\partial}{\partial x_j}\left(\mu \frac{\partial \bar{u}_i}{\partial x_j}\right)-\frac{\partial \bar{p}}{\partial x_i}-\frac{\partial \tau_{ij}}{\partial x_j} \tag{2}$$

$$\frac{\partial \rho \bar{Y}_s}{\partial t}+\frac{\partial}{\partial x_j}\left(\rho \bar{u}_j \bar{Y}_s\right)=\frac{\partial}{\partial x_j}\left(\frac{\mu}{Sc}\frac{\partial \bar{Y}_s}{\partial x_j}\right)-w_s-w_{sgs}-\frac{\partial g_{sj}}{\partial x_j} \tag{3}$$

$$\frac{\partial \rho \bar{h}}{\partial t}+\frac{\partial}{\partial x_j}\left(\rho \bar{h} \bar{u}_j\right)=\frac{\partial}{\partial x_j}\left(\frac{\mu}{\mathrm{Pr}}\frac{\partial \bar{h}}{\partial x_j}\right)-\frac{\partial q_j}{\partial x_j} \tag{4}$$

The Arrhenius expression of the one-step global reaction kinetics for w_s is

$$w_s = 8.345\times 10^9 \rho^2 Y_{fu} Y_{ox} \exp[-1.26\times 10^8/(RT)] \tag{5}$$

In this paper, w_{sgs} , known as the SGS reaction rate, is neglected.The boundary conditions for the surrounding gas flow at the surface of a combusting droplet, accounting for the effect of Stefan flux [2], are taken as follows

$$\lambda_w\left(\frac{dT}{dr}\right)_w=\rho_w v_w q_e=\frac{G}{4\pi r_w^2}q_e \tag{6}$$

$$-D_w\rho_w\left(\frac{dY}{dr}\right)_w+Y_s\rho_w v_w=\alpha\rho_w v_w \tag{7}$$

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For LES, the grid sizes in *x*, *y* and *z* directions are 10μm for the case of d_p=100μm and 400μm for the case of d_p=1000μm. The time step is taken as 0.00001s, which is chosen based on the computation test. Within each time step the convergence can be reached after 10 to 20 iterations. The grid number is 1000000. The mesh type is hexagon. For the numerical procedure, the pressure-implicit with splitting of operators (PISO) algorithm is used for p-v corrections, the second order implicit difference scheme for the time-dependent term, and the quadratic upwind interpolation of convective kinematics (QUICK) difference scheme for the convection and diffusion terms are adopted.

Results and Discussion

Figure 1 gives the simulated instantaneous temperature maps around a combusting ethanol droplet under different relative velocities, showing different flame structures, similar to the experimental results reported by Zhou [2] and recent PLIF measurement results for a combusting acetone droplet made in Ref.[5], as shown in Fig.2. There are three different combustion regimes: fully-enveloped, partially-enveloped and wake flames for different inlet velocities and droplet sizes. The velocity vectors around the combusting droplet (Fig.3) are different from those around a non-combusting particle, showing clearly the Stefan flux near the droplet surface. Figure 4 gives the instantaneous vorticity map, showing the asymmetrical coherent structures in the wake behind the droplet, also different from that of a cold particle. It is seen that in case of combustion the fuel vapor concentration distribution is narrower and longer that that in case of the droplet without combustion. Figures 5, 6 and 7 give instantaneous fuel vapor concentration distribution, H_2O concentration distribution and O_2 concentration distribution under the inlet velocity of 4m/s respectively. The H_2O concentrations are higher in the high temperature region.

Conclusions

The numerical simulation confirms three regimes of droplet combustion: fully enveloped, partly enveloped and wake flames. The droplet combustion model used in LES and RANS modeling should be different for different regimes.The fuel vapor concentration distribution is closely related to the size of combusting droplet and inlet velocity. Furthermore, it is also related to the combustion regime and flame structures of single combusting droplets. So, the evaporation rate model should also be improved in simulation of two-phase turbulent combustion.

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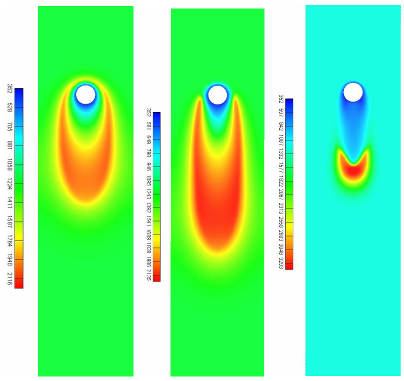

Fig.1 Simulated flame structures （inlet temperature 1200K, droplet diameter 1000μm, inlet velocity 1,2,10m/s respectively）

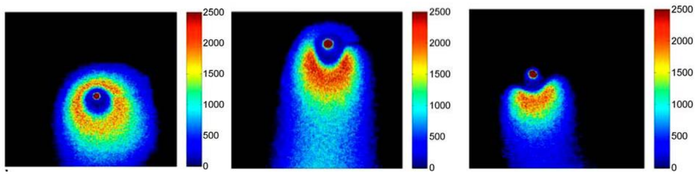

Fig.2 Measured flame structures in Ref. [5]

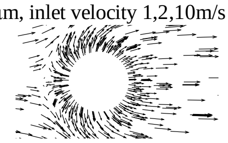

Fig.3: Velocity vectors around the droplet （inlet temperature 1200K, droplet diameter 100μm, inlet velocity 1m/s）

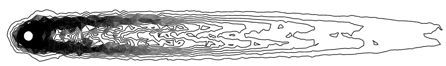

Fig.4: Vorticity maps around the droplet（inlet temperature 1200K, droplet diameter 100μm, inlet velocity 1m/s）

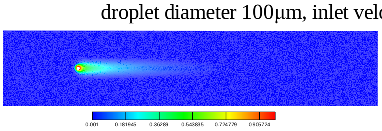

Fig.5 Fuel concentration distribution（inlet temperature 1200K, droplet diameter 100μm, inlet velocity 4m/s）

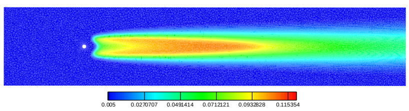

Fig.6 H_2O concentration distribution（inlet temperature 1200K, droplet diameter 100μm, inlet velocity 4m/s）

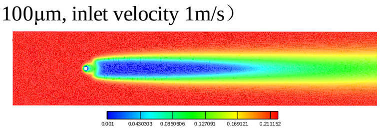

Fig.7 Oxygen concentration distribution（inlet temperature 1200K, droplet diameter 100μm, inlet velocity 4m/s）