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A two-phase turbulent combustion model and its validation for spray flames

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HIGHLIGHTS

- A two-phase turbulent combustion model (FSM) was tested by methanol spray flames.
- FSM model includes the part of individual droplet burning behavior modeling.
- FSM successfully predicted two temperature peaks in the $z = 25$ mm section case 1.
- The traditional model (TM) by author and other workers can only give one peak.
- In these cases, the FSM model predictions are better than those from TM model.

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ABSTRACT

A two-phase turbulent combustion model (FSM) with the inclusion of individual droplet burning behavior was applied in a methanol air spray flame. The FSM model results were compared with the experimental data and results of the traditional two-phase turbulent combustion model (TM). The comparison of the results showed that in most regions the FSM model results were in good agreement with the experimental data. In all the three cases, the FSM model predictions showed the same tendency as the experimental data, which was better than the TM model results. So in the liquid methanol spray flame cases simulated in this paper under atmospheric condition, the FSM model is reasonable for temperature profiles prediction, which could be applied in other liquid fuel combustion simulation in the future.

1. Introduction

In many two-phase flames the droplets burn as single droplets rather than as a cloud, for example the kerosene flame of Katsuki et al. [1] and the acetone counter flow flame of Grisch et al. [2]. The shape of the flame surrounding a burning droplet is determined by the droplet Reynolds number (Re_d) based on the relative velocity between the droplet and the surrounding gas flow. As the droplet Reynolds number increases the flame changes from an envelope flame to a side flame and then a wake flame. The droplet burning condition and flame shape determined by local situation. The work of Grisch produced detailed photographs of single acetone liquid droplets passing through a flame front, an example of which was shown in Fig. 8 in Ref. [2]. There were three photographs showed the passage of a drop of acetone through the flame that did not ignite, whereas other three photographs showed a droplet that did ignite.

In liquid fuel combustion chambers, such as those in most automotive engines, industrial furnaces and aero engines, the liquid fuel is atomized into droplets by nozzles before combustion. Once atomized, the droplets vaporize and combustion takes place. Depending on the droplet loading, a significant part of the combustion occurs as single or individual droplet combustion. During gas turbine combustion chamber (GTC) design, the residence time of droplets in the pre-vaporization zone or the region upstream of the reaction zone, is mainly determined by the droplet auto ignition delay time. Some modern aero engines are fitted with an afterburner, the inlet temperature of the afterburner is approximately 1500 K and the liquid fuel can be ignited by the hot mixture from turbine during very short period, which affects the fuel distribution considerably. The experimental data from Beck et al. [3] demonstrated that the single droplet combustion mode has clear links with the performance of the whole combustion chamber. Also when the gas phase mixture temperature is greater than 950 °C, the metal structure in some combustion chamber may catch fire

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Nomenclature

Romans

A	model constant in ignition delay time scale model ($s(mol/cm^3)^{0.6}$)
B	the Spalding mass transfer number
C_D	the drag coefficient
C_{K,Y_s}	correlation coefficient
C_{ox}, C_{fu}	molecular oxygen and methanol concentrations
Cp_g, Cp_l	the gas and liquid specific heats
d_d	droplet diameter (μm)
d_{d0}	initial droplet diameter (μm)
E	activation energy (kJ/mol)
F_d	drag force per unit droplet mass (N/kg)
h_{fg}	the latent heat of evaporation
K	reaction rate coefficient $K = A\rho^2 \exp\left(\frac{-E}{RT}\right)$
k_e, k_c	model constant (μm^2)
L_S	the sub grid mixing and reaction length scale
Pr_g, Sc_g	the gas-phase Prandtl and Schmidt numbers
R	universal gas constant
Re_d	the Reynolds number based on the relative velocity between the droplet and the gas phase
R_{K,Y_s}	the sub grid scale reaction correlation relation
T_∞	the local ambient temperature
$\overline{T_g}$	the continuous phase temperature
w_{fu}	gas phase fuel reaction rate (kg/s)
$w_{S,s}$	sub grid scale reaction rate for S species
Y	mass fraction

Greeks

μ	the molecular viscosity of the fluid
ρ	gas phase density
ρ_d	the density of the droplet
ρ_g	the density of the gas phase
τ_d	the droplet response time (s)
τ_e	evaporation time scale (s)
τ_i	ignition delay time scale (s)

by droplet ignition and then thermal ablation could happen, which is very dangerous for the aero-engine. Additionally, in the hot-shot ignition method, which was used in the A□l-31Φ, the fuel jet delivers the flame by droplet ignition and burning. So the burning or ignition character of fuel droplet is of importance in combustion chamber design.

The cost of experiments is high and as a result, numerical simulation plays a more and more important role in combustion chamber design, thus modeling development becomes more necessary as are fundamental experiments to examine in detail droplet evaporation and combustion.

During the 1950s, Spalding theoretically analyzed single droplet evaporation and combustion behavior, the governing transfer equations and boundary conditions between a single fuel droplet and gas phase were proposed [4]. In the 1960s, Zhou showed various droplet flame states by experimental results, such as the "parachute flame", as well as ignition phenomenon [5]. Later, Chiu and Liu studied the critical qualification for droplet evaporation/combustion regimes [6]. Then Chiu et al. [7] and Kuo [8] defined droplet cloud/group combustion modes according to the averaged distance between droplets, which showed that in a spray flame or liquid fuel combustion chamber there is single droplet burning with individual flame. Sometimes, the single droplet burning phenomenon cannot be ignored completely.

Russo and Gomez [9] used instantaneous photos, Sonnenfroh et al. [10] the planar laser-induced fluorescence (PLIF) and laser tomography, and Katsuki et al. [1] local OH chemiluminescence and CH-band emission to investigate the combustion in fuel sprays. The experimental results showed individual droplet burning took place in liquid fuel spray flames, and the ignition state condition changed according to local temperature, relative velocity, and turbulence. Chiu [11] has presented the typical droplets combustion modes and pattern in a spray jet flame, in whose theory, the relative Reynolds number and gasification rate were the key factors for the mode change. Faeth and Olson [12] and Bernard and Willis [13] presented droplet ignition experimental data in microgravity environment. It was shown that the local temperature and the ignition delay time had linear relationship in log–log coordinates. Tsue et al. [14] carried out an experimental study and found that the local ambient temperature, pressure, ambient oxygen concentration, and the relative velocity affects the ignition delay time. Stauch et al. [15] used a detailed chemical mechanism with 62 species, 572 elementary reactions to predict the n-heptane droplet ignition delay time and ignition happening position, and analyzed the influence of ambient temperature, pressure and liquid drop diameter. The conclusion was that the ambient temperature was the most important factor, while the droplet diameter had a small effect. Further numerical modeling work by Stauch and Mass [16] examined the ignition delay time on the auto-ignition of heptane/octane droplets, when ambient temperature was lower than 1000 K, the ignition delay time increased with the increase of gas phase octane vapor volume fraction. When ambient temperature was higher than 1000 K, the ignition delay time was independent of the concentration of the liquid phase component in the droplet. Other workers have investigated single droplet combustion in detail, for example, Law [17], Demoulin and Borghi [18], Chigier and McCreath [19], Sirignano [20], Sazhin [21], Reveillon and Vervisch [22] and while many other works on the single droplet burning behavior exist, there is as yet no universal principle for the judgment of droplet combustion modes in the spray flames as well as a simulation model.

A vapor layer forms around the droplet as it evaporates and combustion takes place around the droplet where fuel and oxidant co-exist. In a usual numerical simulation, such as Reynolds averaged Navier Stokes (RANSs) method, the grid size is much bigger than the size of droplet and its flame, thus the burning droplet is treated as a point. Thus, in the dominant two phase combustion simulation methods: the RANS method, Large Eddy Simulation (LES) method and Point source Direct Numerical Simulation (PDNS) method in Euler–Lagrangian coordinates, the droplets are treated as point sinks/sources of mass, momentum and energy.

For the two-phase flow modeling in combustors, there are a number of issues to be addressed in order to improve the accuracy of the current practical combustor simulations, and this paper talks only one of them.

In this paper, a new two-phase turbulent combustion model, i.e. FSM model, with emphasis on the single droplet combustion modes will be tested using methanol air spray jet flames. The comparison between prediction results from the FSM model and the traditional point source two phase combustion model (TM) will be carried out.