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Thermal auto-ignition in high-speed droplet-laden mixing layers

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HIGHLIGHTS

- We investigate thermal auto-ignition in high-speed droplet-laden mixing layers.
- Ignition depends on the combined effects of droplet dispersion and evaporation.
- Contribution of non-premixed flame increases as droplet size increases.
- The droplet size affects the values of the most reactive mixture fraction.
- High spray equivalence ratio enhances scalar dissipation and evaporative cooling.

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ABSTRACT

Numerical simulation is applied to perform fundamental studies of thermal auto-ignition in high-speed droplet-laden reacting mixing layers by means of the hybrid Eulerian-Lagrangian approach. The convective flux terms of the conservative equations of the gas-phase are discretized by an adaptive central-upwind WENO scheme and a sixth-order compact scheme is used for the viscous terms. Effects of initial droplet diameters and spray equivalence ratios are considered. The droplet dispersion associated with the entrainment of large eddies plays an important role in the thermal auto-ignition of fuel sprays. Ignition occurs at the hot boundary of the mixing layers, which is where preferential segregating droplets are evaporated to form fuel vapors for local chemical reactions. Droplets with a medium initial size discussed in this study have the shortest ignition delay time due to the combined effects of droplet dispersion and vaporization, while small droplets closely follow the rotation of the large eddy and cannot traverse into the hot boundary for evaporation to form reactive mixtures. The flame structure, which develops from the ignition kernel, is found to depend on the droplet size; large-sized droplets display a non-premixed flame, and small-sized droplets display a premixed flame. The droplet size also influences the values of the most reactive mixture fraction. A high spray equivalence ratio enhances scalar dissipation and evaporative cooling.

1. Introduction

Spray combustion of liquid fuel in a gaseous oxidizer is ubiquitous in a variety of engineering applications, such as propulsion devices and energy conversion systems. The flow is turbulent in a large number of situations, and combustion of liquid fuel in the background turbulent flow reveals a complex physical process, including evaporation of spray droplets, flame structures and droplet-turbulence-flame interactions. A comprehensive illustration of spray combustion helps to develop a range of combustion devices and is critical to improving fuel efficiency. Recently, the investigation of high-speed propulsion systems has faced difficulties due to the high flow velocity in the combustor chamber, which limits the residence time available for the mixing of fuel and oxygen as well as the chemical reaction, even if high intensity turbulence contributes to the mixing process. Combustion stabilization in such technological applications potentially relies on the thermal ignition of the fuel-air mixture. Therefore, ensuring stable combustion requires an understanding of the thermal ignition dynamics of high-speed fuel spray combustion.

Ignition is important for the study of liquid-fuel spray combustion. The mechanisms of ignition have been widely investigated, including chemical kinetics [1] and turbulent combustion [2]. Compared with the state-of-the-art knowledge available regarding the ignition of non-premixed gaseous mixtures, investigations of two-phase flow ignition are scarce. Therefore, the dynamics of the ignition of dispersed fuel sprays are not thoroughly understood

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Nomenclature

B_M	mass transfer number (–)
c_L	specific heat of liquid fuel (J kg^{-1} K^{-1})
c_p	specific heat of mixture gas (J kg^{-1} K^{-1})
d_d	droplet diameter (m)
D_k	diffusion coefficient of kth species (m^2 s^{-1})
Da_v	Damköhler number (–)
e_t	specific total energy (J kg^{-1})
h	specific enthalpy (J kg^{-1})
L_k	Knudsen layer thickness (m)
L_V	latent heat of droplet evaporation (J kg^{-1})
m	mass (kg)
M_c	convective Mach number (–)
Nu	Nusselt number (–)
N_c	Number of droplets in one computation cell
P	pressure (Pa)
Pr	Prandtl number (–)
q	heat flux (J m^{-2} s^{-1})
R	universal gas constant (J K^{-1} mol^{-1})
Re_d	droplet Reynolds number (–)
S_i	source term
Sc	Schmit number (–)
Sh	Sherwood number (–)
St	Stokes number (–)
T	temperature (K)
$T_{B,L}$	liquid boiling temperature (K)
t_a	droplet acceleration time (s)
t_c	chemical reaction time (s)
t_v	droplet vaporization time (s)
u	velocity (m/s)
W	molecular weight of mixture gas (kg/mol)
Y_k	mass fraction of kth species (–)
Z	mixture fraction (–)
δ	mixing layer thickness (m)
λ	thermal conductivity (W m^{-1} K^{-1})
μ	dynamic viscosity (Pa s)
ρ	density (kg m^{-3})
Φ	equivalence ratio (–)
χ	scalar dissipation rate (s^{-1})

[2–4]. Experimental measurements could be helpful, but they often only offer partial information. Hence, the processes of atomization, vaporization, ignition and stable combustion of liquid fuel have been the focus of many numerical modeling efforts since they are fundamental in plenty of applications [5–9]. Direct numerical simulation (DNS) and large eddy simulation (LES) of multiphase combustion [10–19] are necessary approaches that offer essential information by resolving the full set of partial differential equations describing the physics of the problem with and without sub-grid-scale turbulence models. However, these numerical methods are hindered by many complicating factors because many complex phenomena in multi-physics processes contain a series of disparate temporal and spatial scales that are associated with the chemistry and multiphase nature of the turbulent flow in most applications.

For spray combustion, liquid fuel is usually injected at a high speed and breaks up to form small droplets. The surrounding gas or co-flow with high temperature heats the liquid fuel. Droplet dispersion induced by local turbulent motion could enhance the heat transfer between the liquid and gas phases. Ignition occurs when the mixing process between the fuel vapor and oxidizer reaches the molecular level in mixing layers. Because the fuel-injection velocities in most applications are larger than the burning velocity of premixed mixture, combustion stabilization pertains to the auto-ignition of the fuel-oxygen mixture. Therefore, stable combustion is controlled by the complicated interactions between turbulent transport, droplet dispersion and vaporization as well as chemical reaction. Early investigations focused on gas-phase fueled flows [20,21] and concluded that ignition is most likely to occur where the local mixture fraction is near the most reactive mixture fraction and the local scalar dissipation rate is quite low. Wang and Rutland [14,22] found that auto-ignition is delayed with an increasing initial global equivalence ratio as well as that ignition kernels always localize at a condition of lean mixture, low scalar dissipation rate, and low vorticity magnitude. Schroll et al. [23] demonstrated that the highest reaction rates occur at the locations where the mixture fraction is close to the most reactive mixture fraction and is independent of the droplet size. Borghesi et al. [24] observed that turbulence accelerates ignition because it promotes fuel-air mixing, which eventually results in lower values of scalar dissipation. Martínez-Ruiz et al. [25] investigated the spray ignition characteristics in laminar mixing layers and found that two different ignition modes, a thermal-runaway mode and gradual ignition mode, are encountered according to the thermochemical properties of the fuel. However, the above studies are limited to subsonic flows. The thermal ignition and dynamics of spray flames in spatially developing supersonic flows have yet to be analyzed.

Thermal ignition is very sensitive to the boundary conditions, and could be facilitated by the increment of temperature. Hence, in the current research, the turbulent mixing layer, which separates hot and cold streams, is applied as the flow configuration, and thermal ignition could occur at the edge of hot boundary formed in the shearing motions associated with the rolling-up and entrainment of large eddies. The fuel chosen is n-decane ($C_{10}H_{22}$) because it has low volatility, which facilitates ignition analysis compared to more volatile fuels.

We examine the roles of droplet dispersion, evaporation and turbulence mixing during the thermal auto-ignition. These parameters applied in the present study are correlated with the establishment of ignition kernels. In addition, the initial droplet size and spray equivalence ratio are varied to scrutinize the effects of evaporative cooling and scalar mixing on ignition.

A hybrid Eulerian-Lagrangian formulation, which has been previously utilized for studying the spray combustion problems [26,27], will be applied to describe the supersonic droplet-laden shear flows. The conservation equations of the gas-phase, which include source terms modeling the counter-acting force as well as heating and vaporization from droplets, combine a one-step Arrhenius reaction model that is applied for the chemical reaction. Lagrangian droplets are tracked as sub-grid point sources, and contributions of the mass, momentum and energy from the droplet-phase are introduced as source terms into the Eulerian gas-phase.

The present paper is organized as follows. The mathematical equations are first presented in Section 2. The numerical procedure and the computational details are described in Section 3. In Section 4, the interactions among vortex motion, droplet evaporation and thermal ignition are examined in detail. The initial droplet size and spray equivalence ratio are changed to investigate the