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Direct numerical simulation on supersonic turbulent reacting and non-reacting spray jet in heated coflow

Tai Jin, Kun Luo *, Qi Dai, Jianren Fan

State Key Laboratory of Clean Energy Utilization, Zhejiang University, Hangzhou 310027, PR China

HIGHLIGHTS

- 3D direct numerical simulation of a supersonic spray jet flame is conducted.
- The gas-droplet flow is captured with the hybrid Eulerian–Lagrangian approach.
- Comparative study of the non-reacting and reacting case has been conducted.
- Contributions of premixed flame occupy more than 50% downstream of the flame.
- The conditional scalar dissipation rate increases due to combustion.

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ABSTRACT

Comparative studies of three-dimensional spatially-developing supersonic turbulent spray reactive and non-reactive flows have been conducted by direct numerical simulations. The gas-droplet flow system has been captured with the hybrid Eulerian–Lagrangian approach. High-resolution bandwidth-optimized weighted essentially non-oscillatory (WENO) scheme of spatial discretization and total variation diminishing Runge–Kutta temporal integration are used to capture the compressible turbulent flow. The flow motions of droplets are tracked in the Lagrangian frame. Arrhenius-type finite-rate chemistry is employed for the chemical reaction. The decay of the mean axial velocity at the centerline has been found much slower for the reacting case. The half-width of the spreading reacting jet is larger than the non-reacting case. The velocity of droplet has been found to be increased compared with the droplet at the same position in non-reacting flow. Heat release mainly occurs in the subsonic region. Premixed and diffusion modes are found to coexist in the present flame. Heat release contributed by premixed flame to the total heat release occupies more than 50% and peaks at 71.4% downstream of the flame. Combustion also affects the turbulent intensity of the flow field. Reynolds stress has been found to be slightly larger in the mixing layer with intense heat release. The fluctuation of temperature, mixture fraction has been found to be amplified significantly in the reacting flow.

1. Introduction

Potential requirements for hypersonic transport vehicle at high Mach speeds both in defense and civil aviation areas have greatly motivated research efforts toward supersonic combustion ramjet engine. Liquid hydrocarbon fuels are promising for this kind of engines since it has high heat release per unit mass, high energy density per unit volume, safe and easy for long term storage [1]. In such engines, liquid fuel is injected into the combustion chamber as a thin column or sheet, which disintegrates to form a large number of liquid droplets. These droplets disperse and evaporate under the influence of the surrounding gas-phase flow, and subsequently mix and react with an oxider. Accurate prediction of the droplet dispersion and evaporation in turbulent flows are of crucial importance in the simulation of those reacting sprays since they are considered a rate limiting process [2]. In particular, spray combustion is a complex phenomenon in which the dispersion of the liquid fuel droplets, their evaporation, and the chemical reacting of the fuel vapor with the oxidizer take place simultaneously and interactively. The description of the physical phenomena involved has motivated numerous experimental and numerical studies, however, the underlying physics governing these processes have not been well understood [3].

Extensive experimental researches on laminar and turbulent spray flames with various fuels have been conducted in simple

* Corresponding author. Tel./fax: +86 571 87951764.
E-mail address: zjulk@zju.edu.cn (K. Luo).

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Nomenclature

ρ	density (kg/m^3)	R_u	universe gas constant (J/mol/K)
u_i	velocity in the i direction (m/s)	$\dot{Q}$	the external heat source
Y_k	mass fraction of species k	S_i	source term
$V_{k,i}$	the i component of the diffusion velocity of species k (m/s)	m_d	droplet mass (kg)
		D	jet core diameter (m)
$\dot{\omega}_k$	mass production reaction rate (kg/m^3/s)	B_M	mass transfer number
W	the mixture molecular weight (kg/mol)	C_p	specific heat of mixture gas (J kg^{-1} K^{-1})
σ_{ij}	stress tensor (kg/m/s^2)	$T_{B,L}$	liquid boiling temperature
$f_{k,j}$	the body force (m/s^2)	X_s	Vapor molar fraction
T	temperature (K)	ξ	mixture fraction
P	pressure (Pa)	FI	Flame index
e_t	specific total energy (J/kg)	Lv	latent heat of droplet evaporation (J kg^{-1})
q_i	the heat flux (J/m^2/s)	χ	scalar dissipation rate (1/s)

and complex geometrical configurations, which has greatly promoted understanding of the fundamental physics. However, the concurrent processes of liquid phase dynamics and evaporation, turbulence, as well as combustion strongly interact with each other, which makes experimental measurement very challenging and much more difficult for supersonic spray combustion. The development of computational tools able to describe accurately such flows can provide useful insight into the effect of the control parameters on the flame topology, species mass fractions and velocity fields and aid the design of efficient and low-emission combustors. Various numerical methods, such as Reynolds-averaged Navier–Stokes simulations (RANS), large-eddy simulations (LES) or hybrid LES/RANS, involved with different closure models dealing with turbulence, turbulence/chemistry interactions and mixing have been developed and applied to study supersonic combustion. However, numerical studies of fluid flows based on the conventional RANS modelling approach could lead to poor predictions of highly unsteady and complex turbulent combustion phenomena due to the intrinsic time- or ensemble-averaging of the governing equations. LES can partly overcome this problem, where the major part of the turbulent motion can be resolved. However, the subgrid variances need to be closed with models which are still under development for supersonic spray combustion. The most accurate and straightforward numerical approach to turbulent combustion problems in the continuum limit is called direct numerical simulation (DNS), where the Navier–Stokes equations are directly solved without averaging or approximation, and all the relevant time and length scales are resolved. Thus, the computed flow field obtained is equivalent to a single realization of a flow or a short-duration laboratory experiment [4].

DNS has been proven as a powerful tool for exploring fundamentals of single-phase turbulent combustion and recently extended to spray combustion. Nakamura et al. [5] conducted two-dimensional direct numerical simulation of spray flames stabilized in a laminar counterflow. Two types of spray combustion have been found in front of and inside the high gaseous temperature region, e.g. premixed-like and diffusion-like combustion. Fujita et al. [6] investigate the effects of equivalence ratio, fuel droplet size, and radiation on jet spray flame through two-dimensional direct numerical simulation, and validated an extended flamelet/progress-variable approach. Wacks et al. [7] conducted detailed parametric analysis of premixed flame propagation in n-decane droplet-laden mixtures through DNS and found that the reaction takes place predominantly under fuel-lean conditions. Luo et al. [8] carried out DNS of three dimensional n-heptane spray flames in a swirl combustor. Note that DNS of turbulent spray combustion at moderate Reynolds numbers are feasible with the present computer power [9], however, these studies are still limited to low speed flow and DNS of supersonic spray combustion has not been reported so far.

In the present study, DNS method has been extended to investigate the three-dimensional spatially-developing supersonic turbulent spray jet flame, as well as the non-reacting case for comparisons. The gas-droplet flow system has been captured with the hybrid Eulerian–Lagrangian approach. Droplets have been treated as sub-grid point sources, which are tracked in the Lagrangian sense, while the gaseous phase is dealt within the Eulerian framwork. Contributions to mass, momentum and energy from the evaporating droplets are introduced as source terms into the Eulerian phase. The fuel is considered to be n-decane ($C_{10}H_{22}$), due to its low evaporation rate, enables easier analysis of flame-droplet interaction compared to more volatile fuels. Arrhenius-type one-step finite-rate chemical reaction is employed. The mathematical formulations are first described in Section 2, followed by the numerical methods and computational details in Section 3. In Section 4, detailed comparisons of the non-reacting and reacting case have been conducted to investigate the interactions among turbulence, combustion and evaporation. Effects of combustion on the flow field, turbulent fluctuations, scalar dissipation rate, as well as the droplet dispersion are investigated. Finally, conclusions are made.

2. Mathematical formulation

An Eulerian–Lagrangian framework for dispersed multiphase flows is adopted. The governing equations for continuous gas-phase include the continuity equation, the three dimensional Navier–Stokes equations, the transport equations of chemical species and the total energy, as well as the equation of state, which can be formulated as:

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho u_i)}{\partial x_i}=S_m, \tag{1}$$

$$\frac{\partial(\rho Y_k)}{\partial t}+\frac{\partial}{\partial x_i}(\rho Y_k u_i)=-\frac{\partial}{\partial x_i}(\rho Y_k V_{k,i})+\dot{\omega}_k+S_{Y_k}, \tag{2}$$

$$\frac{\partial(\rho u_j)}{\partial t}+\frac{\partial}{\partial x_i}(\rho u_i u_j)=\frac{\partial \sigma_{ij}}{\partial x_j}+\rho\sum_{k=1}^{N}Y_k f_{k,j}+S_{ui}, \tag{3}$$

$$\frac{\partial}{\partial t}(\rho e_t)+\frac{\partial}{\partial x_i}(\rho u_i e_t)=-\frac{\partial q_i}{\partial x_i}+\dot{Q}+\frac{\partial \sigma_{ij}u_i}{\partial x_j}+\rho\sum_{k=1}^{N}Y_k f_{k,i}(u_i+V_{k,i})+S_e, \tag{4}$$