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Numerical analysis of gaseous hydrogen/liquid oxygen flamelet at supercritical pressures

Taehoon Kim [a], *Yongmo Kim* [a,*], *Seong-Ku Kim* [b]

[a] *Department of Mechanical Engineering, Hanyang University, 17, Haengdang-Dong, Sungdong-Ku, Seoul 133-791, Republic of Korea*
[b] *Space Propulsion Division, Korea Aerospace Research Institute, Daejeon 305-333, Republic of Korea*

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ABSTRACT

Supercritical conditions are typically encountered in high-pressure combustion devices such as liquid propellant rockets and gas turbine engines. Significant real fluid behaviors including steep property variations occur when the fluid mixtures pass through the thermodynamic transcritical regime. The laminar flamelet concept is a robust and reliable approach that correctly accounts for real fluid effects, the large variation in thermophysical properties, and the detailed chemical kinetics for turbulent flames at transcritical and supercritical conditions. In the present study, the flamelet equations in the mixture fraction space are extended to treat the flame field of general fluids over transcritical and supercritical states. Flamelet computations are carried out for gaseous hydrogen and cryogenic liquid oxygen flames under a wide range of thermodynamic conditions. Based on numerical results, the detailed discussions are made for the effects of real fluid, pressure, and differential diffusion on the local flame structure and the characteristics encountered in liquid propellant rocket engines.

1. Introduction

Because of its high specific impulse and clean combustion, hydrogen has been widely utilized as a propellant in liquid rocket engines. The liquid rocket engines are characterized by high chamber pressure which results in the improved engine performance, and increased nozzle expansion ratio. Moreover, since the nozzle expansion ratio at the flow separation under main stage operation is increased by elevating the chamber pressure, the design limitations associated with flow separation can be considerably relaxed [1,2].

As provided in Table 1, most of the recently developed hydrogen fueled rocket engines are operated at supercritical pressures much higher than the critical pressures of oxygen (50.4 bar) and hydrogen (13 bar). Hydrogen fueled rocket engines have generally adopted a simple type of coaxial shear injectors because of fast conversion rate from chemical to thermal energy of hydrogen/oxygen mixture. Prior to injection into the combustion chamber, liquid hydrogen is fed to regeneratively cooling channels of the chamber and heated by absorbing high heat flux through the chamber wall from high-temperature combustion gas. Therefore, hydrogen is injected at a high velocity of hundreds meter per second in a gaseous state around at 300 K through outer annulus while oxygen is discharged at a low velocity of a few meter per second from central passage in a cryogenic liquid state less than its critical temperature.

In case of the cryogenic liquid propellants such as LOx (liquid oxygen), the injection condition that the pressure exceeds critical pressure but the injection temperature is

* *Corresponding author*. Tel.: +82 2 2220 0428; fax: +82 2 2297 3432.
E-mail address: ymkim@hanyang.ac.kr (Y. Kim).
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Nomenclature

Roman symbols

a, b	parameters of SRK EOS
c_p, $c_{p,k}$	constant pressure specific heat of mixture and species k
D_i	mass diffusion coefficient of species i
h, h_k	enthalpies of mixture and species k
Le_i	Lewis number of species i
p	Pressure
p_c	critical pressure
X	mole fraction
q_{rad}	radiative heat loss
R_u	universal gas constant
t	time
T	temperature
T_c	critical temperature
Z	mixture fraction
W	molecular weight
Y	mass fraction

Greek symbols

χ	scalar dissipation rate
α	third parameter of SRK EOS
$\overline{\kappa}_{ij}$	binary interaction coefficient
λ	thermal conductivity
ρ	density
$\dot{\omega}_k$	chemical reaction rate of species k
ω_i	acentric factor

Subscripts

i, j, k	species index
st	stoichiometry

below critical temperature, is specifically designated as transcritical [3]. After the injected LOx at transcritical state is abruptly heated via intense mixing with the ambient hot combustion products, it eventually reaches the supercritical fluid state. In the supercritical fluids, the liquid and gas are indistinguishable in terms of the thermodynamic and transport properties. In the transcritical state, the surface tension nearly vanishes, and the solubility is close to that of a gas, while the density and thermal diffusivity are comparable to that of a liquid. These real fluid properties are characterized according to their liquid-like densities, gas-like diffusivities, and pressure-dependent solubilities. Near the critical conditions, the surface tension and heat of vaporization approach zero, and the constant-pressure specific heat increases substantially. A sequence of recent experiments [4,5] has shown that cryogenic liquid sprays injected at supercritical conditions have no clear inter-phase boundary. Thus, liquid atomization, droplet breakup, droplet-turbulence interaction, and vaporization of the existing spray combustion processes no longer occur at supercritical conditions. Additionally, the supercritical combustion of cryogenic liquid propellants is dominantly controlled by turbulent diffusion and is characterized by extremely high density gradients, thermodynamic non-ideality and anomalies in the transport properties.

According to these experimental evidences, the recent supercritical combustion models for the cryogenic liquid propellants are conceptually based on a single-phase mixture model of general fluids accounting for thermodynamic non-ideality and anomalies of transport properties [3–9]. Recently, Ribert et al. [6] suggested a comprehensive model for studying laminar counterflow diffusion flames for general fluids in subcritical, transcritical, and supercritical states. Their model incorporates a unified treatment of fundamental thermodynamic and transport theories into the one-dimensional counterflow flame solver to treat detailed chemical kinetic mechanisms and multispecies transport [10]. They numerically analyzed the effects of pressure and strain rates on the local structures of the turbulent non-premixed flames in all thermodynamic states. By utilizing the library pre-constructed through the counterflow diffusion flame model, a large eddy simulation for turbulent combustion of liquid oxygen and gaseous methane in the vicinity of a splitter pate under supercritical conditions has been carried out [3].

The modeling concept based on laminar flamelets has been widely applied to practical applications such as turbulent jet flames [11–13], direct injection diesel engines [14], and rocket injectors [7,9]. The main idea of flamelet models is to view the local flame structures of turbulent flames as ensembles of laminar flamelets which are stretched and wrinkled by turbulent flows [15]. In the context of the laminar flamelet model, the effects of turbulence on the flamelets are mapped only on the scalar dissipation rate which governs the characteristic diffusion time within flamelets. In terms of the flamelet equations, there are two different approaches: the one-dimensional counterflow diffusion flame model [6,10] in the spatial domain and the direct flamelet equation model [15] in the mixture fraction domain. The direct flamelet equations in mixture fraction space are derived by asymptotic analysis of the species and energy transport equations transformed into coordinates attached to an iso-surface of the mixture fraction [15]. The counterflow diffusion flame model which allows direct comparison of experimental measurements has

Table 1 – Representative engines of LH_2/LOx propellant rockets [1].

Engine	SLV (stage)	Chamber pressure[a]	Engine cycle	Country
RD-0120	Energia (core)	21.8	SC[b]	Russia
SSME	Space Shuttle (main)	18.9	SC	USA
LE-7	H-II (first)	12.7	SC	Japan
Vulcain 2	Ariane-V (core)	11.5	GG[c]	France
RS-68	Delta IV (booster)	10.1	GG	USA
Vinci	Ariane-V (upper)[d]	6.0	Expander	France/Germany

a Unit: MPa.
b Staged combustion.
c Gas-generator.
d Planned.