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A non-premixed combustion model based on flame structure analysis at supercritical pressures

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ABSTRACT

This work presents a study of non-premixed flames at supercritical-pressure conditions. Emphasis is placed on flame stability in liquid rocket engines fueled with liquid oxygen and gaseous hydrogen. The flame structure sensitivity to strain, pressure, temperature and real-fluid effects was investigated in detailed opposed-jet flames calculations. It is shown that the flame is very robust to strain, that the flamelet assumption is valid for the conditions of interest, and that real-fluid phenomena can have a significant impact on flame topology. At high-pressure supercritical conditions, small pressure or temperature variations can induce strong changes of thermodynamic properties across the flame. A substantial finding was also that the presence of water from combustion significantly increases the critical pressure of the mixture, but this does not lead to a saturated state where two-phase flow may be observed. The present study then shows that a single-phase real-fluid approach is relevant for supercritical hydrogen–oxygen combustion. Resultant observations are used to develop a *flamelet* model framework that combines detailed real-fluid thermodynamics with a tabulated chemistry approach. The governing equation for energy contains a compressible source term that models the flame. Through this approach, the solver is capable of capturing compressibility and strain-rate effects. Good agreements have been obtained with respect to detailed computations. Heat release sensitivity to strain and pressure variations is also recovered. Consequently, this approach can be used to study combustion stability in actual burners. The approach preserves the density gradient in the high-shear region between the liquid-oxygen jet and product rich flame region. The latter is a key requirement to properly simulate dense-fluid jet destabilization and mixing in practical devices.

1. Introduction

Practical devices such as gas turbines, diesel engines and rockets operate at elevated pressures that approach and/or exceed the thermodynamic critical point of the propellants. Under these conditions, injected liquid jets undergo a transcritical change of state as fluid temperatures rise above the critical temperature of the local mixture. For this situation, diminished inter-molecular forces promote diffusion dominated mixing processes prior to atomization and injected jets vaporize in the presence of exceedingly large thermophysical gradients. Well-mixed diffusion flames evolve as a consequence and intense property gradients approach the behavior of a contact discontinuity. Significant real-gas effects and transport anomalies coexist locally in colder regions of the flow, with ideal gas and transport processes occurring within the flame zone [1]. The focus for the present work is development of a combustion model for use with the Large Eddy Simulation (LES) technique [2–7]. This method is very promising to study flame stability, combustion – acoustic coupling, and emissions in actual devices (complex geometry), with detailed thermodynamics and transport.

The goal of this work is to facilitate studies of flame stability in rocket engines fueled with liquid propellants (oxygen and hydrogen) at high pressure. In this type of application, propellants are injected separately and flames are located within the mixing regions. For the present study, an average chamber pressure of 70 bar has been selected, which is above the critical pressures of both reactants ($P^c_{O_2} = 50.4$ bar and $P^c_{H_2} = 12.9$ bar [8]). In addition to a predictive combustion model, sophisticated models to deal with thermodynamics and transport are required and must be an integral part of the model formulation. The ultimate objective of this work is to develop a combustion model able to capture all processes involved.

Previous experimental and numerical studies reveal that the *flamelet* approach is relevant to simulate the flame-turbulence interaction in rocket engines. Experimental investigations carried out at supercritical pressure (with respect to oxygen), in rocket-like test rigs that use coaxial injectors [9–16], have shown that the flame stabilizes directly at the injector post in the mixing layer

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Nomenclature

Abbreviations

GH_2	gaseous hydrogen
Lox	liquid oxygen
st	stoichiometric condition
BC	boundary condition
DNS	direct numerical simulation
LES	large Eddy simulation
LIF	laser induced fluorescence

Symbols

χ	scalar dissipation rate
δ_{flm}	flame thickness
$\dot{\omega}_i$	molar production rate of the species i
$\dot{\omega}_T$	chemical heat release
$\dot{Q}_s$	chemical heat release per unit flame surface area
γ	heat capacity ratio
λ	thermal conductivity
μ	dynamic viscosity
ν	molecular viscosity
ρ	density
τ_c	chemical timescale
τ_χ	diffusion timescale
τ_κ	Kolomogorov timescale
$\tau_{acoustic}$	acoustic timescale
τ	viscous stress tensor
a	strain rate
C_v	heat capacity at constant volume
C_{p_i}	heat capacity at constant pressure of the i^{th} species
D_a	Damköhler number
D_i	diffusion coefficient of the i^{th} species
D_{th}	thermal diffusion coefficient
E	total non-chemical energy
e_s	sensible energy
H	distance between the opposed-jet exits
h_i	sensible enthalpy of the ith species
h_t	enthalpy of the mixture
$h^\circ_{f_i}$	heat of formation of the ith species
Le_i	Lewis number of the ith species
M	Mach number
N	number of species in the mixture
P	pressure
P^c	critical pressure
P^r	reduced temperature
R	ideal gas constant
Re	Reynolds number
T	temperature
t	time
T^c	critical temperature
T^r	reduced temperature
V	molar volume
V_{corr}	velocity correction from the Hirschfelder and Curtiss approximation [28]
W_i	molar mass of the ith species
x,y,z	spatial coordinates
X_i	molar fraction of the ith species
Y_i	mass fraction of the ith species
Z	mixture fraction
Z_H	mixture fraction based on the H element
Zc	compressibility factor
$\mathbf{I}$	identity matrix
$\mathbf{q}_i$	diffusion flux of the ith species
$\mathbf{u}$	velocity vector

Sub-and super-scripts

$\circ$	reference state
ad	adiabatic
F	conditions at the fuel boundary
H_2	conditions at the H_2 boundary
inj	injection conditions
model	output from the combustion model
O	conditions at the oxidizer boundary
O_2	conditions at the O_2 boundary
ref	reference quantity
table	output from the look-up table

between the fuel and the oxidizer streams. This indicates that combustion occurs in a pure non-premixed mode. Singla et al. [16] used Laser Induced Fluorescence (LIF) of the *OH* radical to study the flame structure close to the injector post tip. In this region, the flame is very thin and does not exhibit local extinction. Further downstream, the flame forms close to the oxygen stream and its thickness varies depending on the local strain rate.

The inner structure of $Lox - H_2$ flames has been studied numerically by Ribert et al. [17] and Juniper et al. [18]. Laminar counterflow flames were used to investigate pressure and strain rates effects. It was shown that the flame is very robust to strain over a large range of sub- and super-critical pressures. In addition, Ivancic and Mayer have investigated timescales based on experimental and numerical works [19]. They found that the Kolomogorov timescale has a magnitude of $\tau_\kappa \approx 1$ μs. The characteristic timescale of chemistry can be approximate by: $\tau_c \approx (\rho Y_i)/(W_i \dot{\omega}_i)$, where i is the index of the least reactive species in the flame and $\dot{\omega}_i$ its molar production rate. A chemical analysis of $H_2 - O_2$ combustion at elevated pressure shows that $\tau_c \approx 0.01$ μs. This comparison shows that the Damköhler number $D_a = \tau_\kappa/\tau_c \gg 1$, which implies that the flame is thin and robust and can be viewed locally as a laminar reacting layer insensitive to unsteady effects (i.e. the *flamelet* approximation is valid).

To date, the *flamelet* approach was successfully used by Zong et al. [20] for gaseous-methane/liquid-oxygen combustion in the context of LES at rocket conditions. Schmitt et al. [21] employed a *presumed PDF approach* coupled with a *flamelet* tabulation to represent a methane–Lox flame at elevated pressure in an experimental rocket engine. LES results were in good agreement with experimental observations. A similar method was used by Matsuyama et al. [22,23] to model the flame in a $Lox - GH_2$ rocket engine, and good agreements with experimental shadowgraphs were obtained. In the RANS framework, several numerical studies employed *Flamelet* models for high pressure combustion, with relative success [24,25]. However, in all these investigations, the impact of high-pressure non-linear effects on the *flamelet* approach is never discussed. In particular, the question of how the look-up table is generated must be clarified for supercritical combustion. Given these limitations, the objectives of the present study are:

- Study the flame structure of hydrogen–oxygen diffusion flames at the conditions typically observed in rocket engines, to determine the relevant modeling parameters.
- Investigate the impact of high-pressure phenomena on the modeling approach.
- Develop a *flamelet* model that accounts for these phenomena and test its performance.

To achieve these objectives, we present the theoretical and numerical framework in Section 2 followed by analysis of the flame