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On large eddy simulation of blended CH_4–H_2 swirling inverse diffusion flames: The impact of hydrogen concentration on thermal and emission characteristics

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ABSTRACT

Large eddy simulation (LES) is applied to investigate blended CH_4–H_2 swirling inverse diffusion flames. In this regard, two different compositions of fuel stream including 30% and 80% molar fraction of hydrogen are utilized. Two distinct swirl numbers of 0.667 and 1.33 are applied to the central air stream. The considered configuration for studying swirling inverse flames is extracted from the well-known DLR (Deutsches Zentrum Luft- und Raumfahrt) burner with modifications to allow investigating inverse flames. The DLR-A benchmark is regarded as a reference to contrast Large Eddy Simulation (LES) and Unsteady Reynolds Averaged Simulation (URAS) predictions. It is found that LES results outperform URAS computations in a sufficiently fine grid. Investigating blended CH_4/H_2 inverse flames revealed that the jet penetration length is reduced by an augmentation in hydrogen concentration. This is ascribed to the increased mixing with hydrogen enrichment which leads to decreased flame length as well. It is found that with curtailed concentration of hydrogen, the major axis of vortical structures is aligned with the flow direction. In the other words, the eddies are flattened and the lateral size of mixing region is reduced. The consequence is an enhancement in flame length. A noticeable decrease in the mass fraction of carbon monoxide pollutant is observed with hydrogen enrichment. Reduction in inflow carbon atoms and rapid CO oxidation owing to excessive air in the mid- and far-field regions are authorized as the contributing factors. The lowered peak temperature in presence of enhanced hydrogen concentration is attributed to the related reduction in thermal power.

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Nomenclature

χ	scalar dissipation rate
$\tilde{f}$	Favre filtered mixture fraction
σ	laminar Schmidt number
C_s	Smagorinsky constant
$\widetilde{f''^2}$	Favre filtered mixture fraction subgrid variance
χ_q	scalar dissipation rate of quenching
$<u'v'>$	shear stress component
R	characteristic length
G_x	axial flux of the axial momentum
MR	momentum ratio
U	axial velocity
X	molar fraction
$\bar{\rho}$	filtered density
ν	viscosity
σ_t	turbulent Schmidt number
$\dot{\omega}_k$	chemical source term
Δ	local filter width
X	molar fraction
S	swirl number
G_ϕ	axial flux of the angular momentum
ϕ	equivalence ratio
τ_{kk}^{sgs}	trace of the subgrid stress tensor
W	circumferential velocity
x	distance from the injection plane

Introduction

Large eddy simulation (LES) techniques are widely regarded as a viable replacement for Reynolds-averaged simulation (RAS) approaches to compute the non-reactive turbulent flows far from rigid boundaries. The situation is less pronounced for reactive flows in the presence of chemical reactions and heat release occurring in the unresolved (fine) scales. Besides, LES and RAS methods mostly incur comparable challenges in the context of including thermochemistry terms. Therefore, many LES techniques for reacting flows are derived from the already established theories. A review of the pioneering contributions is performed by Vervish and Poinsot [1].

In LES, a spatial filtering is exerted to the governing equations for the purpose of filtering out the sub-grid scale (SGS) motions from the large-scale counterparts. The large-scale motions which pass the greatest amounts of the kinetic energy are resolved explicitly; whereas the fine (unresolved) scales are modeled. The chemical reactions take place after molecular mixing of reactants. Hence, combustion occurs mostly in the subgrid scales [2]. As such, combustion models are postulated so as to predict accurately the chemical behavior of turbulent reacting flows. To distinguish between large scales of motion and small ones, some kind of averaging must be done. In LES, this operator is a filter which is a locally derived weighted average of flow properties over a volume of fluid, instead of ensemble kind in RAS [3].

Most of the sub-grid scale models have many parallels with their RAS counterparts. The majority of LES studies have employed eddy viscosity sub-grid scale which was first proposed by Smagorinsky [4] and developed further by Lilly [5] and Deardorf [6]. Smagorinsky model assumes that small scales are in equilibrium and dissipate instantly all the energy received from the resolved scales. The advantage of the Smagorinsky model is probably dissipating energy at virtually right overall rate which stabilizes the simulation process [7]. Variant LES combustion models have been proposed and investigated for the non-premixed mode. These models principally feature steady and unsteady flamelets [8,9], Flamelet/progress variable [10], transported filtered density functions [11] and partially stirred reactor [12] approaches. Among these models, one of the currently employed tabulation techniques is the laminar flamelet model proposed by Peters [13]. This model assumes a short chemical time-scale such that reactions take place at a thin layer around the stoichiometric mixture. The steady flamelet model further considers that the reacting structure is in steady situation. This model has been successfully applied to swirl-induced non-premixed flames [14].

Latterly, employing blended hydrocarbon-H_2 fuels has been emerged as a viable procedure to diminish emission level while improving combustor performance [15]. Burning of hydrogen does not leave CO, CO_2 and unburned hydrocarbon (UHC) pollutants. Nevertheless, safety issues have restricted the utilization of hydrogen as a single fuel. The mixture of hydrogen-hydrocarbon is considered as an alternative solution with improved performance, emission levels and fuel economy [16]. Extensive experimental researches have been implemented on effective characteristics of hydrocarbon-hydrogen flames including reactants temperature, hydrogen content and flame stabilization and orientation in the presence of swirl [17]. Tabet et al. [18] reported an increased mixing with hydrogen addition in non-premixed flames of methane/hydrogen. Furthermore, they predicted enhanced NO level with hydrogen addition. Mishra and Kumar [19] studied laminar LPG-H_2 diffusion flames and with preheated reactants and observed a reduction in flame length with H_2 addition. This was attributed to an increased gas temperature. Moreover, an augmentation in soot free length fraction was observed with hydrogen addition to the fuel stream. Kim et al. [20] investigated the characteristics of hydrogen enriched methane flames at constant heat load with varying swirl intensities. They indicated that the lean stability limit is extended in presence of further hydrogen. They reported reduced stability limit at higher swirl number to the fuel-air mixture operating at decreased adiabatic flame temperatures. Moreover, they found that the higher combustibility of hydrogen provides faster chemical reaction, higher temperature and reduced recirculation in the reaction zone [21]. Mira Martinez et al. [22] employed the Large Eddy Simulation (LES) technique to reproduce the flame shape of hydrogen-enriched reacting jets. Their findings indicated that the gradient diffusion model is not trustworthy as a sub-grid scale model for LES computations of mixtures featuring hydrogen. Kashir et al. [23] investigated the impact of swirl intensity on characteristics of blended methane-hydrogen bluff-body stabilized swirl diffusion flames. They predicted flame length reduction with H_2 addition to the fuel stream. However, this reduction rate was inversely related to the swirl number. They reported

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