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Effect of fuel composition and differential diffusion on flame stabilization in reacting syngas jets in turbulent cross-flow

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ABSTRACT

Three-dimensional direct numerical simulation results of a transverse syngas fuel jet in turbulent cross-flow of air are analyzed to study the influence of varying volume fractions of CO relative to H₂ in the fuel composition on the near field flame stabilization. The mean flame stabilizes at a similar location for CO-lean and CO-rich cases despite the trend suggested by their laminar flame speed, which is higher for the CO-lean condition. To identify local mixtures having favorable mixture conditions for flame stabilization, explosive zones are defined using a chemical explosive mode timescale. The explosive zones related to flame stabilization are located in relatively low velocity regions. The explosive zones are characterized by excess hydrogen transported solely by differential diffusion, in the absence of intense turbulent mixing or scalar dissipation rate. The conditional averages show that differential diffusion is negatively correlated with turbulent mixing. Moreover, the local turbulent Reynolds number is insufficient to estimate the magnitude of the differential diffusion effect. Alternatively, the Karlovitz number provides a better indicator of the importance of differential diffusion. A comparison of the variations of differential diffusion, turbulent mixing, heat release rate and probability of encountering explosive zones demonstrates that differential diffusion predominantly plays an important role for mixture preparation and initiation of chemical reactions, closely followed by intense chemical reactions sustained by sufficient downstream turbulent mixing. The mechanism by which differential diffusion contributes to mixture preparation is investigated using the Takeno Flame Index. The mean Flame Index, based on the combined fuel species, shows that the overall extent of premixing is not intense in the upstream regions. However, the Flame Index computed based on individual contribution of H₂ or CO species reveals that hydrogen contributes significantly to premixing, particularly in explosive zones in the upstream leeward region, i.e. at the preferred flame stabilization location. Therefore, a small amount of H₂ diffuses much faster than CO, creating relatively homogeneous mixture pockets depending on the competition with turbulent mixing. These pockets, together with high H₂ reactivity, contribute to stabilizing the flame at a consistent location regardless of the CO concentration in the fuel for the present range of DNS conditions.

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1. Introduction

The integrated gasification combined cycle (IGCC) represents a potential route to a more efficient and environmental-friendly power generation of solid fuels (coal and/or bio-mass). One reason for this is that in the IGCC a synthetic gaseous fuel (syngas) derived from the solid fuel can be burned in a gas and steam turbine combined cycle, which has a higher thermal efficiency than a steam power plant operating with pulverized coal combustion (PCC). Another advantage, in the context of power generation with CO₂ capture, is that

after the water-gas shift (WGS) reaction, the high pressure and CO₂ concentration of the H₂-rich syngas fuel enables an energy-efficient CO₂ capture process. After an initial phase in which the complexity and cost of the IGCC process led to a slow and intermittent deployment of IGCC power plants, interest in the technology has been renewed recently with plants being commissioned in China, Japan and the US [1].

Several problems of practical importance must be addressed in the development of a combustion system capable of efficient, clean and safe combustion of IGCC syngas: in particular, the often varying composition of the fuel, that can contain large fractions of hydrogen, must be taken into account at the combustor design stage, especially if the system must comply with the emissions regulations for threshold levels of CO and NO_x. Some of these problems are well

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understood and utilize well-developed engineering knowledge. However, there are a number of other issues involving complex interactions between the flow field and the reaction kinetics associated with the fundamental combustion process that are far less understood [2]. More specifically, burners are often designed on the basis of complex, poorly understood balances between the flow field, the process of fuel-oxidant mixing and flame propagation. One of the most serious operability issues often preventing modern combustors from operating in a safe, efficient, and reliable manner is flashback when the flame propagates upstream of the design position, where it is supposed to stabilize, and into the premixing duct [3]. Common flashback mechanisms include propagation of the turbulent flame in the core flow of the premixer duct or in its wall boundary layers, oscillations of the flame location due to combustion instabilities or combustion induced vortex breakdown [5]. Regardless of the initiating cause of flashback, once flashback occurs the flame will ultimately reach the fuel injection nozzles. Therefore, understanding and accurate prediction of the flame stabilization mechanism in the near field of fuel jet in cross flow of oxidant are vitally important for gas turbine combustor design. More specifically to applications involving premixed combustion of hydrogen-rich syngas at gas turbine conditions (high pressure, high reactant temperature) mounting evidence indicates that boundary layer flashback constitutes a key challenge [5]. Boundary layer flashback can result in high speed upstream flame propagation, even in the presence of large flow velocities in the downstream direction for the reactants in the bulk region of the duct. This has been shown recently in both experimental and modelling studies [6–8]. Once flashback occurs, it can lead to flame anchoring in the near field of the fuel injection nozzles, rapid increase of material temperatures, with subsequent damage and failure [2]. In order to ensure intrinsic flashback safety, flame stabilization in the near field of the fuel injection nozzles needs to be understood.

A transverse jet in cross-flow (JICF) configuration is often used to achieve a high level of fuel-air mixing within a confined volume and short residence time, and hence it is used in many engineering applications including gas turbines in IGCC. However, the JICF generates a complex three-dimensional flow field involving a variety of flow structures spanning a broad range of length and time scales: shear layer vortices, wake vortices, horse-shoe vortices, and a counter-rotating vortex pair (CVP) [9]. While these flow structures are pivotal in enhancing mixing and in affecting flame stabilization characteristics, they are challenging to study and characterize due to their strong three-dimensionality. Passive scalar transport in the JICF has been studied experimentally [10] and numerically [11], and these studies have shown that scalar mixing in JICF might not be modeled through a direct analogue with the turbulent flow field. In a reacting JICF heat release due to chemical reactions coupled with organized turbulent motion influence the scalar transport in a manner different than passive scalar transport. Also, preferential diffusion of species, with mass diffusivities varying by as much as five-fold, can modify the scalar mixing characteristics [12,13]. Therefore, flame stabilization depends upon the balance of these transport phenomena.

The issue of flame anchoring and stabilization in the near field of a fuel injection nozzle in JICF was previously studied by Direct Numerical Simulations (DNS). Several parameters that influence the JICF near field flame stabilization were investigated. These parameters include fuel nozzle geometry [14,15] and injection angle with respect to the cross flow direction [16]. Previous experimental [17,18] and DNS [14,15] studies have reported that a flame stabilizes in the near-field of a JICF via partially premixed flame propagation. Indeed, the flow velocity component normal to the mean flame base, measured conditionally at the instantaneous flame base location, was reported to be strongly correlated to the laminar flame speed [17]. In light of this, the fuel composition may be expected to have a dominant influence on flame stabilization since it considerably alters the laminar flame propagation speed and flame thickness. This is particularly true of

syngas used in IGCC since its two components – hydrogen (H_2) and carbon monoxide (CO) – have widely disparate chemical and transport properties. Well resolved DNS with detailed chemical kinetics and transport properties can greatly illuminate the parametric influence of fuel composition.

The present study is a continuation of a series of numerical parametric studies [14–16] to understand key sensitivities in the JICF near field stabilization of multi-component fuel combustion. While previous studies varied fuel nozzle geometry [14,15] and transverse injection angle [16], in the present study the focus is on the effect of composition of hydrogen-rich syngas fuel on flame stabilization characteristics relevant to IGCC. Thus, the present study augments the existing parametric studies. Here, we quantify the relative importance of differential diffusion, turbulent mixing and turbulence–chemistry interaction in achieving flame anchoring. More specifically, the *Chemical Explosive Mode Analysis* (see Section 3) is used in combination with analysis of the TAKENO flame/mixing index.

The remainder of this paper is organized as follows: the numerical methods in the DNS code, S3D, used to perform the present simulations is described in Section 2, followed by a detailed description of the DNS configuration and numerical and thermochemical conditions. Instantaneous and time-averaged results from the reacting DNS are discussed in Section 3. Finally, conclusions and recommendations for further work are presented in Section 4.

2. Direct numerical simulations

The Sandia DNS code S3D [19] is used to simulate the combustion of two H_2/CO -air flames aerodynamically stabilized in the near field of the transverse jet immediately downstream of the fuel nozzle. The code solves fully-compressible conservation equations for mass, momentum, total energy and species continuity. The chemical reactions are described by a skeletal mechanism for H_2/CO -air combustion involving $N = 12$ species and 29 elementary reactions [20]. Nitrogen is inert in this context and therefore, NO_x formation reactions are not included. The species specific heats are modeled as polynomial functions of temperature as described in CHEMKIN and TRANSPORT [21], and mixture-averaged transport coefficients are used [22]. Radiative heat transfer is not considered in the present simulations. Spatial derivatives are obtained using an eighth-order central finite difference scheme which gradually reduces to a third-order one-sided difference stencil on the open boundaries [23]. A tenth-order explicit spatial filter is applied to remove any spurious high-frequency fluctuation in the solution [23]. Time integration is achieved using a six-stage fourth-order explicit Runge–Kutta method [23].

The numerical configuration is shown in Fig. 1. The computational domain is a cuboid with dimensions, $L_x \times L_y \times L_z = 25 \times 20 \times 20$ mm³, respectively. The Navier-Stokes Characteristic Boundary Conditions (NSCBC) are implemented [24,25] for non-reflecting inflow ($x = 0$) and outflow ($x = L_x$ and $y = L_y$) planes and a no-slip isothermal, solid surface wall ($y = 0$) boundaries while the z boundaries are periodic. The wall is assumed to be impermeable, such that the wall-normal mass flux of all species is identically zero. The jet nozzle shape is round with a diameter, $d = 1$ mm. The center of the nozzle is located on the spanwise symmetry plane, $z = L_z/2$, and at a streamwise location of $x = 5.5$ mm. The governing equations are discretized using $1408 \times 1080 \times 1100$ Cartesian mesh points in the streamwise x , transverse y and spanwise z directions, respectively. The mesh is uniform in the x and z directions and non-uniform in the y direction to satisfy the resolution requirements near the solid wall located at $y = 0$. The non-uniform mesh is refined in the wall-normal direction near the wall using a hyperbolic tanh mapping, resulting in an increasing wall normal spatial resolution of 10.2 to 24.3 μ m. The first point off the wall is at $y/\delta_{vis} = 0.5$, where δ_{vis} is the thickness of the viscous sublayer of the boundary layer. There are two points within $y/\delta_{vis} = 1$ and 13 points within $y/\delta_{vis} = 10$, satisfying the

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