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Liftoff and blowout characteristics of laminar syngas nonpremixed flames

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ABSTRACT

Liftoff and blowout behavior of nonpremixed syngas flames is investigated using a time-accurate CFD code with a detailed description of transport and chemistry. Lifted flames are established in coflowing laminar jets using N_2 dilution in the fuel jet. Results focus on the effects of syngas composition and temperature on the liftoff, stabilization, and the edge (triple) flame structure. For a given syngas mixture, as the N_2 dilution exceeds certain value, the flame lifts off from the burner rim and propagates along the stoichiometric mixture fraction line, and its structure changes from diffusion to double flame. With further dilution, the flame liftoff height increases rapidly, the base structure transitions from double to triple flame, and its stabilization involves a balance between the triple flame speed and local flow velocity. The temporal evolution of propagating jet flame also exhibits a similar behavior. The transition from diffusion to double and then to triple flame is examined using state relationships in mixture fraction coordinate. As H_2 fraction in syngas and/or temperature is increased, the N_2 dilution required for flame liftoff and blowout increases. The ratio of the triple flame speed to the unstretched premixed flame speed also increases with the increase in H_2 fraction. For H_2 fraction above 30%, the flame liftoff and blowout become less sensitive to syngas composition and temperature.

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Introduction

Lifted flames occur in a wide range of combustion devices, including gas turbines, diesel engines and stationary power systems. The liftoff of nonpremixed and partially premixed flames has been a subject of numerous investigations, and different mechanisms have been proposed for their stabilization. Chung and Lee [1] employed a cold jet theory and showed that the Schmidt number (Sc) plays an important role in flame liftoff, and stable lifted flames are possible only for fuels for which Sc<1. This implied that lifted propane and n-butane flames can be stabilized, whereas methane and ethane flames blowout directly from the burner-stabilized mode. Ghosal and Vervisch [2] extended Chung and Lee's analysis and showed that a lifted laminar flame is possible for a fuel for which Sc is greater than a critical value, which is less than unity. However, Kioni et al. [3] and Plessing et al. [4] established lifted methane flames using nitrogen dilution.

Takahashi and Katta [5] proposed that the nonpremixed flame stabilization involves the presence of an ignition or reaction kernel that synergistically provides radical species upstream, enhancing reaction rates for some key elementary reactions in a small stabilization region. In case of preheated

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reactants, a related mechanism suggested for anchoring lifted flames is autoignition, which is controlled by mixing and chemical kinetics effects [6]. Wichman and Ramadan [7] stated, on the contrary, that upstream radical transport is not a necessary condition, and that flame stabilization can result just due to the existence of a premixing zone of sufficient reactivity. A more common viewpoint for both laminar and turbulent flames is the edge-flame stabilization involving the propagation of a triple flame [3], and a balance between the local flow velocity and the triple flame speed. Qin et al. [8] distinguished between near and far field region stabilization. In the near region, the liftoff height was observed to vary linearly with increasing inflow velocity, whereas in the far region, it exhibited nonlinear behavior with respect to velocity.

Briones et al. [9] and Aggarwal [10] reported numerical and experimental results for dilution-induced liftoff and blowout of methane flames. They provided a more unified viewpoint, involving near field stabilization through the presence of an ignition kernel and far field stabilization through the presence of a triple flame. At certain level of dilution, depending on other conditions, a nonpremixed methane flame is lifted, and its base exhibits a double flame structure (i.e., containing rich premixed and nonpremixed reaction zones) in the near-field region, where the flame stabilization depends on a balance between the reaction rate and the scalar dissipation rate. With further increase in dilution level, the flame becomes weaker and stabilizes at a location that has a lower scalar dissipation rate. As the liftoff height increases, the flame base exhibits a triple flame structure, containing a rich premixed reaction zone (RPZ) on the fuel side, a lean premixed zone (LPZ) on the oxidizer side, and a nonpremixed zone (NPZ) sandwiched between the RPZ and LPZ. The flame stabilization mechanism then involves a balance between the triple flame speed and local flow velocity.

While previous studies have provided a significant database and fundamental understanding of flame liftoff and stabilization, most of this research has considered pure fuels, whereas most practical fuels contain a mixture of compounds with noticeable differences in their reactivity and transport properties. The objective of the present study is to examine the liftoff and blowout characteristics of laminar, nonpremixed syngas flames. It is important to note that the liftoff and blowout of turbulent diffusion and partially premixed flames are often described by the propagation of triple flamelets [6,9,11,12]. The choice of syngas is based on several considerations. First, syngas being a mixture of CO and H_2) represents a fuel blend for which relatively little research has been reported dealing with liftoff and blowout behavior. Second, it represents a cleaner and renewable fuel, and there is significant interest in using it for both stationary and mobile power generation. It is also considered a sustainable energy source as it can be produced from a variety of biomass and other renewable sources [13]. Third, its oxidation chemistry is fairly well established [14], and its combustion characteristics have been extensively investigated [15,16]. However, the liftoff and blowout characteristics of syngas flames have not been examined, although Chung and coworkers have reported simulations of auto-ignited lifted syngas [17] and methane [18] jet flames in heated coflowing air. It is also important to note that the main constituents of syngas, namely H_2 and CO, have widely disparate reactivity and diffusivity, and thus it is of interest how this disparity influences the liftoff behavior. A computational study is performed using a time-accurate implicit algorithm with a detailed description of chemistry and transport processes. Syngas lifted flames are established in axisymmetric coflowing jets using nitrogen dilution in the fuel stream. Results focus on the flame liftoff, stabilization, and blowout characteristics, including liftoff height and base structure at different heights for various syngas compositions. The effect of inflow temperature on flame liftoff and blowout is also examined.

Computational model

Simulations of jet diffusion flames are performed using a 2-D CFD code, UNICORN (UNsteady Ignition and COmbustion using ReactioNs), which is capable of performing direct numerical simulations (DNSs) of reacting flows. Details are provided elsewhere [9,10]. The numerical algorithm solves u- and v-momentum equations, continuity, and enthalpy- and species-conservation equations on a staggered-grid system. Using cylindrical coordinates (r, z), these equations in a generalized form can be written as

$$\frac{\partial(\rho\Phi)}{\partial t}+\frac{\partial(\rho v\Phi)}{\partial r}+\frac{\partial(\rho u\Phi)}{\partial z}=\frac{\partial}{\partial r}\left(\Gamma^{\Phi}\frac{\partial\Phi}{\partial r}\right)+\frac{\partial}{\partial z}\left(\Gamma^{\Phi}\frac{\partial\Phi}{\partial z}\right)-\frac{\rho v\Phi}{r}+\frac{\Gamma^{\Phi}}{r}\frac{\partial\Phi}{\partial r}+S^{\Phi} \quad (1)$$

Here ρ is the mixture density, t the time, and u and v the axial (z) and radial (r) velocity components, respectively. The general form of the equation represents conservation of mass, momentum, species, or energy conservation, depending on the variable used for Φ. The transport coefficient Γ^{Φ} and the source terms S^{Φ} appearing in the governing equations are described in Ref. [19]. Introducing the overall species conservation equation and the state equation completes the equation set. The syngas oxidation chemistry is modeled using the San Diego (SD) mechanism [20], which contains 52 species and 544 elementary reactions. Validation of the mechanism is discussed in the next section.

The thermodynamic and transport properties appearing in the governing equations are considered temperature and species dependent. The transport properties such as viscosity, thermal conductivity and binary molecular diffusion coefficients for each species are evaluated using Chapman–Enskog treatment for colliding molecules and Lennard–Jones potentials and reduced temperatures as described in Ref. [21]. Mixture viscosity and thermal conductivity are then estimated using the Wilke and Kee expressions, respectively. Molecular diffusion is assumed to be of the binary-diffusion type, and the diffusion velocity of a species is calculated using Fick's law and the effective-diffusion coefficient of that species in the mixture. To account for thermal radiation from the flame [9,22], a sink term based on an optically thin gas assumption is included in the energy equation in the form $q_{rad}=-4\sigma K_p(T^4-T_o^4)$, where T denotes the local flame temperature, σ is the Stefan–Boltzmann constant and K_p accounts for the absorption and emission from the participating gaseous species (CO_2, H_2O, CO and H_2).

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