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Numerical study of laminar nonpremixed methane flames in coflow jets: Autoignited lifted flames with tribrachial edges and MILD combustion at elevated temperatures

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ABSTRACT

Autoignition characteristics of laminar nonpremixed methane jet flames in high-temperature coflow air are studied numerically. Several flame configurations are investigated by varying the initial temperature and fuel mole fraction. At a relatively low initial temperature, a non-autoignited nozzle-attached flame is simulated at relatively low jet velocity. When the initial temperature is higher than that required for autoignition, two regimes are investigated: an autoignited lifted flame with tribrachial edge structure and an autoignited lifted flame with Mild combustion. The autoignited lifted flame with tribrachial edge exhibited three branches: lean and rich premixed flame wings and a trailing diffusion flame. Characteristics of kinetic structure for autoignited lifted flames are discussed based on the kinetic structures of homogeneous autoignition and flame propagation of stoichiometric mixture. Results showed that a transition from autoignition to flame propagation modes occurs for reasonably stoichiometric mixtures. The autoignited lifted flame with Mild combustion occurs when methane fuel is highly diluted with nitrogen. The kinetic structure analysis shows that the characteristics of Mild combustion can be treated as an autoignited lean premixed lifted flame. Transition behavior from Mild combustion to nozzle-attached flame was investigated by increasing the fuel mole fraction. As the maximum flame temperature increases with decreasing liftoff height, the kinetic structure showed a transition behavior from autoignition to flame propagation of a lean premixed flame.

1. Introduction

Methane is the dominant constituent of natural gas, shale gas, and landfill gas. It has a high hydrogen to carbon ratio and a large research octane number, making it suitable for spark-ignition engines with a high compression ratio for energy efficiency and greenhouse gas emission. Natural gas is used extensively for gas turbines in combined cycle power generation. Understanding the autoignition and flame stabilization of methane fuel is essential for optimizing its application.

Various experimental and computational studies have been conducted to investigate the autoignition phenomenon. For example, shock tubes, rapid compression machines, and flow reactors have been used to measure the ignition delay time of methane under homogeneous mixture conditions [1–5], based on which chemical kinetic mechanisms were developed and validated [6–8].

Recently, autoignition phenomena under inhomogeneous conditions have begun to draw attention for their practical applications, such as to diesel spray ignition [9] and to the moderate or intense low-oxygen dilution (Mild) combustion [10,11] that is associated with high dilution and high preheating of combustible mixtures to reduce soot and NOx emissions. In this regard, a nonpremixed jet flame can be a canonical flame demonstrating autoignition behavior under inhomogeneous conditions at high temperatures.

Autoignited turbulent lifted flames of various fuels, including methane, have been investigated experimentally and numerically in axisymmetric coflow configurations [12–16]. A strong link has been established between the autoignition kernel and the tribrachial (triple) point of turbulent lifted flames [14]. Furthermore, OH (flame marker) and CH_2O (autoignition precursor) images were used to identify the heat release rate (HRR) profiles that can distinguish an autoignition flame structure [14]. In addition, intermediate species, including CH_2O, HO_2, H_2O_2, and H_2, have been shown to be important indicators of the pre-ignition phase [13,15].

Recently, laminar flame stabilization in high-temperature coflow jets has been investigated in non-autoignited and

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autoignited regimes [17–23]. Experimental studies of autoignited lifted flames have been performed for various gaseous fuels, including methane, ethane, ethylene, propane, *n*-butane, and mixtures of carbon monoxide and hydrogen (CO/H_2) and methane and hydrogen (CH_4/H_2) [17–20]. When the initial temperature, T_0, was below the autoignition temperature, T_{auto}, an external ignition source was required to stabilize a lifted flame and its edge was observed to have a tribrachial structure, consisting of lean and rich premixed flame wings and a trailing diffusion flame that all extend from a single location [24–26]. In this case, flame stabilization is controlled by the balance mechanism between the propagation speed of tribrachial flame edge, which is closely linked to stoichiometric laminar burning velocity, and local flow velocity along a stoichiometric contour [26]. Mixing layer analysis and the associated tribrachial flame structure have been studied theoretically [25,27,28], and the Schmidt number of the fuel has been shown to have the potential to affect lifted flame stabilization in free jets [17,24,29]. Lifted flames with tribrachial edges under low-temperature conditions have also been studied numerically [30–34]. In addition, several computational studies have investigated the effects of fuel dilution and partial premixing on low-temperature flame stabilization and extinction [35–37].

When the initial temperature is greater than the autoignition temperature ($T_0 > T_{auto}$), a flame can be generated by autoignition phenomenon without requiring any external ignition source. The resulting autoignited lifted flames can be categorized into two regimes; autoignited lifted flames with tribrachial edges and autoignited lifted flames with Mild combustion [17,18]. For the former, liftoff height increased non-linearly with fuel jet velocity, while for the latter, under high nitrogen-dilution conditions, liftoff height increased reasonably linearly with fuel jet velocity. In these regimes, an ignition delay time representing fuel's reactivity was found to be a key factor controlling the lifted flame behavior rather than laminar burning velocity, which is important in non-autoignited lifted flames.

A computational study on high-temperature coflow jets can facilitate the understanding of autoignition phenomena in more detail. For autoignited lifted flames, CO/H_2 flames and dimethyl ether (DME) flames have been analyzed [21,38], both for the autoignited lifted flames with tribrachial edge. As far as the authors are aware, autoignited laminar lifted flames with Mild combustion has never been analyzed yet. In the present study, autoignited laminar lifted flames of methane fuel are studied numerically by adopting a reduced kinetic mechanism. Both autoignited lifted flames with tribrachial edges and Mild combustion are considered, along with the transition behavior. The autoignition process and the kinetic structure of autoignited flames are analyzed by comparing its structure with those of homogeneous autoignition and propagating premixed flame.

2. Numerical simulation

A set of time-dependent conservation equations in a two-dimensional axi-symmetric coordinate (x, y) was adopted to simulate autoignited flames in coflow jets and a non-autoignited flame was investigated to provide baseline data. The computation was carried out by an in-house code (RUN2D) with the low Mach number approximation, which has been successfully applied previously for the analyses of various flame configurations [21,29,30]. A finite difference procedure with staggered grids was adopted by the second-order central difference scheme. The 6-stage, 4th-order explicit Runge–Kutta scheme was used for time integration. Details have previously been reported [30].

For computation efficiency, a reduced mechanism [39] was adopted having 19 species with 15 lumped steps. This mechanism was validated for ignition delay time, laminar flame speed, and partially stirred reactor models for methane oxidation. Thermodynamic and transport properties were calculated by CHEMKIN and TRANSPORT packages [40] and mixture-averaged diffusion coefficients were used. The calculation domain was 6.65 × 20 cm in radial (x) and axial (y) coordinates with 112 × 1536 non-uniform grids to improve the resolution in the jet mixing layer and near nozzle region. Radially, 64 uniform grids were placed within 6.65 mm from the center of the nozzle ($\Delta x \sim 119\,\mu m$) and the remaining 48 non-uniform grids were distributed in the outer domain by gradually increasing the grid size. The grids along the vertical axis were uniformly distributed for positions above 1.8 cm from the nozzle tip ($\Delta y \sim 133\,\mu m$), while a finer grid system was used below the domain. The fuel nozzle had $d = 3.76$ mm i.d., with 0.5 mm thick, and protruded 1 cm above the coflow air exit, complying with a previous experiment [17]. This protrusion was to minimize the boundary layer effect when air was passing through a honeycomb in the experiment. The grid dependence was checked by doubling the number of grids in both directions to 224 × 3072, and no observable differences were noticed in the flame structures and lifted flame behaviors.

3. Results and discussion

Autoignited methane flames have previously been observed experimentally at initial temperatures over 940 K [17]. Based on those results, flame stabilization characteristics were investigated. The coflow air velocity was fixed at 1.1 m/s, similar to the experimental condition [17]. The inlet parameters, including initial temperature, T_0, jet velocity, U_0, and fuel mole fraction, $X_{F,0}$, were varied depending on the case investigated. Three cases were tested: a non-autoignited nozzle-attached flame at $T_0 = 800$ K, an autoignited lifted flame with tribrachial edge at $T_0 = 1120$ K, and an autoignited lifted flame with Mild combustion at $T_0 = 1100$ K. In addition, the transition from a Mild combustion regime to a nozzle-attached flame was investigated by varying the degree of fuel dilution. In the present study, the range of the Reynolds numbers $Re = U_0 d/\nu$ is 46–530, where ν is the kinematic viscosity of fuel stream.

3.1. Non-autoignited nozzle-attached flame

At the relatively low initial temperature of $T_0 = 800$ K, an external ignition source was required to generate a flame experimentally [17]. For such a non-autoignited methane flame, no stable lifted flame was observed. This was explained based on an unstable nature of a lifted flame when the Schmidt number of fuel is smaller than unity as discussed extensively previously [17,24,25,29]. As the jet velocity increases, a nozzle-attached flame blows off directly without having a lifted flame mode. This type of nozzle-attached flame was simulated as the baseline test.

After a cold flow field was calculated for $U_0 = 1.0$ m/s and $X_{F,0} = 0.16$ ($Re = 46$), an ignition source was applied by assigning a spherical high-temperature region of 2500 K with a 3 mm radius and 3 cm above the nozzle along the centerline. After a transient ignition, a stationary nozzle-attached flame was obtained and the temperature profiles, heat release rate (HRR), and several species mole fractions are shown in Fig. 1.

The temperature field shows that the attached flame height is 1.1 cm. This height is considered to be reasonably similar to the experimental observation of 1.4 cm considering that the simulation was conducted without accounting for the nozzle heating effect. It has been shown in detail in [41] that simulations with heated and cold nozzles show quite different velocity profiles at the nozzle exit by the fuel heating effect and subsequent buoyancy effect