Combustion and Flame 198 (2018) 305–319

Contents lists available at ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

Differential diffusion effect on the stabilization characteristics of autoignited laminar lifted methane/hydrogen jet flames in heated coflow air

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ARTICLE INFO

Article history:
Received 22 June 2018
Revised 3 August 2018
Accepted 25 September 2018

Keywords:
Autoignition
Liftoff height
Flame stabilization
Tribrachial edge flame
MILD combustion

ABSTRACT

The characteristics of autoignited laminar lifted methane/hydrogen jet flames in heated coflow air are numerically investigated using laminarSMOKE code with a 57-species detailed methane/air chemical kinetic mechanism. Detailed numerical simulations are performed for various fuel jet velocities, U_0, with different hydrogen ratio of the fuel jet, R_H, and the inlet temperature, T_0. Based on the flame characteristics, the autoignited laminar lifted jet flames can be categorized into three regimes of combustion mode: the tribrachial edge flame regime, the Moderate or Intense Low-oxygen Dilution (MILD) combustion regime, and the transition regime in between. Under relatively low temperature and high hydrogen ratio (LTHH) conditions, an unusual decreasing liftoff height, H_L, behavior with increasing U_0 is observed, qualitatively similar to those of previous experimental observations. From additional simulations with modified hydrogen mass diffusivity, it is substantiated that the unusual decreasing H_L behavior is primarily attributed to the high diffusive nature of hydrogen molecules. The species transport budget, autoignition index, and displacement speed analyses verify that the autoignited lifted jet flames are stabilized by autoignition-assisted flame propagation or autoignition depending on the combustion regime. Chemical explosive mode analysis (CEMA) identifies important variables and reaction steps for the MILD combustion and tribrachial edge flame regimes.

1. Introduction

Numerous experimental and numerical studies of autoignition of various fuel/air mixtures have been conducted not only because it is one of the most important combustion phenomena [1,2], but also because it appears in many practical combustion devices such as diesel engines, homogeneous charge compression ignition (HCCI) engine, and its variants [3–7]. In general, autoignition in an ideal HCCI engine occurs under adiabatic condition due to its homogeneities in both temperature and composition. However, autoignition in variants of HCCI combustion including stratified charge compression ignition (SCCI) [8,9] and reactivity controlled compression ignition (RCCI) [5,10,11] combustion occurs non-adiabatically due to their mixture stratification and/or direct-fuel injection to control overall ignition timing and mitigate excessive pressure rise rate (PRR) in an engine cylinder. Similarly, autoignition in the diesel combustion occurs non-adiabatically due to its inherent mixture stratification. Therefore, the liftoff characteristics and stabilization mechanisms of turbulent lifted jet flames at high pressures and temperatures have been a long-time research topic to understand the fundamentals of the diesel combustion [1,3,12–14].

The characteristics of autoignited laminar lifted jet flames in heated coflow air have also been investigated due to their distinct features from those of non-autoignited lifted jet flames and their potential as a building-block configuration for understanding turbulent lifted jet flames at high pressures and temperatures. For instance, stabilization mechanisms found from autoignited laminar lifted flames under various conditions can be useful for understanding those of turbulent lifted jet flames featured by complicated and transient nature. Chung and coworkers [15–17] found

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https://doi.org/10.1016/j.combustflame.2018.09.026
0010-2180/

that an autoignition kernel in a laminar nonpremixed fuel jet in heated coflow air can develop into a stationary lifted flame or a nozzle-attached flame depending on the inlet conditions of the fuel jet and coflow air. They also elucidated that a stationary autoignited laminar lifted jet flame can exist regardless of the Schmidt number of the fuel jet, which implies that ignition delay can play a critical role in stabilizing laminar lifted jet flame under autoignitive conditions [16]. A tribrachial edge flame, or Moderate or Intense Low-oxygen Dilution (MILD) combustion features in the autoignited laminar lifted jet flames; the former appears when the fuel mole fraction in the fuel jet, $X_{F,0}$, is relatively high while the latter occurs at relatively-low $X_{F,0}$. The leading edge of the autoignited laminar lifted jet flames with tribrachial edge consists of lean/rich premixed flame wings and a trailing nonpremixed flame [18]. However, when the fuel jet is excessively diluted with an inert gas such as nitrogen, the conventional tribrachial edge flame does not exist and its flame structure changes to that of a MILD combustion with faint blue color without exhibiting a clear tribrachial structure [15–21].

From previous studies of autoignited laminar lifted jet flames [15,16], their liftoff height variation has been intensively investigated together with their flame structure characteristics. The liftoff height, H_L, of autoignited laminar lifted jet flames is found to be functions of the fuel jet velocity, U_0, and the 0-D adiabatic ignition delay of the stoichiometric fuel/air mixture based on the inlet condition, $\tau_{ig,\,st}$: i.e., $H_L \sim U_0\tau^2_{ig,st}$. This correlation was originally devised by Choi et al. [15] considering thermal balance between heat release from autoignition and heat loss by diffusion in a jet mixing layer. As such, H_L increases with increasing U_0 for the same fuel and oxidizer jet conditions. This correlation is in good agreement with experimental data for autoignited lifted flames with tribrachial edge structure of various single component fuel jets [16]. For an autoignited lifted jet flame with a MILD combustion, the H_L correlation was modified incorporating the ignition strength of the fuel jet [16]: $H_L \sim U_0\tau^2_{ig,st}Y_{F,0}$, where $Y_{F,0}$ is the fuel mass fraction at the inlet [16]. For both H_L correlations of tribrachial edge flames and MILD combustion, we can readily observe a quadratic dependence of H_L on $\tau_{ig,st}$, which implies that the adiabatic 0-D ignition delay can play a critical role in stabilizing autoignited laminar lifted jet flames.

In a previous experimental study of autoignited laminar lifted methane/hydrogen jet flames [17], however, an unusual liftoff height variation with U_0 was observed; H_L decreases with increasing U_0 at relatively-low inlet temperatures and relatively-high hydrogen content. As such, the decreasing H_L with U_0 does not follow the conventional autoignited laminar liftoff height behavior of $H_L \sim U_0$. It was conjectured that the unusual H_L behavior might be attributed to differential diffusion between methane and hydrogen molecules in the fuel jet. Moreover, due to the unusual characteristics of the autoignited laminar lifted methane/hydrogen jet flames, another unique feature of the flames was identified that the flame structure changes from a lifted flame with tribrachial edge to a MILD combustion with decreasing U_0 although the fuel jet is not excessively diluted with an inert gas. According to previous studies of autoignited laminar lifted flames with a single component fuel such as methane and propane, the transition from a tribrachial edge flame to a MILD combustion was typically observed when the inlet fuel mole fraction is significantly low, or $X_{F,0} \sim O(0.01)$ [15,18]. In the autoignition of methane/hydrogen jets in heated coflow air, however, a gradual transition from a tribrachial flame to a MILD combustion was observed with decreasing U_0 even though the fuel jet is not highly diluted with nitrogen ($X_{F,0} \sim O(0.1)$).

Therefore, the objective of the present study is two-fold: (1) to understand the liftoff characteristics of autoignited laminar lifted methane/hydrogen jet flames, especially the reason of the occurrence of the decreasing behavior of H_L with U_0, and (2) to elucidate the flame stabilization and structure characteristics of the autoignited laminar lifted jet flames by performing 2-D detailed numerical simulations for different inlet fuel jet conditions and hydrogen mass diffusivities. The MILD combustion featured by very faint blue flame has many advantages in reducing soot and NOx due to its low flame temperature, and in achieving high thermal efficiency through its high reactant temperature [22,23]. In the context of utilizing low flame temperature, the MILD combustion is quite similar to low temperature combustion (LTC) adopted in advanced IC engines. In the present study, therefore, the characteristics of autoignited laminar lifted flames with MILD combustion will also be investigated.

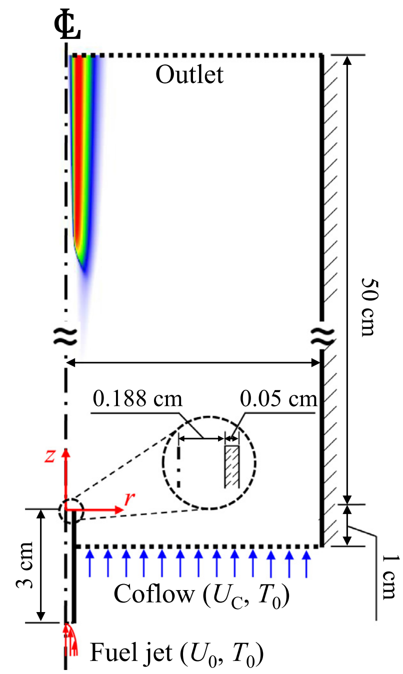

Fig. 1. Schematic of the computational domain for simulations of autoignited laminar lifted methane/hydrogen jet flames in heated coflow air.

2. Numerical methods

Detailed numerical simulations of autoignited laminar lifted methane/hydrogen nonpremixed jet flames in heated coflow air are performed in an axisymmetric coflow burner configuration, which has been adopted in several previous experimental and numerical studies [15–18,21]. The steady compressible Navier-Stokes, species continuity, and energy equations are solved using laminarSMOKE [24,25], which is an open-source code based on OpenFOAM [26] for simulations of multi-dimensional compressible laminar reacting flows with skeletal/detailed chemical mechanisms. For the detailed description of laminarSMOKE, readers are referred to Refs. [24,25].

Figure 1 shows a schematic of the computational domain adopted in this study. The domain size is 6.65 cm × 50 cm in the radial $r-$ and the axial $z-$directions. The inner diameter and thickness of the fuel nozzle are 3.76 mm and 0.5 mm, respectively. To take into account the effect of the finite thickness of the fuel jet nozzle on the flow, 3 cm long fuel nozzle is added to the main computational domain, which protrudes 1 cm above the coflow air inlet as shown in Fig. 1. Note that the configuration of the computational domain is identical to those of previous experiments and simulations [15–18,21].

No-slip and adiabatic boundary conditions are used for all the solid boundaries and symmetric boundary conditions are used for $r = 0$. For the inlets, the fuel inlet velocity is specified as that of a