Combustion and Flame 168 (2016) 75–82

Contents lists available at ScienceDirect

Combustion and Flame

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

Flame dynamics in oscillating flows under autoignitive conditions

Sili Deng[a], Peng Zhao[a,b], Michael E. Mueller[a,*], Chung K. Law[a]

[a] Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ 08544, USA
[b] Department of Mechanical Engineering, Oakland University, Rochester, MI 48309, USA

ARTICLE INFO

Article history:
Received 15 February 2016
Revised 1 April 2016
Accepted 2 April 2016
Available online 5 May 2016

Keywords:
Flame dynamics
Nonpremixed coflow flame
Autoignition
Negative temperature coefficient (NTC)
Dimethyl ether (DME)

ABSTRACT

The structure and dynamics of laminar nonpremixed dimethyl ether (DME)/air coflow flames were investigated at elevated temperatures and pressures. Computations with detailed chemistry were performed for DME and heated coflow air at 30 atm with uniform but sinusoidally oscillating inlet velocities. These unsteady cases were compared with the steady results from Deng et al. (2015)[14] to elucidate the effect of oscillation frequency on the flame dynamics. To benchmark the unsteady cases, a normalized displacement velocity was defined to differentiate flame propagation from autoignition, and this definition was validated against the steady cases. In the oscillating reacting flow, transition between a multibrachial autoignition front and a tribrachial flame occurs periodically. However, unlike the harmonic velocity oscillation, the combustion mode transition is hysteretic. The oscillation cycle starts with the largest inlet velocity, with the multibrachial thermal structure, located downstream, being governed by autoignition chemistry. As flow velocity decreases, the autoignition front moves upstream and transitions to a tribrachial flame near the lower velocity limit, similar to the steady flow, as autoignition chemistry becomes weaker with decreasing upstream residence time. As the flow velocity increases again, the tribrachial flame is convected downstream, and, ultimately, due to the radical and heat accumulation in time, autoignition eventually occurs and becomes the dominant pathway. The finite induction time for autoignition results in the hysteretic behavior during the decreasing- and increasing-velocity cycles, which diminishes at lower oscillation frequency as there is more time for chemistry to respond to the hydrodynamic changes and consequently approach steady state. At the relatively low oscillation frequencies investigated in the current study, first-stage NTC chemistry is less affected by flow dynamics with only second-stage autoignition and flame chemistry, which accounts for the majority heat release, coupled with the flow oscillation.

1. Introduction

Fuel injection and its subsequent mixing and reaction with either a coflowing air stream or a highly turbulent oxidizing environment is an integral process in the operation of many combustors. Due to experimental and computational limitations, simplifications are usually made to obtain fundamental understanding of these reacting flows that are then extrapolated to more complex conditions. For example, laminar nonpremixed coflow flames at normal ambient temperatures have been studied to elucidate the coupling between fluid dynamics and chemistry, leading to the observation that, in the fuel and oxidizer mixing layer, a two-dimensional tribrachial structure (also known as triple flame) [1] is obtained. Specifically, both lean and rich premixed flame branches and a trailing diffusion flame tail intersect at a triple point. Based on the observation of such tribrachial laminar flames, the partially premixed flamelet model [2] was proposed to explain lifted flames in nonpremixed turbulent jets [3].

Previous studies have indicated that nonpremixed coflow flame structure can be modified in unsteady flows. For example, in the experimental investigation of Strawa and Cantwell [4], flow instability and flame breakup was achieved by imposing a small-amplitude, periodic velocity fluctuation to nonpremixed jet flames at elevated pressures and low Reynolds numbers. Later, in the computational study of Sánchez-Sanz et al. [5], perturbation frequency effects on the thermal and chemical properties of the flame in such periodically time-varying flows were evaluated. Three regimes were found depending on the flame's Strouhal number, $S = Df/2U$, with D and f denoting the fuel jet diameter and perturbation frequency, respectively. For small Strouhal numbers ($S = 0.1$), perturbations can travel far downstream, resulting in an oscillating flame. Flame surface flickering was observed when $S \simeq 0.2$,

---

[*] Corresponding author.

E-mail addresses: silideng@gmail.com (S. Deng), muellerm@princeton.edu (M.E. Mueller).

http://dx.doi.org/10.1016/j.combustflame.2016.04.001
0010-2180/

and vigorous flame pinch-off was observed at $S = 0.5$. Larger values of S confine the oscillation to the jet's near-exit region with the pulsation having minimal effects on temperature and concentration values. The unsteadiness in flickering flames also increases pollutant formation, such as soot [6] and carbon monoxide [7]. Mohammed et al. [8] followed by Dworkin et al. [9] conducted computational and experimental studies of 20 Hz periodically-forced methane/air coflow diffusion flames. Acetylene production increased [8] and the oxidation of CO to CO_2 was inhibited [9] in the downstream region of the flame at certain times during the flame's cyclic history.

Although demonstrating unsteady effects on flow-chemistry coupling, these experimental and computational investigations mainly focused on simple fuels, such as methane, and were limited to nonautoignitive conditions. However, as demonstrated by Chung and co-workers through a series of experiments on laminar lifted C_0 to C_8 flames in heated coflow, autoignition can be activated even at atmospheric pressure [10,11]. Although flames were initiated by autoignition, the lifted height did not always correlate well with the ignition delay time. Computationally, Krisman et al. [12] demonstrated that, under more realistic engine conditions of elevated temperature and pressure with practical fuels that have more complex chemical kinetics, the transport-chemistry coupling becomes more complicated. Depending on the conditions, either the traditional tribrachial flame or autoignition can be dominant. Their findings were confirmed and further discussed by Deng et al. [13,14] through a series of computational studies of nonpremixed dimethyl ether (DME)/air coflow flames at 30 atm with varying inlet velocities and coflow temperatures, recognizing that DME possesses the low-temperature chemistry (LTC), negative temperature coefficient (NTC) behavior. A regime diagram was proposed demonstrating that the tribrachial flame is favored at lower inlet velocity and higher coflow temperature, while autoignition is dominant at higher inlet velocity and relatively lower coflow temperature.

In the present study, unsteady nonpremixed DME/air coflow flames under autoignitive conditions are computationally studied to elucidate the coupling between unsteady fluid dynamics and chemical kinetics. Various oscillation frequencies were imposed on the inlet velocity, with the maximum and minimum velocities maintained the same as those in the previous steady study [14], which correspond to an autoignition front and a tribrachial flame, respectively. The current study focuses on low frequency oscillation ranging from 25 to 100 Hz, which covers buoyancy-driven instability frequencies [8,9] and acoustic-driven oscillation frequencies in gas turbines [15]. The objective of the current study is threefold. The first objective is to capture the transition in combustion mode. As the steady cases correspond to different combustion modes, it is expected that, at certain frequencies of velocity oscillation, the dominant combustion process will shift between the nonpremixed tribrachial flame mode and the autoignition mode. The second objective is to assess the thermal and chemical differences during such transition and to elucidate the transition mechanism. The third objective is to demonstrate the effects of oscillation frequency on the coupling of fluid dynamics and chemical kinetics.

2. Computational details

The geometry in this work is the same as that in Deng et al. [14]. Briefly, axisymmetric coflow flames at 30 atmospheres were computed, in which a 300 K DME stream is surrounded by a 900 K air stream. The diameter (D) of the fuel nozzle is 0.8 mm, which is 20 times the thickness of the adiabatic, no-slip wall, separating fuel and coflow. The outer diameter of the coflow is 3.9 mm. Adiabatic, slip wall conditions were specified at the outer radial boundary. The same inlet velocities were imposed for both streams and are uniform in space and sinusoidally oscillating in time. The maximum (8.0 m/s) and minimum (2.4 m/s) velocities were set to match the fastest and slowest steady cases as in Deng et al. [14]. Three oscillation frequencies (25, 50, and 100 Hz) were investigated, with the maximum Strouhal number, based on the velocity and jet radius, estimated to be less than 0.02 to avoid flame pinch-off. The domain length is 15 mm, with a convective outflow boundary condition. The computational results were not affected by further widening or lengthening of the domain. Discretization of the domain was guided by previous convergence studies [13], with a 3072 (x) by 176 (r) grid. Uniform spacing in the axial direction was set to $\Delta x = 4.8$ μm, and nonuniform spacing in the radial direction was set to minimum $\Delta r = 2.5$ μm to resolve the mixing layer near the thin wall. The grid stretch rate is less than 3%.

The Navier–Stokes equations with buoyancy effects in the streamwise direction and the conservation equations of mass, species, and temperature were solved. The species diffusivities were determined assuming constant, nonunity Lewis numbers and kept the same as in Deng et al. [13]. The conserved scalar mixture fraction (Z) was specified as unity and zero for the fuel stream and coflow, respectively, and was computed by solving a conserved scalar transport equation with unity Lewis number [16]. DME was chosen as the fuel, for it is one of the simplest fuels that has NTC chemistry [17], as noted earlier. A skeletal mechanism of 39 species [18], which was reduced from the well-validated detailed mechanism of Zhao et al. [19], was adopted as the chemical model.

A low-Mach number code NGA [20] was adopted to solve the discretized governing equations on a staggered mesh. A second-order centered scheme was used for the momentum equations, while a third-order WENO scheme [21] was used for the scalar equations. An iterative second-order semi-implicit midpoint scheme was adopted for temporal integration [22] utilizing Strang splitting between transport and chemistry in the scalar equations [23]. The chemical source terms for the species and temperature equations were integrated using the CVODE package [24].

3. Results and discussion

In this section, the thermal structure of the unsteady nonpremixed DME/air coflow flame is first described and compared qualitatively with the previous steady study by Deng et al. [14]. The definition of normalized displacement velocity is then introduced and validated against the steady cases to differentiate the combustion modes. Finally, oscillation frequency effects on the evolution of the combustion modes are analyzed.

3.1. Thermal structure

As the largest and smallest inlet velocity cases were designed to match the two extreme cases in Deng et al. [14], which are of different thermal structures, it is expected that similar thermal structures will be obtained. Furthermore, these thermal structures might transition back and forth in response to the oscillating flow field. Indeed, such transitions were observed for all three frequencies. For example, the evolution of the thermal structure of the 100 Hz case, in terms of the heat release rate profile, is demonstrated in Fig. 1. The oscillation cycle starts with the largest inlet velocity of 8.0 m/s, and the minimum inlet velocity (2.4 m/s) is achieved at half cycle.

At 8.0 m/s, the multibrachial thermal structure is located furthest downstream. The leading point, which is defined as the most upstream point that has the heat release rate value of 10^{12} W/m^3, is located at mixture fraction $Z = 0.24$. As the inlet velocity decreases, the multibrachial structure moves upstream, without obvious change of the leading point location, in terms of mixture