Combustion and Flame 162 (2015) 4471–4478

Contents lists available at ScienceDirect

Combustion and Flame

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

Stabilization of laminar nonpremixed DME/air coflow flames at elevated temperatures and pressures

Sili Deng, Peng Zhao, Michael E. Mueller*, Chung K. Law

Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ 08544, USA

ARTICLE INFO

Article history:
Received 17 June 2015
Revised 25 August 2015
Accepted 26 August 2015
Available online 29 September 2015

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

ABSTRACT

The structure and stabilization mechanism of laminar nonpremixed autoignitive DME/air coflow flames was investigated at elevated temperatures and pressures. Computations with detailed chemistry were performed for DME and heated coflow air at 30 atm with uniform inlet velocities (2.4, 3.2, and 8.0 m/s) imposed for both streams. The heat release rate profiles are first examined for each case to demonstrate a multibrachial thermal structure. Species concentrations and temperature were sampled along mixture fraction iso-contours, and Chemical Explosive Mode Analysis (CEMA) was performed to identify the controlling chemistry at representative points. One-dimensional Lagrangian Flamelet Analysis (LFA) was also performed and compared with the two-dimensional computations to elucidate the relative importance of diffusion processes parallel and normal to the mixture fraction gradient. Various coflow temperatures with different inlet velocities are examined to elucidate their influences on the multibrachial structure as well as the stabilization mechanism. NTC (negative temperature coefficient)-affected inhomogeneous autoignition and the coupled effects with premixed flame propagation on stabilization are further studied. It is found that, at high coflow boundary temperatures or low inlet velocities, the classical tribrachial flame structure is achieved, and autoignition contributes less to the stabilization due to reduced heat and radical accumulation. The kinematic balance between the local flow speed and flame propagation speed is the dominant stabilization mechanism. On the contrary, kinetic stabilization is achieved at lower coflow temperatures or higher inlet velocities as autoignition becomes dominant. Due to the transition of the dominant chemical pathways during autoignition, the kinetically stabilized structure is usually multibrachial. The transition of different stabilization mechanisms can be made by changing either the boundary velocity or temperature of the coflow. Based on these results and previous work (Deng et al., 2015) [12], a regime diagram is constructed that identifies the possible stabilization regimes: blow out, kinetically stabilized, autoignition-propagation-coupled stabilized, kinematically stabilized, and burner stabilized.

1. Introduction

Two-dimensional tribrachial structures (also known as triple flames) [1] are observed in nonpremixed laminar lifted flames at nonautoignitive conditions. The dynamic balance between the local flame propagation speed and the incoming flow speed at the triple point is generally considered as the stabilization mechanism [2]. However, practical engines operate at elevated pressures and temperatures. As a consequence, the propensity for autoignition is significantly enhanced, and, therefore, the thermal and chemical structure of the tribrachial flame, as well as the stabilization mechanism, could be affected by the autoignition process. For example, experimentally, Chung and co-workers have investigated autoignited lifted propane/nitrogen [3], methane/hydrogen [4], and other neat C_1–C_4 hydrocarbon flames [5], and compared their lift-off heights with homogeneous autoignition delay time. Furthermore, the autoignition process of most large hydrocarbons under practical engine conditions could possibly lie in the negative temperature coefficient (NTC) regime, in which the overall ignition delay time increases as the initial temperature increases. The NTC phenomenon is relevant to engine knock [6] and has been extensively studied in homogeneous systems [7]. As Law and co-workers [8–10] recently demonstrated, ignition characteristics in a nonpremixed system can also be affected by NTC chemistry, especially at elevated pressures and/or extended residence times. These computational and experimental studies were conducted in the nonpremixed counterflow system where the residence time is well characterized. When the flow residence time and NTC chemistry timescales are comparable, the two processes are strongly coupled, resulting in modified system response, such as autoignition behavior.

---

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

http://dx.doi.org/10.1016/j.combustflame.2015.08.019

To investigate autoignition with NTC chemistry effects in nonpremixed lifted flame stabilization, Krisman et al. [11] recently conducted a numerical study of dimethyl ether (DME)/air nonpremixed flames at 40 atmospheres and elevated air coflow temperatures (700–1500 K) and observed multibrachial thermal structures. The autoignition response in the two-dimensional computation was compared with that of homogeneous autoignition under the same initial conditions. A transport budget analysis of methoxymethylperoxy ($CH_3OCH_2O_2$) and hydroxyl (OH) radicals, which represent the low and high temperature chemistry, respectively, was performed to differentiate deflagration from autoignition. The stabilization points of the multibrachial structure was determined with $CH_3OCH_2O_2$ and OH radical mass fractions for low and high temperature autoignition chemistry, respectively, and varied as boundary temperature and velocity changed.

More recently, to further elucidate the chemical structure of the multibrachial structure and the roles of autoignition and flame chemistry in the stabilization mechanism, the authors [12] performed a numerical study of nonpremixed DME/air coflow flames. Chemical Explosive Mode Analysis (CEMA) was adopted to identify locally dominant reactions, and Lagrangian Flamelet Analysis (LFA) was adopted to identify the dominant combustion mode. The comparison with the two-dimensional computation was able to quantify the relative importance of transport processes parallel and normal to the mixture fraction gradient and elucidate the dominant stabilization mechanism. For increasing coflow boundary temperature at constant inlet velocities, the stabilization mechanism transitioned from kinetic to kinematic stabilization.

In the present study, nonpremixed DME/air coflow flames at elevated temperatures and pressures were further studied. The objective of the current work is fourfold: first, to elucidate transport effects on stabilization, parallel to the previous work [12], which focused on chemical effects; second, to demonstrate the effects of NTC chemistry on the multibrachial structure; third, to understand the transition between *kinetic* and *kinematic* stabilization mechanism and the coupling effects; and, fourth, to structure a complete regime diagram that includes both chemical and transport effects.

As a final note, practical engine conditions are highly turbulent, and the autoignition phenomenon depends on both chemistry and turbulent mixing. For example, in a DNS study, Yoo et al. [13] observed the cyclic movement of the stabilization point of a turbulent lifted ethylene jet flame in highly-heated coflow, which is a consequence of consecutive autoignition events in the high-speed jet and coflow. When fuels involve more complicated chemical characteristics, such as NTC effects, turbulence plays different and potentially competing roles. As demonstrated in a more recent computational work by Echekki and Ahmed [14], although scalar dissipation rate tends to delay ignition due to heat and radical loses from nascent kernels, enhanced mixing ensures much larger volumetric heat release rate after ignition. However, neither of these works has considered high pressure regimes and analyzed the complicating effects of NTC in detail. Therefore, in order to better understand flame stabilization and provide insights for future studies on turbulent lifted flames at elevated temperatures and pressures, the current work focuses on laminar conditions.

2. Computational details

An axisymmetric DME stream at 300 K is surrounded by heated coflow air at 30 atmospheres. The fuel nozzle diameter D is 0.8 mm, and the fuel and air are initially separated by an adiabatic, no-slip wall with thickness $D/20$. The diameter of the coflow is 3.9 mm with adiabatic, slip wall boundary conditions. This diameter was chosen to be wide enough such that further widening of the domain did not influence the computational results. Uniform inlet velocities of 2.4, 3.2, and 8.0 m/s for both streams were specified. The outlet boundary condition is a convective outflow, which is a Neumann condition at steady-state.

Table 1
Computational domain and number of grid points.

Inlet velocity [m/s]	2.4	3.2	8.0
L_x [mm]	3.5	3.5	15
N_x	1536	1536	3072
N_r	176	176	176

The governing equations, transport model, and chemical model were adopted to be the same as in Deng et al. [12]. In brief, the Navier-Stokes equation with buoyancy effects in the streamwise direction and the conservation equations of mass, species, and energy were solved. The species diffusivities are determined assuming a constant, nonunity Lewis number and kept the same as in the previous work [12]. The conserved scalar mixture fraction Z is specified as unity and zero for the fuel stream and coflow, respectively, and is computed by solving a conserved scalar transport equation with unity Lewis number [15]. A DME skeletal mechanism of 39 species [16], which was reduced from the well-validated detailed mechanism of Zhao et al. [17], was adopted as the chemical model.

The governing equations with the low-Mach number formulation are solved using NGA [18]. The momentum and scalar equations are discretized with a second-order centered scheme and a third-order WENO scheme [19], respectively, on a staggered mesh. An iterative second-order semi-implicit Crank–Nicolson scheme is adopted for temporal integration [20]. The chemical source terms for the species and energy equations are integrated using the CVODE package [21].

Leveraging previous grid convergence studies [12], uniform grid spacing in the axial direction was set to $\Delta x = 2.2$–$4.8\ \mu$m, depending on the case. Nonuniform grid spacing in the radial direction was set to minimum $\Delta r = 2.5\ \mu$m to resolve the mixing layer near the thin wall, and the grid stretch rate was less than 3%. Details about the numerical discretization are summarized in Table 1.

3. Transport effects

Transport effects on nonpremixed coflow flame stabilization were demonstrated by fixing the coflow temperature at 900 K while varying the uniform inlet velocities as 2.4, 3.2, and 8.0 m/s. The 3.2 m/s case was computed in previous work [12].

3.1. Thermal and chemical structure

The heat release rate profiles for the three cases are shown in Fig. 1. A qualitative determination of the stabilization point is the most upstream point on the largest heat release contour (the leading point), colored by red. The mixture fraction iso-contours of $Z_{st} = 0.1005$, $Z = 0.2$, and $Z = 0.3$ are delineated in solid black lines, from right to left.

When the inlet velocity is the lowest, 2.4 m/s, a tribrachial thermal structure is observed very similar to that of the classical triple flame. The triple point at $Z = 0.15$, where the three large heat release branches intersect, is also the stabilization point. Some heat release can be found upstream of the tribrachial thermal structure for the partially reacting mixture at elevated temperature but is much less than the heat release from the flame structure. As the inlet velocity increases to 3.2 m/s, another branch with large heat release is found attached to the tribrachial structure around $Z = 0.2$. The stabilization point is, again, the same as the triple point. This structure has been analyzed in our previous work [12]. However, as the inlet velocity further increases to 8.0 m/s, the stabilization point is no longer on the tribrachial structure. Instead, it is found to be near $Z = 0.25$ and is the intersection point of two trailing heat release branches. Attached to the leaner branch, there is a tribrachial structure that