The evolution of autoignition kernels in turbulent flames of dimethyl ether

Andrew R.W. Macfarlane*, Matthew Dunn, Mrinal Juddoo, Assaad Masri

School of Aerospace, Mechanical and Mechatronic Engineering, The University of Sydney, J07 - Mechanical Engineering Building, NSW 2006, Australia

ABSTRACT

Simultaneous planar laser-induced fluorescence (PLIF) imaging of CH_2O and OH was performed at a repetition rate of 10.kHz, jointly with chemiluminescence to explore autoigniting dimethyl ether (DME) flames in a hot vitiated coflow burner. The focus of the study is the imaging of the flame stabilization region and the temporal evolution of ignition kernels upstream of the flame base. Results detail the evolution of kernels throughout their formation, growth and final merging with the flame base. The ignition events were explored for a range of different fuel premixing and dilution ratios over two coflow temperatures which result in different lift-off heights. Images of CH_2O and OH over the entire flame length show that not only is the lift-off height much higher at low coflow temperatures, but that the fluctuations are more intense and the region of kernel formation is larger both radially and axially. In these autoignition stabilized flames, increased premixing leads to the lift-off height and location of the maximum kernel formation rate being further downstream. Transient 1-D simulations of hot coflow products opposed against jet fuel mixtures identify that the overlap of CH_2O and OH PLIF signals are a reliable marker of heat release in autoignition kernels. Measurements indicate that for the high coflow temperature cases, on average, the heat release of individual kernels is low, despite the high total kernel formation rate. This can be correlated to the slow growth rate and elongated aspect ratio of the kernels. For low coflow temperature cases, kernels are growing faster and have high heat release rates with near unity aspect ratios.

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1. Introduction

Dimethyl ether (DME) is a promising alternative to conventional fossil fuel-derived diesel in compression ignition engines [1]. Another application of DME is in land-based gas turbines where it can potentially replace compressed natural gas (CNG) and liquefied petroleum gas (LPG) as a cleaner fuel [2]. DME has several desirable combustion properties such as a high cetane number, low autoignition temperature and a low sooting propensity by virtue of the fuel bound oxygen. However, due to the multiple competing chemical pathways leading to autoignition [3], the low-temperature chemistry of DME is significantly more complicated compared to simpler fuels such as methane and syngas.

The autoignition combustion process compared to freely propagating flames contains significant differences in terms of low-temperature chemistry and chemical time scales; and as such has received considerable attention both numerically and experimentally for a variety of fuels. Experimental studies have mostly focused on three jet in hot coflow burner (JHC) configurations, which provide conditions that are comparable to practical applications such as: exhaust gas recirculation (EGR) in gas turbines. These three burner configurations are: (i) The jet in a hot vitiated coflow (VCB) investigated by Cabra et al. [4,5], Gordon et al. [6,7], Oldenhorf et al. [8–11] and Arndt et al. [12,13], (ii) fuel jet in heated air, Markides and Mastorakos [14] and, (iii) Mild combustion by Medwell and Dally [15–17]. The JHC is studied extensively using hydrogen [5,7,18,19], methane [9,20] and more recently heptane [21], which have shown qualitatively similar stability with the lift-off height being strongly dependent on the temperature of the coflow. High-speed imaging of chemiluminescence as well as laser-induced fluorescence (LIF), have also shown that autoignition is initiated by the formation of kernels upstream of the flame base [6]. Oldenhof et al. [8,9] have used ignition statistics to identify autoignition as the main stabilizer, indicating ignition kernels form upstream then grow and convect downstream to meet the flame base. Ardnt et al. [22,23] have used pulsed methane jets in a hot vitiated coflow to confirm that ignition occurs in very lean mixtures where the scalar dissipation rates are low.

Using heated air to initiate autoignition, Markides and Mastorakos studied the effect of turbulence on ignition delay times. They have shown that increasing the turbulent length scale by altering the fuel nozzle diameter increases the ignition delay time [32]. However, increased Reynolds number for the same jet diameter increases entrainment of hot coflow fluid and hence lowers the location where initial reactions occur [33]. In the third configuration of Mild combustion, autoignition remains the dominant mode of stabilization. However, Medwell et al. [16] highlight an 'apparent' lift-off height upstream of a faintly attached OH tail to the exit nozzle. This is in contrast to the more distinct OH gradient at the flame base in the case of the JHC burner.

Numerical studies on the autoignition of turbulent flames may be classified in two broad categories: direct numerical simulation (DNS) and either large eddy simulations (LES) or RANS with a relevant combustion model. DNS studies have established that autoignition events occur mostly in regions of lean mixture fractions (most reactive mixture fractions) and at low scalar dissipation rates [24,25]. Echekki and Chen [26] have shown kernels to initiate in lean mixtures but the flame propagation crosses stoichiometric contours leading to burning of richer mixtures. Sreedhara and Lakshmisha [27] have shown vortex shedding in 3-D DNS produces faster ignition delay times than 2-D DNS. Cao and Echekki [28] performed 3-D DNS, indicating lean autoignition kernels initially propagate in a similar most reactive mixture fraction field then extending into rich regions; a conclusion also supported by Echekki and Chen [26]. Further details on autoignition propagation and the coflow burner topic may be found in the review by Mastorakos [29]. DNS studies by Yoo et al. [3,30] used chemical explosive modes to demonstrate that lifted hot coflow flames are stabilized by autoignition. The oscillation and upstream 'jumps' in the flame base are due to kernel merging events, where premixed stabilization is not responsible for any upstream propagation.

Large Eddy (LES) and Reynolds Average Navier Stokes (RANS) simulations of autoigniting flames have been performed for the various burner configurations mentioned earlier. Using RANS with a composition probability density function (PDF) and detailed chemical kinetics Gordon et al. [31,32] analysed the concentration of radicals and transport budgets in JHC flames at different coflow temperatures. Numerical simulations have identified that a radical build-up (HO_2, H_2O_2 and CH_2O) occurs in the lead-up to autoignition [33]. There is a transition from a convective-reactive balance when autoignition prevails to a diffusive-reactive balance when premixed flame propagation is the dominant mode of stabilization [34]. Laminar DME autoigniting flames [35] have shown a transition from autoignition to flame propagation stabilization for increased coflow temperatures. Further PDF methods by Masri et al. [36] showed the ignition and hence stabilization to be largely controlled by chemistry rather than mixing rates. LES simulations [20,37,38] of autoigniting methane flames have confirmed the concept of the most reactive mixtures being responsible for initiating autoignition.

Existing knowledge on autoignition acquired from earlier studies should carry across to DME, notwithstanding the additional complexities of chemical kinetics. The formaldehyde radical (CH_2O) has been used as a low-temperature and ignition marker in high-pressure experiments [39] to identify the first and second stages of ignition for DME [40]. Imaging of OH and CH_2O LIF was performed simultaneously [17,41–44] to identify low and high-temperature regions, where their spatial overlap is employed as a marker for heat release [45] as is done in this work.

Reliable chemical kinetic mechanisms are needed to compute the autoignition delay times which are subsequently used to predict lift-off heights in laminar [46,47] and turbulent [48] autoignition flames. Since DME displays mild negative temperature coefficient (NTC) behaviour and has significant low-temperature re-

actions [49] there are potential difficulties in obtaining reliable mechanisms to correctly predict ignition delay times. Three mechanisms for DME are commonly applied (NUIG Mech_56.54 [50], NUIG Aramco Mech 1.3 [51], and Zhao et al. [52]) with the former showing the best agreement with measured data [53,54]. Reduced mechanisms such as Pan et al. [55] remove certain minor pathways to minimize computational cost compared to the large parent NUIG Mech_56.54 [50] mechanism. The reduced mechanism has been shown [55] to represent experimental delay times for DME at a range of ignition temperatures, where species, OH and CH_2O are also well represented.

The simplest reactor is typically the 0-D homogenous constant pressure reactor, which can identify delay times and additionally demonstrate negative temperature coefficient behaviour described by Li et al. [56]. This was also confirmed by Echekki and Ahmed [57] who demonstrated DME's dual stage ignition. Owing to imposed scalar dissipation from turbulent flow fields, opposed flow simulations between cold fuel and heated oxidants are often used. The opposed flow reactors show S-shaped plots of temperature versus strain rate [58]; with autoignition found to occur only for strain rates below a critical value. Increased DME fuel fraction with N_2 and increased strain rates have the effect of increasing the ignition temperature ranging between 900–1300 K [59]. Transient counterflow flames (used in this study) with a heated oxidant against a fuel jet [13, 40] have been used to identify how increased strain rate or scalar dissipation rate serve to increase delay times.

The current paper builds upon previous work [60] that studied autoignition and flame stabilization processes in DME flames primarily using chemiluminescence as a diagnostic tool. It addresses the influence of ignition kernels and their dependence on the flame base stabilization. A link between the formation rates and relative heat release of autoignition events for varying coflow temperatures and premixing/dilution ratios with DME is observed. Joint PLIF of OH and CH_2O is performed to resolve the flame structure in the stabilization zone and kernel heat release measurements are reported for a range of coflow temperatures.

2. Experimental setup

2.1. Hot coflow burner

The hot coflow burner in this experiment is similar to that studied by Cabra et al. [4,5] and used previously at the University of Sydney [20,60]. The diameter of the coflow is 197 mm with $\sim$1800 $\times$ 1.6 mm diameter holes to stabilize the lean H_2/air flames; the coflow shrouds the central fuel jet, having an inside diameter (D_J) of 4.45 mm. The burner produces a simplified axisymmetric geometry making modelling and optical access very accessible. By varying the shrouded H_2/air equivalence ratio, the required coflow temperature is established such that for this experiment a constant bulk burnt velocity of $U_C = 4$ m/s was maintained. The hot coflow provides a cone of combustion products that remains uncorrupted by laboratory air for about 60 D downstream of the stabilising plate. This region is referred to as the 'valid cone' within which all subsequent measurements are restricted.

Conditions selected for further study are listed in Table 1 along with relevant flame properties. In addition to pure DME, three other mixtures are investigated to study the effects of partial premixing with air and dilution with nitrogen. Table 1 lists two mixtures of DME with air for two volumetric ratios: 1:1 and 3:1 (three parts air and one part DME) and one dilution ratio of DME and N_2 at 3:1 (three parts N_2 and one part DME). Mean lift-off heights and their RMS values for a range of coflow temperatures at the premixing ratios studied here can be found in a previous publication [60]. Each fuel is investigated at two coflow temperatures: a lower temperature (around $T_c = 1250$ K) and a higher temperature coflow of