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Structural differences of ethanol and DME jet flames in a hot diluted coflow

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ABSTRACT

This study compares the flame structure of ethanol and dimethyl ether (DME) in a hot and diluted oxidiser experimentally and computationally. Experiments were conducted on a Jet in Hot Coflow (JHC) burner, with the fuel jet issuing into a 1250-K coflow at three oxygen levels. Planar measurements using OH-LIF, CH_2O-LIF, and Rayleigh scattering images reveal that the overall spatial distribution and evolution of OH, CH_2O, and temperature were quite similar for the two fuels. For both the ethanol and the DME flames, a transitional flame structure occurred as the coflow oxygen level increased from 3% to 9%. This indicates that the flames shift away from the MILD combustion regime. Reaction flux analyses of ethanol and DME were performed with the OPPDIF code, and ethane (C_2H_6) was also included in the analyses for comparison. These analyses reveal that the H_2/O_2 pathways are very important for both ethanol and DME in the 3% O_2 cases. In contrast, the importance of fuel-specific reactions overtakes that of H_2/O_2 reactions when fuels are burnt in the cold air or in the vitiated oxidant stream with 9% O_2. Unsteady laminar flamelet analyses were also performed to investigate the ignition processes and help interpret experimental results. Flamelet equations were solved in time and mixture fraction field, which was provided by non-reactive Large-Eddy Simulation (LES).

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1. Introduction

The ever-rising concern for the environment has increased efforts to improve energy efficiency and reduce pollutant emissions. Amongst advanced combustion technologies, Moderate or Intense Low-oxygen Dilution (MILD) combustion is a promising technology because of its potential to reduce emissions while maintaining a high thermal efficiency [1]. In practical devices, MILD combustion is usually established through a strong recirculation of hot exhaust gases. This leads to volumetric reactions without visible flames under some conditions [1,2]. Hence it is also referred to as flameless oxidation (FLOX®) [1]. Under MILD combustion conditions the peak flame temperature is reduced due to a larger total volume of gases and the altered chemistry at a lower local oxygen concentration. Consequently, this causes a drastic reduction in emissions, particularly in nitrogen oxides [3,4].

Previous studies of MILD combustion [5–9] have mostly focused on common fossil fuels. There are limited studies that investigate MILD combustion of renewable fuels [10,11]. Experimental measurements performed on the Jet in Hot Coflow (JHC) burner revealed a similar reaction zone structure of natural gas, ethylene, and LPG flames when hydrogen was added to the three fuels. This suggests different types of fuels are interchangeable under MILD combustion conditions [12]. Supporting this, Derudi and Rota [4] have reported that the averaged flame temperature and pollutants emissions were similar for methane and LPG flames when they were burnt in the MILD combustion mode. Whilst it is true that some previous studies have shown that for simple fuels the flame characteristics under MILD combustion conditions are very similar [4,12], this is not true for more complex fuels [8,13,14]. For instance, visible flames and high NO_x emissions were reported as distinctive features when heavy fuel oil was used instead of light fuel oil in a MILD furnace [8]. Reddy et al. [13] found that lower NO_x and unburned hydrocarbon emissions were produced when a combustor was fired with a mixture of biodiesel and diesel rather than pure biodiesel. Ye et al. [14] performed a comparative study of ethanol, acetone, and *n*-heptane in a reverse-flow MILD combustor. They found that combustion of acetone and *n*-heptane became unstable at equivalence ratios of 0.7–0.8 and elevated pressures, where visible flames and high emissions were observed [14].

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Meanwhile, stable combustion of ethanol was established under all the investigated conditions [14].

A better understanding of the impact of fuel type on the flame structure is required, particularly for fuels that are more complex than methane and hydrogen. Due to increasing interest in reducing the dependence on petroleum-derived fuels and diversifying the energy supply, alternative fuels have received great attention. Combining alternative fuels with MILD combustion would exploit the benefits of both, leading to more efficient combustion with lower emissions. Ethanol (CH_3CH_2OH) and dimethyl ether (CH_3OCH_3), isomers of C_2H_6O, are very promising fuels. Comparing them also provides an opportunity to explore the impact of molecular structure on the flame behaviour under vitiated coflow conditions.

Ethanol (EtOH), a type of alcohol, has a low tendency to generate soot and particulate-matter [15]. Due to its high flame speed it can be burnt at very lean conditions with a relatively low flame temperature [16]. As a consequence, NO_x emissions are suppressed. Ethanol can be produced from a wide range of renewable raw materials. Second generation bio-ethanol is derived from lignocellulosic biomass like wood, which is not in competition with food chain [17]. Its renewable nature, low emissions, and reduced production costs make it an attractive alternative fuel [18].

Dimethyl ether (DME), the simplest ether, is an excellent alternative fuel for transportation and power generation [19]. For instance, DME can be used as a substitute for diesel fuels due to its capacity to abate soot emissions [20]. The existence of an O atom and absence of any C–C bonds in DME contribute to its smoke-free nature [21]. It is also an ideal ignition promoter in engines not only because of its low auto-ignition temperature and high cetane number, but also because of its rapid vaporisation upon injection [20]. It can be manufactured from a variety of resources such as natural gas, wastes, and biomass [20].

Due to the potential utility of DME in gas turbine applications, the comparison between DME and methane (main component of natural gas) has attracted great interest. Lee and Yoon [22] tested DME in a gas turbine, and they reported that lower NO_x emissions were produced from DME than methane. Chen et al. [23] investigated the impact of adding DME to methane-air flames on the ignition characteristics. They found that the ignition delay times of the methane-air mixture were significantly shortened due to a rapid build-up of CH_3 and HO_2 radicals with the presence of DME [23].

Limited comparative studies [24–32] have been performed to investigate the effect of molecular structure on the combustion behaviour of DME and ethanol flames. Most of these studies were focused on the role of the structure of oxygenated fuels in reducing soot precursors and soot particulates.

Previous studies have investigated the autoignition and extinction characteristics of ethanol and DME [25,33]. Wang et al. [25] reported that DME flames were more resilient to extinction than ethanol flames, though this difference decreased as the fuel jet became more diluted with N_2 [25]. Tingas et al. [33] performed an analytical analysis of the autoignition characteristics of ethanol/air and DME/air homogeneous mixtures at an initial pressure of 5 MPa and an initial temperature of 1100 K. This analysis revealed an overall shorter ignition delay in the ethanol/air case. They found that the C–C bond in ethanol is maintained and the hydrogen chemistry plays a dominant role at the early stage of autoignition [33]. In contrast, the autoignition of DME/air is initiated by single-carbon chemistry [33]. As the reaction progresses, similar hydrogen chemistry pathways dominate in both fuels [33]. Formaldehyde was reported to be insignificant in the autoignition dynamics of ethanol/air mixtures, while adding formaldehyde can promote or retard the ignition of DME/air mixtures depending on the initial temperature [34].

There is a paucity of information on ethanol and DME flames under conditions relevant to MILD combustion. Kang et al. [10] investigated NO_x emissions of DME flames in a MILD burner. They found that the NNH-intermediate pathway was the major route for NO_x formation in DME flames under MILD combustion conditions [10]. Rodrigues et al. [11,35] studied the ethanol spray flame structure in a hot and vitiated coflow. An enhanced spray evaporation in the presence of hot coflow led to changes in the atomisation mechanism, with an immediate liquid jet break-up near the atomiser [11]. Moreover, the reduced local oxygen concentration shifted the stoichiometric mixture fraction away from the spray axis, consequently reducing the peak flame temperature [11]. The liftoff heights of the ethanol spray flames were found to be dependent on the droplet convective, vaporisation, and chemical time scales before ignition [35].

The present paper aims to improve the understanding of the impact of fuel structure on MILD flames by performing a combined experimental and computational investigation of ethanol and DME. In order to control parameters independently, a JHC burner was used to emulate a MILD furnace environment where the gas mixture inside the combustion chamber is hot and diluted, with a fuel stream injecting into it. In this configuration, DME or prevaporised ethanol was issued into a hot and diluted coflow with the O_2 level varying from 3% to 9% (by volume). To reveal the flame structure of the two fuels, the distributions of OH, CH_2O, and temperature have been measured instantaneously and simultaneously. Digital photographs and images of OH* chemiluminescence have also been recorded. To help explain the experimental observations, laminar flame calculations using the OPPDIF code and unsteady flamelet simulation have been performed. The purposes of the simulations in this paper are not to directly simulate the experimental flames. Instead, numerical simulations and experimental observations complement each other. The steady-state OPPDIF analysis was performed to compare the chemistry of the two isomers, ethanol and DME, particularly via reaction flux analysis. This configuration is ideally suited to focusing on the fuel chemistry while isolating the impact of turbulence that occurs in the experiments. The unsteady flamelet model was employed to provide information on the transient ignition processes of the two fuels.

2. Experimental details

2.1. Experimental setup and operating conditions

The basic configuration and operation of this JHC burner shown in Fig. 1 are the same as in a previous study [36]. The JHC burner consists of an insulated central fuel jet (ID = 4.6 mm) surrounded by an annular coflow (ID = 82 mm). This coflow is generated from a secondary porous-bed burner located 90 mm upstream of the jet exit plane. The hot vitiated coflow was produced from the combustion of a lean mixture of natural gas (92% methane by volume), hydrogen, air, and nitrogen. The mole fractions of natural gas, hydrogen, air and nitrogen were manipulated to vary the coflow oxygen level from 3% to 9% by volume, while the temperature and C/H ratio were kept constant. The temperature of various coflows (T_{coflow}) was kept at 1250 K. The three hot coflow conditions are summarised in Table 1. To obtain a fully developed turbulent pipe flow, the length of the central fuel jet is more than 100 times the jet diameter. The burner was wrapped with ceramic fibre insulation to minimise heat losses and maintain a constant temperature of the coflow.

As shown in Fig. 1, ethanol was heated and mixed with carrier gas in a Controlled Evaporator and Mixer (CEM). The temperature of the heater inside the CEM was set by the Bronkhorst control unit, which also controlled the mass flow rates of ethanol and carrier gas. The preheat temperature was around 413 K, which is

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