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Ignition features of methane and ethylene fuel-blends in hot and diluted coflows

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ABSTRACT

Turbulent flames in the moderate or intense low oxygen dilution (MILD) combustion regime have previously exhibited less susceptibility to lift-off than conventional autoignitive flames in a jet-in-hot-coflow (JHC) burner. This has been demonstrated through laser-based diagnostics and examination of CH^* chemiluminescence. New experimental observations are presented of turbulent flames of natural gas, ethylene and blends of the two fuels, in coflows with temperatures from 1250–1385 K and oxygen concentrations from 3–11% (vol./vol.). Zero- and one-dimensional simulations, as well as turbulent flame modelling, are used to explain the trends seen experimentally with different coflows and fuels. Numerical simulations using simplified batch reactors and opposed-flow flames demonstrate that blending of methane and ethylene fuels is most significant near 1100 K. Near this temperature, pure ethylene exhibits a transition between high and low temperature ignition pathways. Further analyses show that a 1:1 methane/ethylene blend behaves more like ethylene near MILD combustion conditions, and more like methane in conventional autoignition conditions. Two-dimensional modelling results of the turbulent flames are then discussed and explained in the context of the simplified reactor results. The flames confined by the lean flammability-limit in the coflow and high strain-rates in jet shear layer, in agreement with previous work using a semi-empirical jet model. The two-dimensional modelling is additionally able to qualitatively replicate the trends in lift-off height, with normalised heat release rate profiles reproducing, and serving to explain, the effects seen in experimental campaigns.

1. Introduction

Moderate or intense low oxygen dilution (MILD) combustion has been the subject of previous investigations due to its potential to reduce pollutant emissions and increase thermal efficiency in practical systems [1]. This combustion regime has already been successfully implemented in furnaces and burners with strong recirculation [2–4], and similar systems have been suggested for applications such as gas turbines [5], however further fundamental understanding is required for MILD combustion in these applications [6].

Previous experimental studies of non-premixed MILD combustion have been undertaken in jet-in-hot-co-/cross-flow (JHC) burners [7–20]. These studies have investigated the combustion of gaseous, pre-vaporised liquid and solid fuels under MILD combustion conditions, and in the transition between the MILD and conventional autoignitive combustion regimes. Among these, studies of natural gas (NG) and C_2H_4 have demonstrated non-monotonic trends in visual lift-off height with changing oxidant O_2 level [12,19]. These trends are evident in laminar and turbulent flames in the transition between MILD and autoignitive combustion regimes, however, the underlying mechanisms behind these trends remain unresolved [12]. The flame structure and stabilisation mechanisms of non-premixed flames in the transition between MILD combustion and conventional, lifted, autoignitive flames are not very well understood [12,19,21], and exhibit significant instability and sensitivity to ambient conditions [2,12,13,22].

The ignition of MILD flames has been widely investigated in premixed, homogeneous reactors [23–27]. These studies have used different measures of ignition to define ignition delay, such as the time required for a 10-K increase above the unreacted mixture temperature [23–25], or the onset of thermal runaway [26–28]. This initial temperature increase occurs almost simultaneously with thermal runaway in conventional autoignition, however these do not coincide during the more gradual ignition processes in MILD combustion [21]. Ignition processes in MILD combustion, have shown good agreement with a 10-K temperature increase threshold in predicting ignition delay and the onset of

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chemiluminescence [21,23–25]. Although simplified reactors may be used to provide an estimate for the ignition delay of a homogeneous chemical mixture, neither well-stirred nor plug-flow reactors can provide insight on the effects of mixing, strain-rate or diffusion encountered in practical combustion systems.

Numerical modelling of non-premixed MILD combustion has been previously undertaken using opposed-flow simulations to build on the understanding of flame structure and stabilisation. Simplified opposed-flow flames have previously been used to predict species distributions within turbulent flames in mixture fraction (Z) space [7,29], and to explain the distribution of species and heat release rate (HRR) within MILD flames [30,31]. This modelling approach has additionally been used to assess the stability [10,26] and ignition behaviour [10,19,21,27] of MILD flames. These studies have suggested that MILD flames are stabilised through partial premixing of O_2 into the fuel stream [10], however transient analysis of opposed-flow flames determined that this simplified configuration is inappropriate for modelling ignition delay [21] without a reasonable estimate of the underlying physical flow-field [19].

The flow-field of a JHC burner may be modelled using CFD with a Reynolds-averaged Navier–Stokes (RANS) approach. The RANS approach has been used for the validation and verification of combustion models, with MILD combustion shown to require finite-rate chemistry modelling due to Damköhler numbers (Da) of order unity [32,33]. Several modelling attempts have been made to compare combustion models against previously obtained experimental results using RANS and the eddy dissipation concept (EDC) combustion model [32,34–40,33,41–44] or higher-fidelity large-eddy simulations [45–47]. These studies have predominantly been for model validation or focussed on the structure of the flames downstream. Beyond the coflow-controlled region, however, the simulated oxidant composition is heavily dependent on the model boundary conditions and the flame is greatly affected by the entrainment of cold, ambient air [36]. Although RANS modelling studies with adjusted EDC constants have shown reasonable agreement with experimental data [35,39,40], there has been very little work using this approach to develop understanding of flame stabilisation in the MILD combustion regime, or replicating the trends seen experimentally under these conditions [9,12].

Many studies of MILD combustion have focussed on CH_4 – the primary constituent of NG [48], or C_2H_4 – an important intermediate in the combustion of larger hydrocarbons [48,49]. Both of these fuels have previously been studied issuing into identical coflows, suggesting very similar ignition characteristics, however these were mixed with H_2 (1:1 by vol.), serving to stabilise the flames [11]. In the MILD combustion of CH_4, CH_3 recombination serves to slow the overall reaction [25], and non-premixed combustion occurs without any regions of negative HRR [30]. At temperatures below approximately 1000 K, the ignition delay of CH_4 has displayed a negative temperature coefficient (NTC) region due to competition between the CH_3 pathway and a preference for ignition via the H_2 branching pathway at high temperature [24,50]. The oxidation pathway of C_2H_4 in MILD combustion is through H abstraction to C_2H_3 and then to C_2H_2 [48,39]. This process therefore also leads to significant production of H_2 at temperatures near 1000 K, similar to the operating conditions in previous investigations with a JHC burner [9]. The unique environment in MILD combustion suggests that the H_2 ignition pathway may be more pronounced under MILD conditions for both C_2H_4 and CH_4 combustion.

Both CH_4 and C_2H_4 are produced in significant quantities during combustion of larger hydrocarbons [49] and are key species in combustion systems using combinations of NG and other, larger hydrocarbon fuels. Blends of CH_4 and C_2H_4 have been previously studied numerically and experimentally to assess the chemical and physical effects on flame speed of mixtures of these fuels at room temperature and ignition delay of dilute mixtures [51,52]. Analyses of CH_4 and C_2H_4 blends have shown that the flame speed of the mixture is more heavily dependent on kinetic influences than physical effects [52]. Kinetic analysis of different blends of CH_4 and C_2H_4 indicates that C_2 chemistry becomes significant for mixtures with more than 10% C_2H_4 [51]. The same study found that beyond this concentration, the reaction of $C_2H_4 + OH \rightarrow C_2H_3 + H_2O$ overwhelms $CH_4 + OH \rightarrow CH_3 + H_2O$ [51]. Further to this scavenging reaction, the reaction of atomic O with C_2H_4, has been shown to favour CH_3 formation below temperatures near 1000 K [53]. However, it has not been determined how significant concentrations of C_2-species, or the recombination of CH_3 in a blend of CH_4 and C_2H_4 fuels, change the flame behaviour during ignition and flame stabilisation in hot oxidants. The interaction between CH_4 and C_2H_4 under MILD conditions is unknown, although it is relevant for potential fuel blends of NG and larger hydrocarbon fuels.

Simplified reactors have been used to provide insight into the processes involved in ignition under MILD combustion conditions, however further work is required to explain the non-monotonic trends in lift-off height across the boundary of the MILD combustion regime. To meet these needs, this work will investigate trends from experimental observations and compare them against predictions from simplified reactors and RANS modelling. This will be used to assess whether trends in lift-off height may be described as the effects of ignition delay or flame extinction, or whether a more complete description of the flow-field is required. This study will not only investigate trends in the transition between the MILD and autoignitive combustion regimes, but will shed light on the ignition features of CH_4/C_2H_4 fuel blends in a hot and diluted conditions, to advance the current understanding of ignition processes under MILD combustion conditions.

2. Methods

2.1. Experimental observations of turbulent jet flames

Photographs were taken of turbulent flames in a jet-in-hot-coflow (JHC) burner, which has been used widely in previous studies [7–12,18,19]. The JHC burner features a fuel jet issuing from a 4.6-mm-diameter pipe (with a length >100 times the pipe diameter) into a concentric coflow of hot combustion products from an 82-mm-diameter secondary burner. This results in a coflow-controlled environment extending approximately 100 mm downstream. The various compositions of the coflow are given in Table 1. The fuel issuing from the central jet of the JHC burner is natural gas (NG, $\geqslant$92% CH_4), C_2H_4 or a blend in ratios of 1:2 or 2:1 (by vol.). In each case, the jet has a bulk Reynolds number (Re) of 10 000.

Photographs of turbulent flames in the JHC were taken using a Canon EOS 60D SLR camera, fitted with a 50 mm, $f_{\#}$1.8 lens. Photographs were taken with manual settings (including white balance), with the details presented later. Visual lift-off heights were determined by isolating the blue channel of these photographs, inverting them and identifying an "unequivocal" flame base or a weak-to-strong transition, similar to method of Medwell and Dally [12]. Additionally, the first instance of chemiluminescence was also identified from photographs of the same flame. In the absence of soot, the blue channel is taken to indicate CH^* chemiluminescence at 430 nm [54].

2.2. Numerical simulations of simplified reactors and turbulent jet flames

Ignition delays of CH_4, C_2H_4 and CH_4/C_2H_4 fuels were evaluated using stoichiometric, constant pressure, batch reactors using the AURORA routine from the CHEMKIN software package. Ignition