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Structure of spray in hot-diluted coflow flames under different coflow conditions: A numerical study

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ABSTRACT

This work studies the influence of coflow conditions on the structure of the Delft Spray in Hot-diluted Coflow (DSHC) flames, using Large Eddy Simulation (LES) techniques. The developed modeling approach was first applied to three different experimental cases for validation. Major properties such as droplet velocity, SMD, gas phase velocity and temperature can be reproduced with good accuracy. Also, the trends of flame lift-off height and flame width with change of coflow conditions were properly captured. Then the study was extended to four more virtual cases, which differ from each other only by coflow temperature or oxygen concentration. The purpose of this step is to eliminate the simultaneous change of multiple parameters as was done in the experiment and to isolate the influences of coflow temperature and O_2 concentration, which are important parameters for a MILD furnace design and operation. Two reaction regions (RRs) have been identified in the DSHC flame. The inner RR is created by the premixed reaction of ethanol under hot and fuel rich condition. The outer one is formed by the non-premixed reaction of intermediate fuels, e.g. CO and H_2, which are produced in the inner RR. The coflow temperature (T_{cf}) has a significant influence on the DSHC flames. Increase of flame lift-off height by a factor of five was observed when the coflow temperature was decreased from 1400 K to 1200 K. The flame changed from having a two-RRs structure to a triple flame when the coflow temperature is reduced. The outer RR shifted from non-premixed combustion at high T_{cf} to premixed combustion at low T_{cf}. The oxygen mole fraction in the coflow ($X_{O_2,cf}$) alters the role of two RRs. The inner premixed RR is strengthened with increasing $X_{O_2,cf}$. The flame peak temperature is significantly increased in the case with highest $X_{O_2,cf}$. According to Cavaliere and de Joannon's definition [1], all studied cases except the one that has the highest $X_{O_2,cf}$, falls into the MILD regime. But when a restriction of flame peak temperature ($T_{peak} < 1800$ K) is also applied, only the case with the lowest $X_{O_2,cf}$ and moderate T_{cf} can be strictly called MILD.

1. Introduction

Achieving low pollutant emissions while maintaining high efficiency and the required heat flux is a key goal for innovation in combustion research [2,3]. The MILD (Moderate or Intense Low-oxygen Dilution) combustion or "flameless oxidation" [1,4,5], has been such innovation. MILD combustion of gaseous fuels has been intensively studied both experimentally and numerically [6–9]. However, so far there has been much less research on liquid fuel MILD combustion [10–13].

Weber et al. [10] performed an experimental study of MILD combustion of various fuels and found that similar to the case of natural gas, no visible flame is present for the light oils in a vitiated coflow. Mahendra Reddy et al. [14] investigated kerosene combustion in a two stage flameless combustor. Experimental measurements showed that MILD combustion mode was achieved. An order of magnitude of reduction in CO and NO_x emission was also reported. More recently, they [15] performed an experimental study of biodiesel fuel MILD combustion in a high swirl combustor, and found that the emission is drastically reduced when the pure biodiesel is blended with conventional diesel. They concluded that the reason is that the viscosity, surface tension and boiling temperature of biodiesel can be reduced by the blending, which in turn leads to a reduced droplet Sauter Mean Diameter (SMD) and increased evaporation rate. MILD combustion of another biofuel – Butyl Nonanoate (BN) was investigated by Khalil and Gupta [16] under gas turbine condition. 15% reduction in NO emission compared to JP8 was observed, CO emission was also lower than JP8. No startup issues and combustion instabilities were observed. These studies have undoubtedly demonstrated the

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promising performance of the MILD combustion technology for liquid fuels. However, the flame structure, stabilization mechanism and the parameter optimization of the liquid-fueled MILD combustion are not fully understood.

The Delft Spray-in-Hot-Coflow (DSHC) burner was designed to study the fundamental aspects of flameless oxidation of representative biofuels—ethanol and acetone [17]. With different spray and gas phase properties measured and influences of coflow conditions and fuel flexibility studied, the DSHC dataset provides a valuable basis for the development and validation of modeling methods towards the application of MILD spray combustion [18]. The study in this paper is part of a multi-stage project that is dedicated to the numerical study of the DSHC flames, with the goal of developing a reliable modeling approach, and to better understand the mechanism of MILD spray combustion. In our previous studies, different modeling strategies have been applied to the DSHC dataset, and in general, decent results compared to experimental data were obtained [19–21].

For MILD combustion of gaseous fuels, a range of operating parameters, such as coflow conditions, fuel compositions etc., have been shown to affect the establishment of MILD condition [6,22]. To better understand the MILD spray combustion, similar parameter studies for liquid fuels are necessary. Recently, Ye et al. [13] investigated the combustion of pre-vaporized liquid fuel in a reverse-flow combustor. MILD combustion mode was successfully realized for all studied fuels (ethanol, acetone and n-heptane). They found that the air jet velocity, pressure and carrier gas of the liquid fuel all influence the combustion stability and emission levels. From experimental visualization [23] and previous numerical studies [19,20] it was confirmed that the DSHC flames are lifted from the spray injector exit. The lift-off phenomenon in spray combustion results from the disparity between time and length scales for different processes, e.g., evaporation, convection and reaction [24,25]. The coflow conditions, e.g. temperature and oxygen concentration, all have a certain influence on the lift-off height through the influence on these time scales. For example, increasing coflow temperature can significantly shorten the droplet evaporation and reaction time scale, therefore leading to a reduction of lift-off height. The decrease of O_2 concentration in the coflow, leads to the formation of the mixture condition that is less favorable for ignition, hence the flame can only be stabilized further downstream. A clear insight in the influence of these parameters on flame structures may provide valuable references for the design of liquid-fueled combustion systems that are intended to work in MILD conditions.

In the DSHC burner, the hot-diluted coflow is generated by a secondary burner that operates on a lean mixture of Dutch Natural Gas (DNG) and air [18]. A limitation of this configuration is that the coflow temperature and O_2 concentration can only change simultaneously, increase of one is always accompanied with decrease of the other. However these two can be independent parameters in a real MILD furnace, by different degrees of air preheating and internal recirculation [4]. Computational Fluid Dynamics (CFD) is an ideal tool to carry out parameter studies that are not possible or difficult to do with experiment. In this paper, three experimental cases from the DSHC dataset with various coflow conditions are first simulated and the results are carefully compared with available experimental data. The purpose of this first step is to check the reliability of the proposed numerical approaches and the developed solver [21], and its capability in capturing the trend of flame properties with change of coflow conditions. Based on the confidence obtained in the first step, some virtual cases that differ from each other only by one coflow parameter (temperature or O_2 concentration) are simulated.

The remaining of the paper is structured as follows: the experimental dataset and numerical approaches are first presented in Section 2, a description of the cases that will be studied in the present paper is also given in this section. The results and discussions will be given in Section 3 along the line of first experimental validation and then numerical parameter study. Main findings of this study are summarized in Section 4.

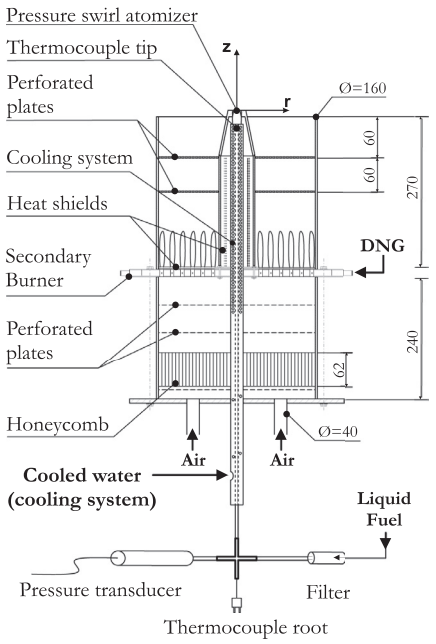

Fig. 1. Schematic of the DSHC burner [17].

2. Experimental setup and modeling approaches

2.1. Experimental setup

The schematic of the DSHC burner is shown in Fig. 1. The liquid fuel (ethanol) is injected into the hot-diluted coflow by a pressure-swirl atomizer. The hot-diluted coflow is generated by a secondary burner matrix to emulate the diluted air by recirculated combustion products in a large scale MILD combustion furnace. Comprehensive laser diagnostic measurements, including Laser Doppler Anemometry (LDA), Phase Doppler Anemometry (PDA) and Coherent Anti-Stokes Raman Scattering (CARS) have been conducted. Gas phase velocity components, temperature and O_2 volume fraction have been measured along the radial direction at coflow exit ($\mathcal{Z} = 0$ mm). Droplets properties (velocity, diameter, number concentration and mass flux) have been measured along the radial direction at different axial locations ($\mathcal{Z} = 8, 10, 12, 15, 20, 30, 35, 40, 45$ mm). Gas phase temperature has been measured with CARS technique along the radial direction at different axial locations ($\mathcal{Z} = 15, 20, 30, 40, 50, 60$ mm). For further details about the DSHC burner and the database, the readers are referred to [17,23]. The experimental data will be compared with simulation results for validation purpose.

2.2. Simulation cases

As explained in the introduction, in this paper we first simulate three cases from the DSHC dataset, namely the case "H_I", "H_{II}" and "H_{III}" [23]. These three cases all use ethanol as fuel, and the coflow consists of hot combustion products generated by the secondary burner. The main parameters for these cases are described in Table 1. Subscript "*cf*" refers to the property of coflow, and the last two columns are the turbulent intensity and mass flow rate of the liquid fuel. One may notice that the coflow temperature and O_2 mole fraction shown in Table 1 are different from those reported in