Combustion and Flame 196 (2018) 416–423

Contents lists available at ScienceDirect

Combustion and Flame

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

Characterization of ozone-enhanced propane cool flames at sub-atmospheric pressures

Mohammadhadi Hajilou, Erica Belmont*

Department of Mechanical Engineering, The University of Wyoming, 1000 E. University Ave., Laramie, WY, USA

ARTICLE INFO

Article history:
Received 24 January 2018
Revised 3 July 2018
Accepted 3 July 2018

Keywords:
Low temperature oxidation
Negative temperature coefficient (NTC)
Cool flame
Propane
Directed relation graph (DRG)

ABSTRACT

A recently developed experimental setup for the study of cool flames was employed to investigate low temperature combustion of propane. Cool flames were stabilized though ozone activation using a laminar flat flame Hencken burner at sub-atmospheric pressures. Propane cool flame stability was observed to be highly sensitive to pressure, and a pressure stability map is presented for a range of equivalence ratios (ϕ) from 0.17 to 1.0 in 0.17 increments and a range of reactant flow rates. Based on the stability map, a propane cool flame of $\phi = 0.17$ at 17.3 kPa was chosen for further study. Flame lift-off height above the burner surface was measured and two operating regimes of burner-stabilized and freely propagating flames were observed. The intersection of these two regimes was used to estimate the cool flame propagation speed. Temperature measurements of the cool flame were taken and used in fixed-temperature numerical flame simulations. Additionally, flame temperatures and propagation speeds are presented for all equivalence ratios and pressures where stable, freely propagating flames were observed in the stability map. In order to enable non-fixed temperature, freely propagating cool flame simulations to be performed, reduction of a chemical kinetics model using the Directed Relation Graph method (DRG) in conjunction with reaction rate sensitivity analysis was performed. Experimentally determined propagation speed, temperature and species concentrations at partial equilibrium were compared to numerical simulations with reasonable agreement and results are discussed.

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1. Introduction

Both high and low temperature oxidation kinetics have a significant role in the combustion of hydrocarbon fuels, and a detailed understanding of chemical kinetics can aid in yielding higher thermal efficiency in engines and other combustors and lowering pollutant production [1]. Several works have reported on the importance of low temperature fuel oxidation to engine knock in internal combustion engines [2–5]. Although various studies have been performed to investigate chemical kinetics of high temperature oxidation [6–9], low temperature fuel oxidation, where negative temperature coefficient (NTC) behavior is observed, is still lesser understood [10]. Improved understanding of low temperature oxidation, or cool flames, requires both experimentation and development of chemical kinetics models, and comparison of numerical results with experimental results for model validation [1,10–13].

In this regard, there exists a need for an experimental platform which can be employed to investigate low temperature oxidation of fuels under strongly coupled chemistry-transport conditions. Many experimental platforms, such as Rapid Compression Machines (RCMs) [14,15], have been widely used to measure low temperature ignition delays as well as species concentrations at highly diluted mixture conditions to suppress heat release, which culminates in weak chemistry-transport coupling. In a recent work by Hajilou et al. [16], an experimental setup was developed and utilized for the study of freely propagating dimethyl ether (DME) cool flames, in which a flat flame laminar Hencken burner facility was used as a platform [17,18] and ozone (O_3) enhancement was employed [19–21] to produce stabilized freely propagating DME cool flames for the study of flame lift-off heights, propagation speed, stability, and temperature and species measurements. The aforementioned experimental setup used in this study for characterization of propane cool flames utilizes undiluted mixtures, resulting in highly coupled chemistry and transport for model validation in a reactive-diffusive system. O_3 plays a crucial role in cool flame stabilization, in that O_3 decomposes in the upstream region of the cool flame via $O_3\ (+M) = O + O_2\ (+M)$ with low activation energy, producing O atoms in the preheat zone of the flame [16,20]. These O atoms participate in H-abstraction reactions with the fuel molecule, and low temperature chemistry is initiated through a radical recombination reaction of the fuel radical with

* Corresponding author.
E-mail address: ebelmont@uwyo.edus (E. Belmont).

https://doi.org/10.1016/j.combustflame.2018.07.001
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O_2 ($R + O_2 = RO_2$). Next, OH radicals are produced through chain branching reactions of RO_2 that accelerate the cool flame chemistry, which is slow in comparison with high temperature oxidation.

Many attempts have been made to model and understand the low temperature oxidation of alkanes [22–25]. Propane (C_3H_8) has been reported to be the smallest alkane demonstrating NTC behavior, and propane cool flame propagation speeds under reduced-gravity conditions were investigated by Foster and Pearlman [26] for an equimolar mixture of propane/oxygen. Moreover, Fairle et al. [27] performed an experimental and numerical study on equimolar propane cool flames in reduced-gravity conditions and derived a reduced kinetics model for their work. Multi-stage ignition of cool flames was shown, and it was observed that oscillatory behavior in cool flames can occur under non-adiabatic conditions.

There exist three combustion regimes in the course of full hydrocarbon fuel oxidation: cool flame, which incorporates the NTC behavior; double flame, which is a transitional stage between cool flame and hot flame; and hot flame, which encompasses high temperature oxidation [28,29]. As was mentioned in a previous work by Hajilou et al. [16], a trailing hot flame downstream of the cool flame is avoided in the utilized experimental setup. This phenomenon is in contrast to what was reported by Ju et al. [28] who, in a numerical study, discussed the existence of a trailing hot flame after the cool flame was ignited. It was explained in [16] that, due to the uniqueness of the experimental setup, the trailing hot flame is quenched downstream of the cool flame due to ambient gas entrainment in the far-field. This permits a stabilized cool flame to be achieved in the absence of a trailing hot flame. The role of flow residence time on cool flames was studied in [30,31], where it was suggested that one method to attain a steadily propagating planar cool flame in numerical simulations was to abbreviate the downstream flow time, thereby inhibiting the transition to a hot flame. This suggested mode of hot flame suppression aligns with the experimental technique utilized in [16] and the current study. Due to the transition that will occur in an adiabatic system with infinite flow field, fixed temperature simulations were performed in [16], where an experimental temperature profile was measured and the energy equation was not solved so as to avoid the transition from cool flame to hot flame observed in non-fixed temperature simulations.

In the study of combustion kinetics, whether in fixed or non-fixed temperature simulations, many methods have been developed to reduce chemical kinetics models, such as the method of Directed Relation Graph (DRG) [32–35]. Generally, mechanism reduction is performed to improve the usability of these models in large scale simulations. Lu and Law [32] reported the use of auto-ignition simulations for low to mid-high temperature oxidation and perfectly stirred reactor (PSR) simulations for high temperature oxidation in the implementation of DRG. In cases where there was a need to include the NTC regime in the reduced mechanism as well, the starting temperature was chosen in the NTC regime [33]. Reduction of chemical kinetics models for propane cool flames to capture the multi-stage ignition phenomenon was performed by Fairlie et al. [27], in which they used CHEMKIN [36] and KINALC [37] along with sensitivity analysis to remove unnecessary species and reactions. Also, Gupta [38] utilized Rate of Production (ROP) analysis to reduce chemical kinetics models for propane cool flames and capture the multi-ignition phenomenon, and the importance of the base mechanism used for the reduction procedure is highlighted in that work. It has been recognized in the literature that chemical kinetics models have some uncertainty regarding the reaction pathways throughout the NTC regime in cool flames. For example, Benson [11] discusses in detail the role of the NTC regime in the oxidation of propane cool flames and notes that, because the cool flame behavior depends on rate of heat release and coupling between chemical kinetics and heat transfer, it is complex and difficult to model. Cord et al. [13] examined low temperature propane oxidation at atmospheric pressure using a jet-stirred reactor and gas chromatography and synchrotron vacuum ultraviolet photoionization mass spectrometry, and discussed that the low temperature propane oxidation mechanism has not been well-established. Thus, it is an objective of this study to provide experimental data for chemical kinetics model evaluation.

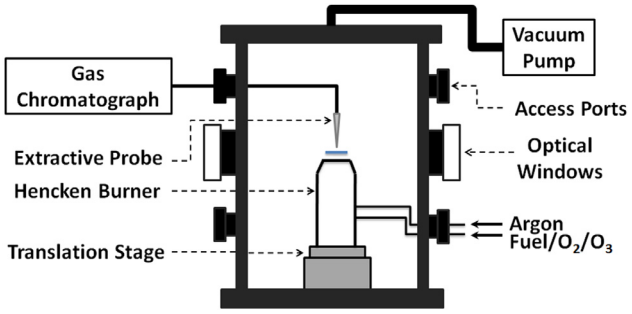

Fig. 1. Schematic of the experimental apparatus utilized in this study, including the pressure chamber, Hencken burner, translation stage and extractive sample probe [16].

The experimental platform utilized in [16] was employed in the present study to investigate the combustion characteristics of ozone-enhanced freely propagating premixed propane cool flames at sub-atmospheric pressures. Due to the sensitivity of propane cool flame stability to pressure, a pressure stability map was developed for a range of equivalence ratios to identify stable operating points, and different pressure stability regimes were defined. Lift-off height measurements of the flame above the burner surface were taken to identify burner-stabilized and freely propagating operating regimes, and the cool flame propagation speed was identified at the intersection of these regimes. Temperature measurements of a lean propane cool flame as a function of height above the burner (HAB) were taken and utilized in fixed temperature numerical simulations. Flame temperatures and propagation speeds of freely propagating propane cool flames were measured for a range of equivalence ratios and pressures based on stability map results. In order to facilitate a non-fixed temperature simulation of the freely propagating flame without the transition of cool flame to hot flame usually seen in non-fixed temperature numerical simulations, a chemical kinetics model was reduced employing the DRG technique, and the propagation speed obtained using the reduced model was compared with the experiments. Lastly, measurements of the quasi-equilibrium products of the freely propagating propane cool flame were taken using gas chromatography (GC) for comparison with numerical simulation results.

2. Materials and methods

2.1. Experimental techniques

Figure 1 shows the experimental setup developed to study the combustion characteristics of cool flames. As was explained in Hajilou et al. [16], the experimental setup consisted of a stainless steel pressure chamber, 87 cm in height and 60 cm in diameter, inside which a Hencken burner (Technologies for Research, Model RT1X1) was mounted on a translation stage, facilitating temperature and species measurements from upstream to downstream of the flame. In order to maintain the pressure in the experiments at a desired level, the chamber was connected to a vacuum pump. Borosilicate windows mounted on the chamber permitted optical access. Pictures of the flame were taken through the chamber windows with a Nikon D90 camera utilizing a NIKKOR 50 mm/f1.8 lens,

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