



# Cool diffusion flames of butane isomers activated by ozone in the counterflow

Adamu Alfazazi<sup>a,\*</sup>, Abdullah Al-Omier<sup>a,b</sup>, Andrea Secco<sup>a,c</sup>, Hatem Selim<sup>a,d</sup>, Yiguang Ju<sup>e</sup>, S. Mani Sarathy<sup>a,\*</sup>

<sup>a</sup> King Abdullah University of Science and Technology (KAUST), Clean Combustion Research Center (CCRC), Thuwal 23955-6900, Saudi Arabia

<sup>b</sup> Department of Chemical Engineering, King Faisal University, Al-Ahsa 31982, Saudi Arabia

<sup>c</sup> Dipartimento di Chimica Industriale "Toso Montanari", Università di Bologna, Viale Risorgimento 4, Bologna 40136, Italy

<sup>d</sup> GE Power, Saudi GE Technology & Innovation Center, Dhahran 34464, Saudi Arabia

<sup>e</sup> Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ 08544, USA

## ARTICLE INFO

### Article history:

Received 11 September 2017

Revised 29 December 2017

Accepted 30 December 2017

### Keywords:

Cool diffusion flames

Counterflow

Butane isomers

Ozone

Mass spectrometer

## ABSTRACT

Ignition in low temperature combustion engines is governed by a coupling between low-temperature oxidation kinetics and diffusive transport. Therefore, a detailed understanding of the coupled effects of heat release, low-temperature oxidation chemistry, and molecular transport in cool flames is imperative to the advancement of new combustion concepts. This study provides an understanding of the low temperature cool flame behavior of butane isomers in the counterflow configuration through the addition of ozone. The initiation and extinction limits of butane isomers' cool flames have been investigated under a variety of strain rates. Results revealed that, with ozone addition, establishment of butane cool diffusion flames was successful at low and moderate strain rates. iso-Butane has lower reactivity than *n*-butane, as shown by higher fuel mole fractions needed for cool flame initiation and lower extinction strain rate limits. Ozone addition showed a significant influence on the initiation and sustenance of cool diffusion flames; as ozone-less cool diffusion flame of butane isomers could not be established even at high fuel mole fractions. The structure of a stable *n*-butane cool diffusion flame was qualitatively examined using a time of flight mass spectrometer. Numerical simulations were performed using a detailed chemical kinetic model and molecular transport to simulate the extinction limits of the cool diffusion flames of the tested fuels. The model qualitatively captured experimental trends for both fuels and ozone levels, but over-predicted extinction limits of the flames. Reactions involving low-temperature species predominantly govern extinction limits of cool flames. The simulations were used to understand the effects of methyl branching on the behavior of *n*-butane and iso-butane cool diffusion flames.

© 2018 The Combustion Institute. Published by Elsevier Inc. All rights reserved.

## 1. Introduction

In efforts to comply with the stringent emission regulations, auto manufacturers are investigating various combustion strategies that produce lower combustion temperatures. Such low-temperature combustion (LTC) strategies e.g. the partially premixed combustion, PPC [1] and gasoline direct injection, GDI [2] are becoming increasingly attractive as they produce less emission and improve overall engine efficiency. One of the challenges of these engines, however, is how to control the heat release during the compression stroke and thus, the ignition timing. Ignition in LTC engines often occurs in two stages, the first stage which occurs

at low temperature and the second stage ignition respectively. Low-temperature cool flames and associated heat release during the first stage affects the heat release, the timing of the second stage ignition, and even knocking [3–5]. Engine studies [3–7] have shown that stratified combustion concepts display ignition phenomenon that is governed by both molecular transport and chemical kinetic processes.

The concept of LTC and controlling oxidation chemistry is well documented for different fuels in homogeneous systems such as jet stirred reactors (JSR), rapid compression machines (RCM) and shock tubes (ST) [8–14]. Many studies were carried out to understand low temperature fuel oxidation and intermediate species produced in these systems. This has influenced the understanding and advancement in building chemical mechanisms used in modeling LTC in these homogeneous systems. However, transport processes are negligible in the aforementioned homogeneous

\* Corresponding authors.

E-mail addresses: [adamu.fazazi@kaust.edu.sa](mailto:adamu.fazazi@kaust.edu.sa) (A. Alfazazi), [mani.sarathy@kaust.edu.sa](mailto:mani.sarathy@kaust.edu.sa) (S.M. Sarathy).

systems, and do not contribute to the evolution of cool flames and low-temperature heat release. In counterflow diffusion systems, where the fuel is initially separated from the oxidizer, the transport timescale is comparable to the reaction time scales. Therefore, both transport and kinetics contribute to the morphology and sustenance of cool flames using the opposed flow configuration [15]. These systems are canonical representations of transport-kinetic couplings present in PPC combustion engines.

Because most of previous studies focused on testing high strain rates, which require high temperature to achieve ignition [16–20], cool flame ignition in the counterflow configuration has received little attention. Nevertheless, initial pieces of evidence from the studies by Zheng et al. [21] and Grana et al. [22] involving hot diffusion flame suggested the existence of low-temperature reactivity in the counterflow flame. Later, Law and Zhao [23] computationally investigated the exhibition of LTC in the counterflow using *n*-heptane as the fuel. They noticed the occurrence of a secondary *s*-curve which is controlled by low-temperature species.

Few experimental studies on low-temperature combustion have been carried out using the counterflow configuration. Sun et al. [24] and Won et al. [25] established dimethyl ether and *n*-heptane cool flames, respectively, using by plasma discharge and ozone sensitization. It was shown that by adding ozone to the oxidizer stream in opposed flow systems, atomic oxygen produced as a result of ozone decomposition in the preheating zone intensely reduces the initiation time scales of low-temperature chemistry [26], thereby extending the flammable region of cool diffusion flames to higher stretch rates. Species measurements of CH<sub>2</sub>O and major reactants and intermediate species in diffusion cool flames by using laser induced fluorescence and a micro-GC showed that the existing low temperature kinetic mechanisms of *n*-heptane and dimethyl ether over-predicted the cool flame temperature and heat release rate. Their numerical simulations further showed that *n*-heptane cool diffusion flames are controlled by transport of species and low-temperature chemistry triggered by breakdown of ozone. Deng et al. [15] examined the low-temperature ignition of dimethyl ether (DME) and measured the intensities of formaldehyde species (HCHO) with the aid of infrared imaging. They provided an experimental evidence of the occurrence of such flame by applying optical detection and measurement in counterflow of heated air stream against diluted N<sub>2</sub>/DME mixture. They used a photomultiplier (PMT) to detect the CH<sub>2</sub>O\* chemiluminescence, which characterizes the low-temperature reaction; while sensitive infrared imaging was used to observe the ignition temperature. They revealed that low-temperature ignition is favored at low strain rates. In a separate study, Deng et al. [27] studied the extinction strain rates and ignition limit of DME/air at high pressures. They observed and quantified the existence of a hysteresis between cool flame ignition and extinction. They noted that heat release from LTC and hysteresis are largely promoted at high ambient pressure and oxygen concentrations.

The major challenge of establishing stabilized cool flames in non-premixed counterflow is the slow initiation chemistry at low temperature, which prevents the fuel from breaking down into small radicals and formaldehyde, thus preventing low-temperature branching reactions and self-initiation of the flame. In a separate study, Reuter et al. [28] compared the extinction limits of cool diffusion flames of large saturated alkanes; from *n*-heptane to *n*-tetradecane. They found that fuels with longer hydrocarbon chain lengths produce stronger cool diffusion flames, but at low strain rates, ozone addition greatly improved the low-temperature chemistry and made the cool flame reactivity independent of the carbon chain length. In the same study, they observed that cool diffusion flames can be sustained for large alkanes at high fuel mole fractions without ozone, but doubted if ozone-less cool flames could be sustained for *n*-alkanes less than *n*-hexane.

Clearly, the experimental method proposed by Won et al. [25] facilitates the establishment of sustaining cool diffusion flames in the counterflow facility in conditions at which cool flames may not be sustained. It also provides a platform to simultaneously study the combined effect chemical kinetics, heat release and transport on low-temperature cool diffusion flames. One of the major revelations from the above studies is that the existing numerical models over-predict the measured cool flame ignition and extinction limits [25,28–30]. This implies that the LTC is still not well developed and the current chemical kinetic models cannot accurately describe the cool flame behavior and its heat release rate, despite their capability to reproduce many homogeneous experiments at low temperatures.

With this in mind, the present study is aimed at employing the counterflow diffusion configuration assisted by ozone addition, to see if butane isomers exhibit low-temperature behavior in transport affected systems. As previously done for hot flames [20,31,32], this study provides an understanding of the influence of methyl branching on extinction limits and initiation of cool diffusion flames at various strain rates. Also, this study investigates the influence of both temperature and ozone concentration on the extinction limits of the tested fuels. Qualitative measurements of characteristic low temperature species as well as other species were obtained using a mass spectrometer. The mass spectrometer contains a sampling system, an ion source, a mass analyzer and a detector all kept under high vacuum condition. Finally, with the aid of molecular transport and detailed chemistry, an analysis is carried out to understand the detailed structure and reactions responsible for the extinction of cool diffusion flames of butane isomers.

The choice of butane isomers as fuels cannot be over emphasized. Butane is a constituent of commercial gasoline and the simplest alkane exhibiting structural isomerism. *n*-butane (RON-94) and iso-butane (RON 102) exhibit different knocking properties in spark ignition engines. Furthermore, *n*-butane is a simple gaseous hydrocarbon that shows a broad range of combustion properties such as negative temperature coefficient (NTC), low-temperature chain branching, cool flame and hot flame [18]. Moreover, accurate kinetic models of butane are necessary to build oxidation mechanisms of higher hydrocarbons. A number of studies have been carried out to understand butane isomers' combustion characteristics. This led to the development of several comprehensive kinetic models for the oxidation of butane [33–39]. Nevertheless, a detailed low-temperature study of butane isomers in a non-premixed diffusive system is still not available. Therefore this study provides additional data for validation of the existing butane models.

## 2. Experimental and numerical procedures

Fig. 1 illustrates the counterflow configuration used in this work. The burner has of two opposing duct nozzles. Preheated Fuel/N<sub>2</sub> mixture is introduced into the upper nozzle, while the oxidizer is injected into the lower nozzle. The upper part of the burner consists of an alumina tube, internal diameter,  $d = 25$  mm, directing preheated fuel stream downward. A preheater and an external Thermcraft heater (1-1/4ID, X8L, 365 W, 115 V, 12" braided leads) heat the fuel stream. A high temperature-resistant insulation surrounds the alumina tube to minimize radiation heat loss. The heaters are electrically controlled with variable transformers to provide constant power.

The oxidizer stream consists of oxygen and ozone. An ozone generator from Ozone Solutions (TG40) generates ozone from pure oxygen (>99.9% purity). A calibrated ozone monitor (2B Technology Model 106-H) is connected to the outlet of the ozone generator before the lower duct of the burner to enable constant and accurate measurement of ozone concentration in the oxidizer stream. This

Download English Version:

<https://daneshyari.com/en/article/6593744>

Download Persian Version:

<https://daneshyari.com/article/6593744>

[Daneshyari.com](https://daneshyari.com)