

Higher Alcohols as Renewable Fuels for Compression Ignition Engines: Vaporization and Combustion of Butanol Droplets

By

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Abstract

With global energy demand on the rise and liquid fossil fuels continuing to dominate the transportation sector, there is an urgent need for cleaner, renewable alternatives for internal combustion engines. Among the various candidates, butanol emerges as a promising option for compression ignition engines due to its high energy content, favorable auto-ignition characteristics, and material compatibility. Additionally, advancements in production technologies are improving its economic viability, further strengthening its potential as a renewable liquid fuel.

In compression ignition engines, liquid fuel is injected into the cylinder and undergoes primary and secondary breakup, forming a spray of fine droplets. In the downstream, more diluted region of the spray, individual droplets interact with the surrounding hot gases, leading to heating, evaporation, and eventually combustion. Studying these isolated droplet processes are critical for developing accurate spray combustion models and optimizing fuel injection strategies to enable the effective use of renewable fuels in compression ignition engines.

To this end, the present research investigates the evaporation and combustion characteristics of single butanol droplets under near engine-like conditions. A fan-stirred chamber is employed to generate a homogeneous and isotropic turbulent environment with a nearly zero mean velocity. A comprehensive parametric study is conducted to examine the influence of key parameters, including droplet size, ambient pressure, turbulence intensity, and ambient gas composition. Additionally, the results for butanol are compared with those of conventional hydrocarbon fuels to assess the role of fuel type. These investigations are presented across four main chapters, each based on a published manuscript.

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List of Abbreviations

Nomenclature

d_0	Initial droplet diameter, μm
r_0	Initial droplet radius, μm
K	Evaporation rate, $\text{mm}^2 \text{s}^{-1}$
K_0	Evaporation rate under stagnant condition, $\text{mm}^2 \text{s}^{-1}$
K_b	Burning rate, , $\text{mm}^2 \text{s}^{-1}$
P_∞	Ambient pressure, bar
T_∞	Ambient Temperature, K
U_{rms}	Root mean square velocity (x direction), m s^{-1}
V_{rms}	Root mean square velocity (y direction), m s^{-1}
V_r	Radial velocity, m s^{-1}
$q^{0.5}$	Turbulence intensity, m s^{-1}
N	Rotational Fan speed, Revolution per minute (RPM)
D_{ab}	Mass diffusivity of a in b, $\text{m}^2 \text{s}^{-1}$
X	Mole fraction
Da	Damköhler Number
Re_t	Turbulent Reynolds number
Sc	Schmidt number
t_{flow}	Turbulent flow characteristic time scale
t_{vap}	Vaporization time scale

L	Integral Length scale, mm
L_f	Longitudinal integral length scale
C_ε	Proportionality constant
Y_i	Mean mass fraction of species i

Greek symbol

ν	kinematic viscosity, $\text{m}^2 \text{s}^{-1}$
ρ	density, kg m^{-3}
η	Kolmogorov length scale, μm
α	Thermal diffusivity, $\text{m}^2 \text{s}^{-1}$

Acronym

PIV	Particle image velocimetry
HIT	Homogeneous isotropic turbulence
RMS	Root mean square
SI	Spark ignition
CIEs	Compression ignition engines
EGR	Exhaust gas recirculation
LOC	Limit of oxygen concentration
TLE	Temporary luminous extinction
LZ	Flame average luminous zone
LHV	Lower Heating Value
SiC	Silicon Carbide

Declaration of the academic achievement

This thesis is organized in accordance with the “sandwich format” as outlined by the Faculty of Graduate Studies at the University of Manitoba. It comprises four individual research papers prepared for publication in peer-reviewed journals. Chapter 1 introduces the research motivations, problem statement, and outlines the major contributions of the thesis. Chapters 2 through 5 present the main experimental studies in the form of complete manuscripts, each including an abstract, introduction, methodology, results, and discussion. Chapter 6 concludes the thesis and provides recommendations for future research. Additional technical details, including PIV measurements, fiber-related information, experimental reliability, and supplementary data, are provided in the appendices.

Chapters 2 to 5 are based on papers that have already been published in peer-reviewed journals. The research was conducted under the supervision of Dr. Madjid Birouk, who provided continuous guidance throughout all phases of the project—from proposal development and experimental design to data analysis and manuscript preparation. Dr. Cameron Verwey contributed to the development of MATLAB codes used for processing PIV data and calculating evaporation and burning rates. He also reviewed some manuscript drafts and assisted in addressing reviewers’ feedback in which he was a co-author, and offered support in resolving some experimental/technical challenges. Mr. Perry Cheung contributed to the work presented in Chapter 5 by conducting the experiments under atmospheric pressure conditions.

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1. **A. Arabkhalaj**, C. Verwey and M. Birouk, “Experimental study of butanol droplet evaporation in a turbulent, high-pressure environment” *Fuel* 353 (2023) 123143. <https://doi.org/10.1016/j.fuel.2023.129143>.
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3. **A. Arabkhalaj**, C. Verwey and M. Birouk, “Experimental study of butanol droplet combustion in a turbulent, elevated-pressure environment”, *Combustion and Flame* 276 (2025) 114150. <https://doi.org/10.1016/j.combustflame.2025.114150>.

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4. **A. Arabkhalaj**, P. Cheung and M. Birouk, “Effect of Ambient Gas Composition on Butanol Droplet Vaporization in Turbulent High-pressure Environments”, *Fuel* 407 (2026) 137285. <https://doi.org/10.1016/j.fuel.2025.137285>.

Chapter 1: Introduction

1.1 Background and scope

Traditional global transportation is predominantly powered by internal combustion engines (ICEs), with more than 99% of the energy demand in this sector being met by such engines. Notably, 95% of this energy originates from the combustion of liquid fossil fuels [1]. Compression ignition engines (CIEs), in particular, are widely employed in transportation owing to their high thermal efficiency, favorable fuel economy, reliability, and durability [2]. However, the use of fossil fuels—especially diesel—in CIEs leads to the emission of pollutants such as NO_x , soot, and particulate matter (PM), all of which pose serious risks to both human health and the environment [3]. Furthermore, increasing global energy demand accelerates the depletion of fossil fuel reserves. These fuels are also unevenly distributed across geopolitical regions, making their supply and pricing vulnerable to political instabilities. These concerns have prompted researchers to explore renewable alternative fuels that could potentially replace diesel. Although diesel has long held a dominant position as a conventional fuel, interest in alternative fuels dates back to the 1980s [4]. Among various candidates, alcoholic fuels have recently gained considerable attention due to their oxygenated nature, which enhances combustion efficiency and reduces harmful emissions [5].

Light alcohols, such as methanol and ethanol, possess high octane numbers and are therefore well-suited for use in spark ignition (SI) engines [6]. Their effective performance in SI engines has led to widespread adoption in several countries. For example, the U.S. Environmental Protection Agency allows ethanol blending in gasoline up to 15% [7], while in Europe, up to 3% methanol can be blended with gasoline [8]. Additionally, high-ethanol blends (up to 85%) or even pure

ethanol are commercially available in countries such as Brazil [9] and Sweden [10]. However, light alcohols are generally unsuitable for CIEs. Their low cetane number, low calorific value, high latent heat of vaporization, low flash point, and resistance to auto ignition negatively affect engine performance [11, 12]. Moreover, blending these alcohols with diesel or biodiesel often results in phase separation [13].

These limitations have shifted research focus toward higher alcohols—longer-chain alcohols containing four or more carbon atoms, such as butanol [14]. Table 1-1 compares fuel properties of diesel with various alcohols. Research indicates that longer carbon chains enhance the ignition quality of alcohols [15]. Higher alcohols also offer advantages over light alcohols, including higher energy density, better cetane number, higher flash point, lower heat of vaporization, and reduced corrosiveness, making them more compatible with CIEs [16]. Furthermore, blends of higher alcohols with diesel are more stable and less prone to phase separation [13].

Table 1-1. Fuel properties of diesel and some alcohols [13]

Fuel Properties	Diesel	Methanol	Ethanol	Propanol	n-Butanol	Pentanol	Hexanol	Octanol
Formula	C ₁₂₋₁₄ H ₂₆₋₃₀	CH ₃ OH	C ₂ H ₅ OH	C ₃ H ₇ OH	C ₄ H ₉ OH	C ₅ H ₁₁ OH	C ₆ H ₁₃ OH	C ₈ H ₁₇ OH
Density (at 15 °C)	840	791.3	789.4	803.7	809.7	814.8	821.8	830
Boiling point (°C)	227	65	78	97	118	138	156	194
LHE (kJ/kg)	250-290	1173.5	918.6	788.7	685.4	504	486	408
Kinematic viscosity at 40 °C (mm ² /s)	2.0-4.5	0.58	1.13	2.96	3.17	3.44	5.32	5.5
Calorific value (kJ/kg)	45.5	20.08	26.83	29.82	32.01	32.16	37.1	38.4
Flash point (°C)	70	12	13	22	35	48	59	81
Cetane number (%)	52	3.8	8	12	17	20	23	38.4
Oxygen (%)	0	49.93	34.73	26.62	21.59	18.15	15.7	12.31

Historically, the production of higher alcohols was limited by high costs, their use in the food industry, and the scarcity of renewable production methods [17]. Low production efficiency and limited public and policy-level awareness further hindered their widespread adoption [18].

However, the past decade has seen renewed interest in higher alcohols as sustainable fuel candidates. Advances in biotechnology and catalysis have enabled various production pathways, including fermentation using novel *Clostridium* strains [19], genetic engineering of microorganisms such as *Escherichia coli* [20], *Cyanobacteria* [21], and *Saccharomyces cerevisiae* [22], as well as catalytic conversion of syngas through higher alcohol synthesis (HAS) [23].

Moreover, higher alcohols can benefit from the infrastructure developed for light alcohol production such as ethanol [24]. In some cases, they even require less energy during production than light alcohols, as biological conversion processes can be terminated earlier [12]. Consequently, the availability of higher alcohols is expected to improve, with reduced reliance on food crops and increasingly mature production technologies [25, 26].

Among the various higher alcohols explored for use in CIEs, butanol has garnered significant attention due to its favorable physicochemical properties and superior engine compatibility [27]. There are four isomers for butanol, and among them, n-butanol has been considered as a fuel in CIEs due to its higher heating value [14]. In recent years, the potential of n-butanol is being investigated extensively in different kinds of CIEs as it shows excellent features like a great reduction in NO_x and smoke emissions and high thermal efficiency [28]. In the following section some of these studies are briefly reviewed.

1.2 Literature on using butanol in CI engines

A few studies are dedicated to running CIEs with neat higher alcohols, such as butanol [29]. These studies revealed that it is possible to run CIEs with butanol in a limited range of conditions with engine modification. These modifications include the replacement of plastic and rubber parts with alcohol tolerant substances [30], use of high-pressure injectors for direct injection of butanol [31]

along with a fuel cooler and preheated air [32], and the addition of a lubricity improver to butanol [33]. On the other hand, there are many studies on using higher alcohols in binary and ternary blends in CIEs. Binary blend refers to the mixture of two fuels, such as butanol and diesel, and ternary blend refers to a mixture of three fuels, such as butanol-diesel-biodiesel blend or vegetable oil-biodiesel-butanol [34]. As it is mentioned, higher alcohols can create more stable blends with diesel rather than light alcohols [35], so various blends of alcoholic fuels with diesel and biodiesel are tested in CIEs [26]. Results showed that it is possible to safely use up to 45% of butanol in blend form with diesel in CIEs without any engine modifications [34]. The dual fuel injection technique is another method for using butanol in the CIEs [26, 34]. Reviewing the literature shows that this technique has several advantages over the alcohol/diesel blending strategy. First, it is reported that a higher volume of alcohol can be used in this technique compared to the blending strategy (up to 10%) [36, 37]. Second, it is possible to regulate the butanol fraction based on load conditions [38]. Third, it is possible to switch the engine operation from a dual-fuel mode to a single fuel if required [26]. Fourth, evaporation of butanol in intake air can cause a cooling effect and increase the density of the mixture [39]. Therefore, more mixture can enter the engine chamber/cylinder and improve the power output. Fifth, it can minimize the evaporation losses compared to blends [40]. Finally, it is a more effective strategy in reducing NO_x emission when compared to alcohol/diesel blends [37, 38]. Therefore, the mentioned potential of using higher alcohols in CIEs through dual fuel injection technique necessitates further investigation.

In dual fuel injection operation, the engine runs effectively on two fuels, and there are several concepts to achieve this [41-43]. One concept is to separately inject two fuels directly into the cylinder. Another concept (so-called fumigation) is to inject one fuel into the intake and the second fuel into the cylinder. The first concept requires two injectors, which need modification of the head

of the cylinder. On the other hand, the fumigation concept is easier to implement because the first fuel is injected at lower pressure, and no cylinder modification is required [44]. The fumigation concept is already used by port fuel injection of natural gas and direct injection of biodiesel [64], and some studies showed that natural gas can be replaced by higher alcohols such as butanol or pentanol [27, 30].

1.3 Problem definition

Reviewing literature reveals that there is a limitation for using alcoholic fuels in current CIEs. For instance, butanol and pentanol can be used up to 40% with diesel [34]. This limitation is attributed to the physical and chemical characteristics of alcoholic fuels. One problem, which is frequently mentioned in the literature, is the longer ignition delay of higher alcoholic fuels. The ignition delay is determined as the time that elapses between the injection of fuel and the beginning of combustion [45]. Ignition delay has a significant role in the combustion and emission characteristics of engines. Increasing this period results in enhancement of the maximum pressure rise rate and engine noise. A longer delay period will retard the start of the combustion closer to the top dead center, so majority of the fuel burns during the expansion stroke, which results in a reduction of the power developed by the engine. This also increases the unburnt hydrocarbon and smoke emissions, which are frequently reported as a consequence of using higher alcoholic fuels in CIEs. On the other hand, a shorter ignition delay period requires more compression work against the product of the premature combustion. This leads to an increase in the combustion temperature and, subsequently, NO_x formation. Therefore, both longer and shorter ignition delays are not suitable for CIEs, and thus an optimum ignition delay is required for effective performance [45].

Ignition delay is influenced by several physical and chemical processes. The physical processes comprise mainly atomization of liquid fuel, spray break up into droplets, droplet vaporization, and

mixing fuel vapor with air, while chemical processes include preliminary exothermic chemical reactions [46, 47]. It should be noted that physical and chemical processes are not consecutively occurring as there exists some overlap between these two processes [48], which makes it difficult to distinguish their roles. However, there exists a considerable number of published studies dedicated to the role of each process.

From chemical point of view, Koivisto et al. [15] concluded that a longer ignition delay is due to the higher electronegativity of oxygen atoms in alcohols compared to carbon atoms, which results in increasing hydrogen abstraction and isomerization. They also found that the position of the hydroxyl group affects the ignition delay.

However, it is also reported that the physical properties play a major role in combustion behavior as well [49]. One of the earliest studies was the report of Sangiovanni et al. [50], who experimentally investigated the ignition delay of two alcohols, including furfuryl and butyl alcohols. They used a freefalling of stream droplets technique for this experiment. Their results showed that ignition delay significantly increases with decreasing the fuel volatility or droplet size, which are both physical aspects. Santhosh et al. [51] used a diesel engine to investigate the ignition delay of 1-pentanol/diesel with different blends. They showed that longer ignition delay belongs to the higher proportion of 1-pentanol in the diesel blends, which is mainly attributed to the higher latent heat of evaporation of this fuel. They reported that alcoholic fuel such as 1-pentanol has a high latent heat of vaporization and contains a small quantity of water, which absorbs more heat to evaporate, which causes a quenching effect and prolongs the ignition delay. Similar findings were reported by Seelam et al. [52], who studied the performance of a CIE fueled with different 1-hexanol/diesel blends using direct injection method. They reported that a high latent heat and a low H_2O in 1-hexanol fuel blends are the cause of a greater heat for evaporation, which results in

extending the ignition delay. Zubel et al. [49] evaluated the potential of using C8 alcohols, including 1-octanol and its isomer dibutyl ether (DBE), in the CIEs. They reported that the chemical section of ignition delay for these two fuels are in the same order, but due to the difference in volatility and viscosity, the physical portion of ignition delay makes a difference. Therefore the 1-octanol has a relatively long ignition delay rather than DBE. Zhang et al. [53] studied the effect of turbulence intensity on ignition delay of n-pentanol/diesel droplet under a high temperature of 900 K. They showed that under low turbulence intensity, the ignition delay slightly decreases, which is attributed to increasing the vaporization rate. However, under high turbulence intensity, the ignition delay sharply increases due to the heat and radicals transported by turbulence.

These aforesaid investigations confirm that, the physical processes play an important role in the ignition delay of alcoholic fuels. Furthermore, the role of droplets evaporation process is highlighted among physical processes, where it is reported that turbulence intensity, fuel volatility, ambient pressure and temperature, and latent heat of vaporization, all of which can influence the ignition delay. Moreover, since fuel vapor diffusion around droplets controls the ignition process of a combustible mixture [54], it is important to investigate and understand the vaporization behavior droplets.

Fuel spray injection lies at the core of combustion engine operation. In CIEs, liquid fuel is atomized by a high-pressure jet into a cloud of fine droplets, significantly increasing the surface area for evaporation and promoting better fuel–air mixture formation. As such, spray evaporation plays a critical role in establishing the initial conditions for combustion. However, accurately analyzing spray evaporation is inherently challenging due to the need for substantial approximations and modeling assumptions [55]. Although engine-based studies provide valuable insights under realistic operating conditions, their results are often influenced by non-controllable parameters

such as spray geometry, local temperature and pressure gradients, and in-cylinder turbulence [16]. Given that the sub-grid structure of a fuel spray consists of individual droplets [56], it is widely accepted that single droplet evaporation studies can effectively capture the fundamental physical and chemical phenomena governing fuel injection [57]. A key advantage of a single droplet configuration is that all influencing parameters—such as ambient conditions, droplet size, and composition—can be precisely controlled. This ensures that the observed behavior can be directly attributed to the fuel properties alone [16]. Furthermore, experimental data obtained from single fuel droplet studies continue to play a vital role in the development and validation of numerical models for spray combustion and evaporation, despite the significant progress made in computational modeling capabilities [58-60].

Following the ignition delay period, combustion is initiated when local thermodynamic and mixture conditions—specifically temperature and equivalence ratio—become favorable. This process often begins at the spray front, where individual droplets ignite first due to their exposure to high temperature, oxidizing environments [61]. Understanding the combustion behavior of these isolated droplets is of both fundamental and practical importance. With the ongoing development of advanced combustion technologies aimed at cleaner and more efficient utilization of liquid fuels, a deeper understanding of the underlying physical and chemical processes—particularly at lower combustion temperatures—has become increasingly critical. Single droplet combustion offers a powerful methodology for gaining such insights. Under idealized and controllable experimental conditions, isolated droplets eliminate the complexities associated with droplet–droplet interactions in spray flames. This makes it possible to study fundamental processes such as heat and mass transfer, ignition, flame structure, and extinction in a more precise and reproducible manner [62]. Such controlled experimentation not only enhances the physical

understanding of liquid fuel combustion but also provides high-quality data for validating and refining spray combustion models [63]. Therefore, investigating the combustion behavior of single droplets is essential not only for advancing fundamental combustion science but also for improving the predictive capabilities of computational models used in the design and optimization of modern combustion systems.

1.4 Motivations

Studying the evaporation and combustion of single droplets has practical advantages that have attracted scientists and engineers for decades [56]. First, a single droplet is believed to portray the diluted region of the spray in the far-field of the injector where there is fewer droplets interaction. Second, a single droplet study helps understand complex mechanisms governing spray evaporation and combustion. Third, it provides an opportunity to isolate and study the effects of each influential parameter on the evaporation or combustion process. Although fundamental studies on isolated droplet combustion have attracted attention for over seven decades [65], detailed investigations focusing on the evaporation and combustion characteristics of long-chain alcohols remain limited [66]. Table 1-2 presents a summary of relevant studies found by the author in the literature.

Table 1-2. Summary of studies on butanol droplet evaporation and combustion

Evaporation studies							
Authors	Study	Fuel	d_0 (μm)	P_∞ (bar)	T_∞ (K)	Conditions	Ambient
Law et al. (1987) [58]	Exp. and Num.	Butanol	1000	1.0	297	Stagnant	Humid air
Mandal et al. (2012) [59]	Exp.	Butanol	3000	1.0	300	Stagnant	Air
Sadiki et al. (2014) [60]	Num.	Butanol	1760	1.0	473	Stagnant	Air
Rehman et al. (2016) [61]	Exp. and Num.	Butanol	1500	1.0	400	Laminar ($U=1.4$ m/s)	Air
Yi et al. (2017) [57]	Num.	Butanol - Pentanol	200	20.0	873	Stagnant	N_2
Xi et al. (2021) [62]	Exp.	Butanol	1700	1.0	609	Stagnant	Air
Combustion studies							
Jangi et al. (2009) [63]	Exp. and Num.	Butanol	1000	4.0	293	Laminar ($U=0.4$ m/s)	Air
Ogami et al. (2009) [64]	Exp.	Butanol	1200	4.0	293	Oscillation velocity ($U=2$ and 0.4 m/s)	Air
Bartle et al. (2011) [65]	Exp.	Butanol	1200	1.0	293	Stagnant	Air
Nakaya et al. (2013) [66]	Exp.	Butanol	600	1.0	293	Stagnant	$\text{O}_2 + \text{AR} + \text{CO}_2$
Hoxie et al. (2014) [67]	Exp.	Butanol	610	1.0	293	Stagnant	Air
Alam et al. (2015) [68]	Exp. and Num.	Butanol	560	1.0	293	Stagnant	$0.08 < X_{\text{O}_2} < 0.21$
Xu and Avesdian (2015) [69]	Exp.	Butanol	560	1.0	293	Stagnant	Air

Liu et al. (2016) [70]	Exp.	All Butanol isomers	520	1.0	293	Free fall	Air
Muelas et al. (2017) [16]	Exp.	Butanol	150	1.0	293	Free fall	Air
Coughlin and Hoxie (2017) [71]	Exp.	1-butanol – 1-pentanol	1000	1.0	373	Stagnant	Air

As can be seen in Table 1-2, most of the studies are conducted in atmospheric pressure and stagnant conditions, while droplets experience elevated pressure conditions ($P > 20.0$ bar [72]) and intense turbulence intensity ($>100\%$ [73]) in the real engine conditions. Furthermore, most of these studies investigated droplet evaporation and combustion in air ambient conditions. However, in real applications, droplets evaporate in the presence of vapor fuel and combustion products. Moreover, the studied droplets sizes are usually constant and significantly large compared what practical atomizers generate, which ranges from a few micrometers up to $500\ \mu\text{m}$ [74]. Considering the shortcomings of the previous studies, investigations of the effect of ambient pressure, turbulence environment, effect of droplet size, and ambient compositions on the vaporization and combustion of droplets can provide useful knowledge for better understanding the complex spray vaporization and combustion processes.

1.5 Research objectives

The main objective of this research is to experimentally investigate the evaporation and combustion of n-butanol fuel droplets under near engine-relevant conditions. The study is designed to systematically examine the individual and coupled effects of fuel type, turbulence, pressure, droplet size, and ambient gas composition on single butanol droplet evaporation and combustion. The specific objectives of this research are as follows:

- To characterize the vaporization behavior of n-butanol droplets in turbulent flow fields at elevated pressures and to validate correlations that describe droplets vaporization rate.

- To determine the influence of droplet diameter/size on the vaporization rates under varying turbulence intensities and pressure levels, and to characterize the associated turbulence length scales.
- To investigate the combustion of n-butanol droplets in turbulent, high-pressure environments and to study the effects of varying O_2 and CO_2 concentrations on combustion characteristics, including flame structure and burning rate.
- To compare the evaporation and combustion behavior of n-butanol droplets with that of conventional hydrocarbon fuels, such as heptane and decane, under identical test conditions.
- To examine the coupled effects of ambient gas composition, pressure, and turbulence on the evaporation and burning rates of single n-butanol droplets.

1.6 Outline of the thesis

As mentioned above, the objective of this thesis is to experimentally examine the evaporation and combustion characteristics of n-butanol droplets under conditions relevant to compression ignition engines. By isolating key physical parameters such as turbulence intensity, ambient pressure, droplet size, and ambient compositions, this work aims to enhance our understanding of the physical processes influencing ignition delay and burning behavior of higher alcohols. The experimental results obtained provide valuable insight into the suitability of n-butanol as an alternative fuel and can also serve as reference data for future numerical modelling of the more complex spray combustion process.

This thesis is presented in a sandwich format and comprises four core chapters. Chapters 2 to 5, each consist of a complete manuscript that has been published in peer-reviewed journals.

[Chapter 2](#) presents a comprehensive experimental investigation of n-butanol droplet evaporation in a high-pressure, turbulent environment. This study examined the effects of varying ambient turbulence intensity and pressure on the vaporization behavior of butanol droplet. The work aimed to validate the applicability of the classical d^2 -law under these conditions, determine the role of turbulence and its coupling with ambient pressure on the evaporation characteristics of butanol and compare the results with those of conventional hydrocarbons such as heptane and decane. Additionally, the study assessed the predictive capability of published correlations based on Damköhler and turbulent Reynolds numbers for butanol droplet vaporization.

[Chapter 3](#) presents a study that primarily focuses on the effect of droplet size on the vaporization behavior of n-butanol under ambient turbulent and elevated pressure conditions. This investigation analyzes the interaction between turbulence length scales and droplet diameter/size in determining the evaporation rate. Additionally, the study investigates the effectiveness of turbulence on the vaporization of different fuel types by assessing the influence of their thermophysical properties.

[Chapter 4](#) presents an experimental study on the combustion characteristics of n-butanol droplets in a turbulent, high-pressure environment. This work investigates the coupled effects of pressure, turbulence intensity, and ambient-gas composition on key combustion parameters such as droplet burning rate, and flame morphology. Additionally, the study compares the burning behavior of n-butanol with that of n-heptane under identical conditions to assess the role of fuel properties.

[Chapter 5](#) presents a comprehensive experimental investigation on the evaporation behavior of single butanol droplets under engine-relevant turbulent and high-pressure conditions. The study systematically examines the influence of ambient gas composition—including pure and binary mixtures of N_2 , O_2 , and CO_2 —on the evaporation rate. Furthermore, the effectiveness of turbulence is assessed across different ambient compositions and ambient pressures.

[Chapter 6](#) concludes the thesis with a summary of key findings and provides some suggestions for future research directions.

In addition, supplementary technical details that support the main chapters are presented in appendices. [Appendix A](#) elaborates on the Particle Image Velocimetry (PIV) results used for turbulence characterization. [Appendix B](#) describes the image analysis procedure employed to extract droplet size and evaluate droplet sphericity. [Appendix C](#) discusses the influence of fibers on droplet size measurement and burning rate determination. [Appendix D](#) assesses the independence and reliability of the measured burning rates. [Appendix E](#) provides additional details related to the thesis document.

1.7 References

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Chapter 2: Experimental Study of Butanol Droplet Evaporation in a Turbulent, High-Pressure Environment

2.1 Abstract

An experimental investigation is conducted to study the vaporization behavior of butanol droplets in a turbulent environment at elevated pressure. A single droplet of butanol, with a diameter of 500 μm , is suspended at the intersection point of two micro-fibers positioned in the center of a fan-stirred spherical chamber. The latter is equipped with eight axial fans to generate an isotropic and homogeneous turbulent flow field with nearly zero-mean velocity. In this experiment, turbulence intensity and ambient pressure were varied from 0 to 1.5 m/s and from 1 to 10 bar, respectively, while ambient temperature was kept at room conditions. The experimental findings revealed that the butanol droplet squared diameter exhibited a linear relationship with time for the majority of the droplet lifetime. This observation suggests that the d^2 -law is applicable across all the test conditions explored in this study. Results showed that the vaporization rate of a butanol droplet decreases with ambient pressure and increases with turbulence intensity. The vaporization rate of butanol falls between that of heptane and decane, with closer proximity to decane. Furthermore, the comparison of these fuels indicates that the influence of turbulence on the vaporization rate is more significant for fuels with lower vapor mass diffusivity. Finally, published correlations based on Damköhler and Reynolds numbers are verified and found to hold for the butanol droplet vaporization data.

2.2 Introduction

Global energy demand is expected to increase by 48% in the next 20 years to fulfill the growing human population's needs and rapid socio-economic development [1]. Transportation is one of the main industries that involves energy usage, consuming nearly 30% of all energy produced today [2]. More than 95% of energy in the transportation sector comes from burning liquid fossil fuels [3], which are responsible for environmental problems such as air pollution and global warming [4]. Consequently, transportation has been identified as an important sector for greenhouse gas mitigation in support of global climate commitment [5]. According to the International Energy Agency road map estimation, more than 25% of the total global transport fuel should come from biofuels by 2050 to reduce dependence on fossil fuels [6]. Ultimately, internal combustion engines will continue to play a major role in the transportation sector [7]. Compression ignition (CI) engines, which have higher thermal efficiency, reliability, and durability compared to spark ignition engines [8], are expected to see continued usage in public transportation, power generation applications, and industrial heavy equipment [9]. Therefore, research to develop alternative fuels that are compatible with current CI engines is of paramount importance [10, 11].

Among different alternatives, there is a growing interest in alcoholic fuels. These oxygenated fuels help improve combustion efficiency and reduce air pollution [12]. Light alcohols such as ethanol and methanol have a high octane number, which makes them plausible alternatives for spark ignition (SI) engines [13]. The successful performance of light alcohols in SI engines has been demonstrated and ethanol, in pure form or mixed with gasoline (up to 85%), has been used in countries such as Brazil [14] and Sweden [15]. However, these light alcohols are inappropriate for use in CI engines. They were found to degrade the performance of CI engines [9] due to their low cetane number, low calorific value, low flash point, high latent heat of vaporization, and high

resistance to auto-ignition [16, 17]. Moreover, their mixture with diesel or biodiesel exhibits phase separation [18].

On the other hand, higher alcohols, such as butanol, have several advantages which make them more suitable for CI engines. They have higher energy densities, cetane numbers, and flash points than their light alcohol counterparts [19]. They cause less corrosion and have a better material compatibility with engine components [20]. Additionally, they have lower heats of vaporization and longer carbon chains, which improve fuel ignition [21]. Moreover, higher alcohols have the potential to be used along with diesel to make a homogenous blend without any phase separation [18]. These fuels are sustainable, as they can be produced by several methods such as the fermentation process [22] or via genetically engineered micro-organisms [23]. Therefore, fuel availability would be less of an issue due to a reduced reliance on food crops [24] and maturing production technology and processes [25].

The possibility of using higher alcohols in CI engines has been extensively investigated in the last decade (e.g., [9, 18, 24-26]). It was reported that CI engines fueled by butanol could work properly with less NO_x emission and acceptable efficiency with minor engine modifications [9]. Butanol can be used in CI engines in different ways, including as a standalone fuel [27], with diesel or biodiesel using dual fuel injection technique [28-30], or in binary or ternary mixtures with diesel or biodiesel [31, 32]. A literature review shows that the dual fuel injection technique has several advantages over the alcohol/diesel/biodiesel blending strategy. For instance, compared to the blending strategy, up to 10% more volume of butanol can be used in dual-fuel mode [28, 33]. Also, butanol fraction can be adjusted based on the engine load conditions [34]. Moreover, when required, it is possible to switch the engine operation from dual-fuel mode to single fuel [24]. Furthermore, the evaporation of butanol in the intake air can decrease the temperature and

subsequently increase the density of the mixture, which could enhance engine power [35]. Also, evaporation losses can be minimized in dual mode compared to blend strategies [36]. Dual-fuel mode was found to be a more effective strategy for reducing NO_x emission than the blending technique [33, 34]. Therefore, there is an apparent need to investigate the potential of using high alcohols (such as butanol) in CI engines.

Published studies reported that CI engines fueled by butanol suffer from extended ignition delay [37-39]. The ignition delay of a CI engine is defined as the time elapsed between the injection of fuel and the start of combustion [40]. Prolonged ignition delay increases unburned hydrocarbon emissions [40] and decreases the engine's thermal efficiency [41]. It is known that physical processes, including spray break up, droplet evaporation, and air/fuel mixture, all have a role to play on the duration of ignition delay [42, 43]. Droplet evaporation is reported to be a decisive parameter [44, 45]. Additionally, single droplet evaporation may reasonably portray the essential phenomena involved during the fuel injection process [46], which determines the initial conditions of combustion in the engine cylinder. Therefore, understanding the evaporation behavior of butanol droplets can be very helpful for the promotion of renewable fuels in CI engines.

A literature review revealed that there are only few studies on butanol droplet evaporation. In one of the earliest studies, Law et al. [47] claimed that atmospheric moisture does not affect butanol droplet evaporation rate. Mandal et al. [48] investigated the effect of internal circulation during the evaporation of a single droplet of water and some alcohols, including butanol. Rehman et al. [49] experimentally investigated the evaporation of a single butanol droplet in a laminar flow at atmospheric pressure. Their results revealed that increasing the ambient temperature of laminar flow from 303 K to 343 K significantly decreased the butanol droplet lifetime (by more than 75%). Xi et al. [50] experimentally studied the evaporation of single droplets of butanol, hexadecane, and

their binary mixtures at different ambient temperature and pressure conditions. They showed that the evaporation process for single butanol droplets can be divided in two stages; a minor volume expansion that is attributed to the ambient temperature, and a stable evaporation phase characterized by the classical d^2 -law. Yi et al. [51] developed a numerical model to study the evaporation characteristics of pure diesel and pure higher alcohols such as butanol and pentanol. However, due to the lack of experimental data for higher alcohols, they used methanol and ethanol evaporation data for the validation of their numerical model. A summary of relevant published studies and their test conditions are given in Table 1.

As seen in Table 1, most of these studies were conducted in standard pressure and room temperature environments. Moreover, these studies used thermocouples or glass fibers for suspending the butanol droplet which could significantly influence heat transfer to the droplet and, consequently, alter the vaporization process. In addition, the investigated droplets are significantly large and unrealistic, since most practical atomizers generate droplets ranging from a few micrometers up to 500 μm [52]. The literature also revealed that, due to the lack of experimental data for high alcohols, numerical studies on higher alcohols, such as butanol, resorted to water [53] or light alcohol [51] evaporation data for validation. The present study aims to investigate the evaporation behavior of a single butanol droplet under different turbulence intensity levels at elevated ambient pressure and room temperature conditions.

Table 2-1. Summary of published studies on butanol droplet evaporation.

Authors	Type	d_0 (μm)	P (bar)	T (K)	Condition	Ambient
Law et al. (1987) [47]	Exp. and Num.	1000	1.0	300	Stagnant	Humid air
Mandal (2012) [48]	Exp.	3000	1.0	300	Stagnant	Air
Rehman et al. (2016) [49]	Exp. and Num.	1500	1.0	403	Laminar ($U=1.4$ m/s)	Air
Xi et al. (2021) [50]	Exp.	1700	1.0	Up to 609	Stagnant	Air
Sadiki et al (2014) [53]	Num.	1760	1.0	473	Stagnant	Air
Yi et al. (2017) [51]	Num.	200	20.0	873	Stagnant	N ₂

2.3 Methodology

2.3.1 Overview

Single droplet vaporization experiments were performed in a large, fan-stirred spherical chamber. Butanol droplets (Sigma-Aldrich, 99.9% purity) with a diameter, d_0 , of 500 μm were suspended at the intersection of two microfibers and exposed to turbulence intensities, $q^{1/2}$, up to 1.5 m/s at ambient pressures, P , ranging between 1 and 10 bar. The ambient temperature, T_∞ , was kept constant at 300 K.

While a comprehensive account of the experimental methodology has been previously elucidated by this research group [54, 55], the subsequent sections succinctly outline the fundamental facets. Section 2-2 provides a description of the experimental setup which consists of the high-pressure chamber (vessel), optical windows and ports, fans arrangement for generating the turbulent flow field. Section 2-3 describes the two-dimensional particle image velocimetry (2D-PIV) that is used to characterize the turbulent flow field in the vessel. Section 2-4 reports the injection system used to generate droplets along with the imaging system for capturing the droplet evaporation process. Finally, section 2-5 delineates the experimental procedure employed for determining the droplet vaporization rate.

2.3.2 Fan-stirred spherical chamber

The cross-sectional view of the experimental setup employed in this work is depicted in Fig. 2-1. The test rig is a large, sealed spherical chamber with a volume of 29 L. It is made of stainless steel with an inner and an outer diameter of 380 and 405 mm, respectively. The chamber is equipped with four pairs of axially-opposed fans located at a distance of 200 mm away from one another. The fans are positioned such that the airflow collides in the center of the chamber, thereby generating a turbulent flow field with a negligible mean velocity. The fan speeds are checked

before and after each set of tests with an optical tachometer, which ensures that no fan deviates from the target speed by more than $\pm 0.5\%$. The maximum turbulence intensity of 1.5 m/s is achieved with the fans operating at 3000 rpm.

The chamber also has two pairs of opposed windows positioned 90 degrees apart around the horizontal equator. The windows provide the proper visual access for imaging the evaporation process, PIV measurement, and physical access inside the chamber. In addition to the windows, ten accessory ports are available; four are between the windows around the horizontal equator, and the rest are arranged along the chamber's upper and lower sides. These ports are for different inputs, such as the fuel injector, the fiber-support frame, the pressure gauge, the pressure transducer, the thermocouple, the cartridge heater, the vacuum pipe, the outlet valve, and the safety valve. The nominal chamber temperature is maintained at 300 K using a small, finned cartridge heater and monitored by a K-type thermocouple located 180° from the heater. The heater is employed to maintain the test chamber temperature within the range of 300 ± 1 K during experimentation. A conservative estimate of the overall uncertainty in the reported temperature, considering both the thermocouple (± 2.2 K) and the ADC module (± 1.2 K), is ± 3.4 K. The turbulent flow generated by the fans ensures that the temperature field is reasonably homogeneous.

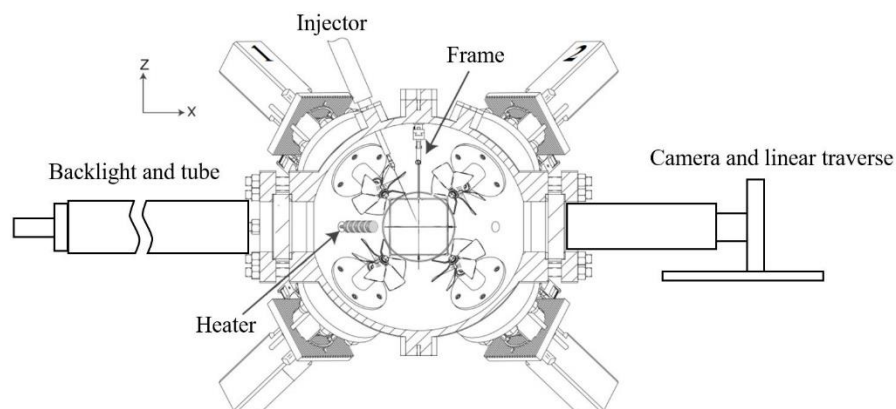


Figure 2-1. Cross-sectional view of the chamber setup.

2.3.3 Flow field characterization

Two-dimension particle image velocimetry (2D-PIV) was used to characterize the turbulent flow field inside the chamber. Although the chamber has been thoroughly analyzed via PIV in past investigations [55, 56], recent modifications to the fan driving mechanisms, along with a new combination of internal components, necessitated a brief confirmation of the flow field quality. A Dantec Dynamics 2D-PIV system, which consists of a Dual Power Nd:YAG laser with 135 mJ double pulse and a FlowSense EO 4M camera, was used. For visualization, the flow field is seeded using micro-sized olive oil droplets generated by a LaVision aerosol generator. Control, synchronization, and acquisition, along with cross correlation of the raw images, were performed by DynamicStudio software.

The turbulent flow is only characterized within a central area of the chamber, where the field of view (FOV) is approximately 80×80 mm. Although the FOV is limited by the size and location of the windows, this region is sufficiently large to provide information about the flow field surrounding the $500 \mu\text{m}$ evaporating droplet. In each PIV test, 2000 pairs of images at a repetition rate of 10 Hz were collected and processed with an interrogation area of 32×32 pixels with 50% window overlap. The pulse delay time was changed depending on the fan speed using the guidelines reported in [57]. In the present study, as reported in [55], 2000 pairs of images were found satisfactory for the convergence of turbulence statistics.

2.3.4 Droplet formation and imaging

The injection system is shown in Fig. 2-1. As seen in this figure, the injector port is located on the top of the chamber to take advantage of gravity. The injector consists of a leadscrew-driven piston, a retractable barrel, a steel needle, and a capillary tube with an inner and an outer diameter of 40 and $60 \mu\text{m}$, respectively. This system is capable of producing small droplets with a size range

between approximately 100 and 1000 μm . To suspend small droplets, maintain a spherical shape, and avoid heat conduction through the suspension system, two intersecting 14 μm silicon carbide (SiC) fibers were employed. These delicate fibers are crossed at 90 degrees and are installed in a frame, which is fixed from the top of the spherical chamber. It should be noted that the cross-fiber, which is used to suspend the droplet, occupies less than 1% of the droplet volume. This volume is deemed too small to impact the accuracy of the droplet size. The droplet evaporation process is captured using a Fastec IL5Q camera coupled to a Questar QM-100 long distance microscope and backlight produced by a 250 W halogen lamp directed through a long metal tube to avoid heating the droplet. This combination gives a spatial resolution of 1.08 $\mu\text{m}/\text{px}$. The image frame rate is fixed at 24 fps, and a shutter speed of 200 μs was selected and held constant.

Systematic error in calculating droplet size is introduced through the camera calibration and droplet edge detection algorithm. Camera calibration was achieved by placing a ball bearing of known diameter in the field of view. Factoring in both the uncertainty of the ball bearing diameter and the repeatability of calibration object positioning, a reasonable estimate of uncertainty associated with the camera magnification is 1%. The error induced by edge detection is estimated by analyzing each droplet image twice; once by applying an Otsu thresholding scheme and again by manually setting an elevated threshold (0.95 in normalized units), which counts nearly all non-white pixels as part of the droplet. In no instance does the thresholding scheme alter the initial diameter by more than 2%. More details about this procedure can be found elsewhere [55].

2.3.5 Experimental Procedure

Prior to performing experiments, the chamber is vacuumed to ~ 0.1 bar to ensure that there is no accumulated moisture or impurities inside the chamber. The chamber is then pressurized using dry nitrogen from a commercial cylinder, where the pressure is monitored by a transducer and held to

$\pm 1\%$ of the desired target. To reduce variability during experiments, the cartridge heater maintained a constant ambient temperature of 300 ± 1 K for all droplet evaporation tests. Once the fans are rotating at the desired speed, the injector is inserted into the chamber and a droplet with a desired initial diameter is deposited onto the intersection point of the cross fiber. The injector is then quickly retracted to avoid interfering with the flow field before recording of the evaporation process begins.

In order to determine the evaporation rate, K , the recorded images are processed using an in-house MATLAB code, where K is calculated based on the slope of the linear evolution of the d^2 -plot, $K = -dd^2/dt$. Previous droplet evaporation studies in turbulent environments reported that there is a noticeable deviation from the d^2 -law towards the end of the droplet lifetime [56, 58], and this behavior is observed in the present experiment. Consistent with the d^2 -law, K is determined by fitting a linear line through the data in the range $0.4 \leq d^2/d_0^2 \leq 1.0$. This range represents a 75% reduction in droplet volume, and the upcoming figures indicate that the evaporative profiles are quasi-linear between these limits. The coefficients of determination, R^2 , for the best fit linear lines universally exceed 0.99. The uncertainty in determining the droplet vaporization rate was estimated using 95% confidence interval. The calculations show that the standard error is less than 5% at all explored test conditions.

2.4 Result and discussion

2.4.1 Turbulent flow field characterization

To evaluate the turbulence characteristics at conditions similar to the droplet evaporation test matrix, PIV tests were performed over a wide range of fan speeds (200 rpm up to 4000 rpm) at three different ambient pressure conditions (1, 4, and 11 bar) and a temperature of 300 K. The PIV data was compiled and then processed using in-house MATLAB codes in order to calculate

the mean velocities, $\langle U \rangle$ and $\langle V \rangle$, and their corresponding velocity fluctuations, u and v . It is assumed that the Reynolds normal stress along the z -coordinate, $\langle ww \rangle$, is equal to the average of the two resolvable counterparts, $\langle ww \rangle = 0.5(\langle uu \rangle + \langle vv \rangle)$. This is a reasonable assumption since the turbulent flow field has excellent isotropy. Turbulence intensity is defined as the square root of the turbulent kinetic energy, $q^{0.5}$, and based on the aforementioned assumption for Reynolds stress, it can be written as $q^{0.5} = (\sqrt{3}/2) \sqrt{(\langle u^2 \rangle + \langle v^2 \rangle)}$.

Figure 2-2 illustrates an example of the mean flow velocity vectors and the corresponding turbulence intensity map at 1 bar. Fig. 2-2a reveals that the flow mean velocity is very low in the central region of the chamber. Fig. 2-2b showcases the level of anisotropy through a transparent overlay, where completely opaque regions indicate an anisotropy level below 10%. In this study, the spatial averages of turbulent statistics are calculated in a circular region around the center of the chamber with a diameter of 10 mm (indicated by the white circle in Fig. 2-2b). This spatial averaging is reported with the “ $\bar{}$ ” notation. The central region of the chamber exhibits a homogenous isotropic turbulent field under this condition, as evident in Fig. 2-2b. This pattern persists across other explored conditions, which will be further examined in subsequent figures.

Fig. 2-3 presents the ratio of the mean velocity over its root mean square (RMS) value for both orthogonal velocity components at different fan speeds. This figure clearly reveals that the mean velocity is a small fraction of the RMS velocity (remaining less than 15% in the worst-case scenario). In absolute terms, the flow mean velocities are very weak and less than 0.1 m/s in most cases. This indicates that the turbulent flow generated in the central area of the chamber can be considered a nearly zero-mean velocity flow field.

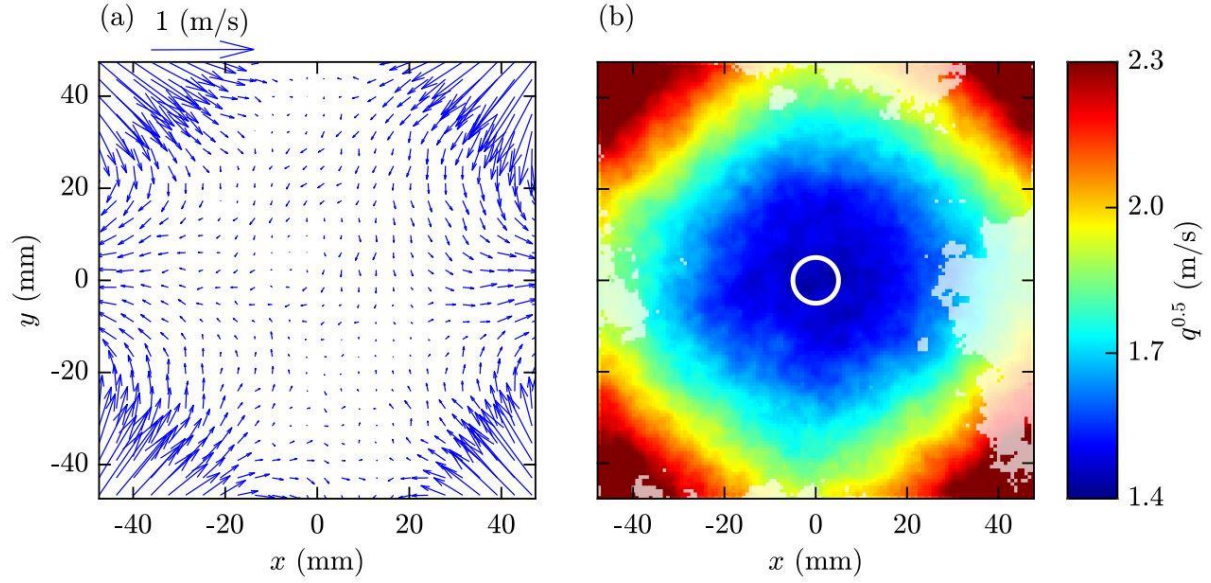


Figure 2-2. 2D profiles of a) mean velocity and b) turbulence intensity at 3000 rpm and 1 bar. The white circle in (b) represents the spatial averaging diameter (10 mm). Fully opaque regions in (b) denote < 10% anisotropy.

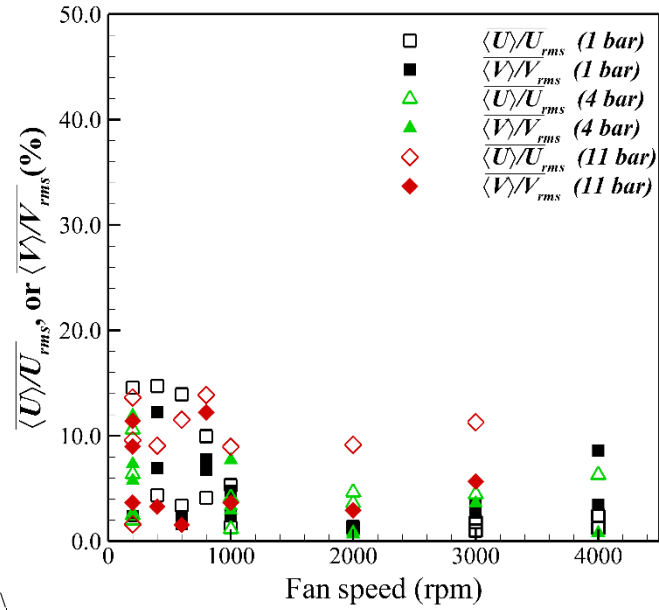


Figure 2-3. Variations of the ratio of the mean velocity component over its corresponding RMS velocity for both orthogonal velocity components with fan speeds for three different ambient pressures. These quantities are the spatial averages within the central zone of 10 mm diameter.

Fig. 2-4a shows that the variation of U_{rms}/V_{rms} with different fan speeds is within 10%. The results reveal that the level of isotropy is not affected when increasing the ambient pressure up to 11 bar. Fig. 2-4b, which depicts the variation of U_{rms}/V_{rms} along the horizontal axis (where $Z = 0$ mm), shows that the level of flow anisotropy is maintained less than 10% within a central zone of a diameter of approximately 40 mm. It should be noted that similar results were obtained along the vertical axis. The spatial variations of U_{rms} and V_{rms} were also investigated and it is observed that there is no noticeable deviation in each direction. Note that the RMS values in Fig. 2-4a are the averages taken in the 10 mm diameter central zone of the chamber, while those in Fig. 2-4b are the local values.

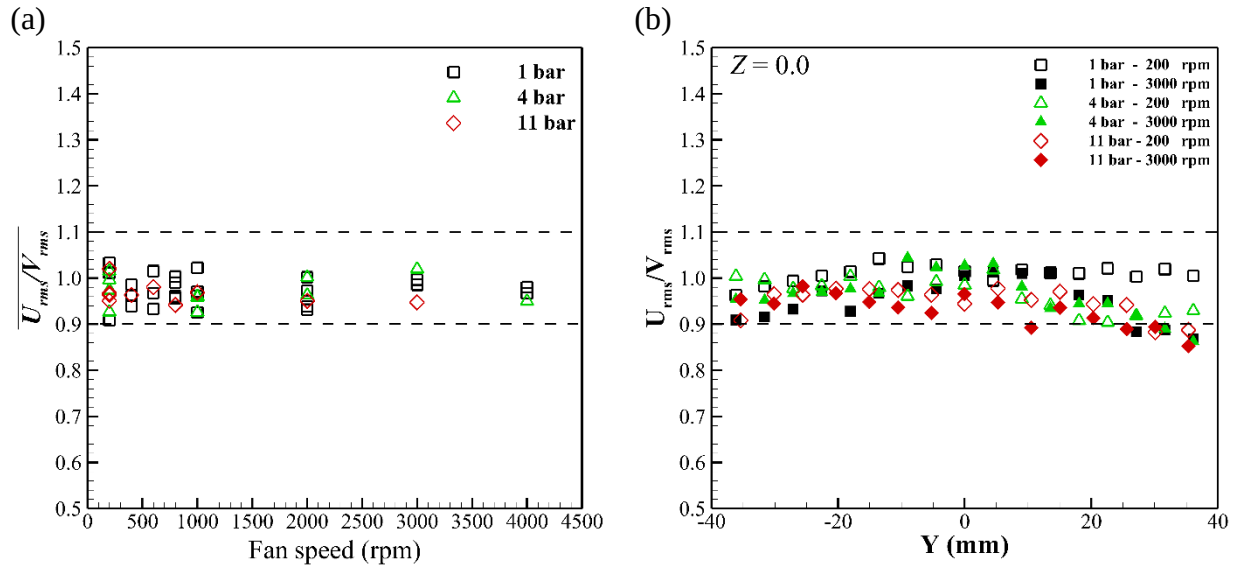


Figure 2-4. a) Variations of U_{rms}/V_{rms} with the fan speed by taking the spatial average in the 10 mm diameter central region of the chamber b) Spatial variations of U_{rms}/V_{rms}

As expected [54], turbulence intensity has been found to vary linearly with the fan speed in the current fan-stirred chamber, where the spatial average of turbulence intensity with the fan speed is expressed as $\overline{q^{0.5}} = 0.0005 \times N$, where N is the fan speed in rpm. Fig. 2-5 shows the local variation of turbulence intensity for various fan speeds within a central circular zone of

approximately 80 mm diameter at a typical ambient pressure. This figure shows that turbulence intensity remains relatively constant within a central zone of approximately 40 mm in diameter for all fan speeds.

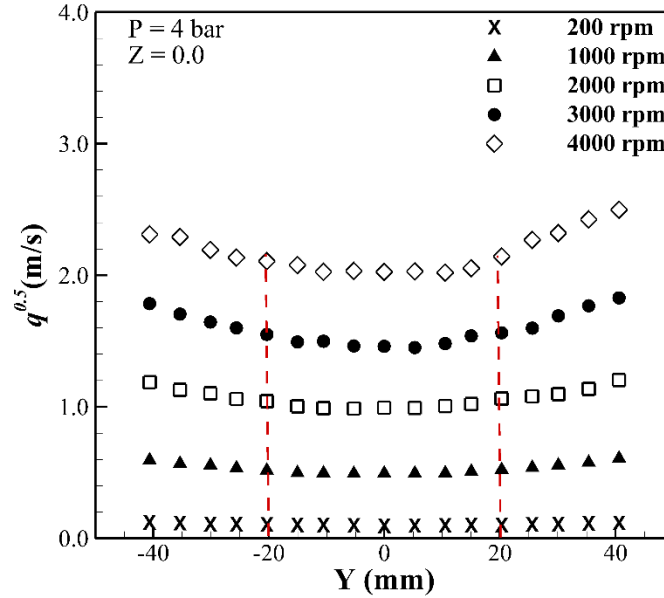


Figure 2-5. Variation of turbulence intensity in the central region of the chamber at different fans speed. The deviation within the region between the two dashed lines is less than 10%.

The integral length scales are calculated by integrations of longitudinal correlation coefficients.

The normalized correlation coefficients are written as [59]:

$$f_x(r, t) = \frac{\langle u(x_0, y_0, t) \cdot u(x_0 + r, y_0, t) \rangle}{U_{rms}(x_0, y_0)^2} \quad (2-1)$$

$$f_y(r, t) = \frac{\langle v(x_0, y_0, t) \cdot v(x_0, y_0 + r, t) \rangle}{V_{rms}(x_0, y_0)^2} \quad (2-2)$$

With the length scales can be calculated as:

$$L_{ux} = \int f_x(r, t) dr \quad (2-3)$$

$$L_{vy} = \int f_y(r,t) dr \quad (2-4)$$

A reasonable estimation of the longitudinal integral length scale, L_f , is obtained as $L_f = 0.5 (L_{ux} + L_{vy})$. It is worth mentioning that, at all explored conditions, the average variation between L_{ux} and L_{vy} is less than 10%. The spatial correlation coefficient $f_x(r,t)$ at different fan speeds and ambient pressures is illustrated in Fig. 2-6. The integral length scale L_{ux} is calculated by numerically integrating these plots. Due to the limited FOV, the correlation coefficient fails to reach zero. In order to carry out the integration, the combined approach suggested by Verwey and Birouk [60] is employed. In this approach, two curves are extended based on the data in the range of 0.2 and 0.4 (shown by the dash-dotted lines in Fig. 2-6). These curves are a linear fit and an exponential fit. The area under the curves is integrated, and the integral length scale is determined as the average of these two values (the numerical value is reported in the legend of Fig. 2-6). Although the integral length scale appears to vary slightly with fan speed, similar to what has been reported in [55], it remains relatively constant, with an average value of about 25.8 mm. Interestingly, this value is in the range of what is typically reported in real combustors [61].

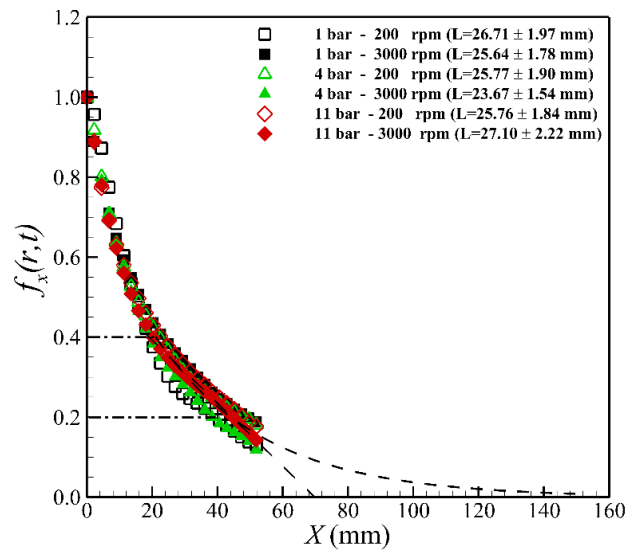


Figure 2-6. The spatial correlation coefficient for different fan speeds and ambient pressure conditions. Dashed lines are fitted to data for 11 bar – 3000 rpm.

The Kolmogorov length scale measures the smallest eddies in the flow, which is on the order of droplet size. It is a function of turbulent dissipation and fluid viscosity, so its calculation is not simple. Therefore, it is assumed that the dissipation rate is equal to the production rate, and based on this assumption, it is calculated using the following relationship [62]:

$$\eta \approx L \left(\text{Re}_{t,L}^{-3/4} \right) = C_\varepsilon^{-1/4} L \left(\frac{q^{0.5} L}{\nu} \right)^{-3/4} \quad (2-5)$$

where C_ε is a proportionality constant on the order of unity. Verwey and Birouk [60] investigated this parameter to show how it may systematically vary with turbulent flow field conditions. Using the exact same chamber, they provided comprehensive results at variable fan speed and pressure conditions, and showed that C_ε approaches 0.5 (this value is used presently in Eq. (2-5) to estimate η). Based on Eq. (2-5), the calculated Kolmogorov length scale decreases with increasing turbulence intensity and ranges from 675 μm at 200 rpm to 88 μm at 3000 rpm at 1 bar pressure. Furthermore, increasing the pressure decreases the kinematic viscosity and consequently reduces the Kolmogorov length scale. For instance, at 11 bar, the Kolmogorov length scale is equal to 120 μm and 16 μm at 200 rpm and 3000 rpm, respectively. A summary of the turbulent flow field characteristics is given in Table 2.

Table 2-2. Summary of the test conditions and turbulence statistics.

d_o (μm)	T (K)	P (bar)	N (rpm)	$q^{0.5}$ (m/s)	L (mm)	η (μm)
500	300.0	1.0 - 10.0	0 – 3000	0 – 1.5	25.8	16 - 675

2.4.2 Effect of ambient pressure on butanol droplet evaporation

This section focuses on the effect of ambient pressure (up to 10.0 bar) on the evaporation of a single butanol droplet in a quiescent atmosphere at room temperature. Fig. 2-7 illustrates the

temporal variation of the droplet normalized squared diameter for different ambient pressures in a quiescent environment. As expected, this figure depicts that increasing the pressure reduces the vaporization rate and consequently prolongs the droplet lifetime. The reduction in the droplet vaporization rate by increasing the pressure at low ambient temperature is in accordance with published data of conventional fuels [63] and light alcohol [64]. This phenomenon is attributed to two main reasons. First, it is known that the evaporation rate is mainly controlled by mass diffusion at low ambient temperature. In this condition, increasing the pressure attenuates mass diffusion by suppressing the mass fraction of fuel vapor at the droplet surface, thereby reducing the vaporization rate. Second, increasing the ambient pressure enhances the droplet surface temperature. Elevating the droplet surface temperature diminishes the temperature gradient at the droplet surface [65], which consequently causes a reduction in the rate of heat transfer. This causes a decrease in the droplet evaporation rate.

Another observation in Fig. 2-7 is that the temporal variation of the normalized squared diameter follows a predominantly linear trend, with a deviation occurring towards the latter stages of droplet lifetime. This deviation is insignificant at moderately elevated pressure (up to 5 bar) and becomes more apparent with increasing ambient pressure (i.e., higher than 5 bar). Gan et al. [66] reported that this deviation occurred for heavy fuels with a high boiling point. Verwey and Birouk [67] investigated the vaporization of heptane and decane droplets and showed that increasing the ambient pressure accelerated the onset of d^2 -deviation, which is more pronounced for the less volatile fuel (decane). One possible explanation is that increasing the pressure decreases the mass diffusion and enhances the importance of natural convection on the vaporization rate, which is not considered in the development of the d^2 -law [68]. Moreover, less volatile fuels are more influenced by natural convection due to their weak vapor generation and poor diffusion.

Nonetheless, the linear portion of the droplet lifetime is sufficient for the calculation of the vaporization rate over the interval $(0.4 \leq d^2/d_0^2 \leq 1.0)$.

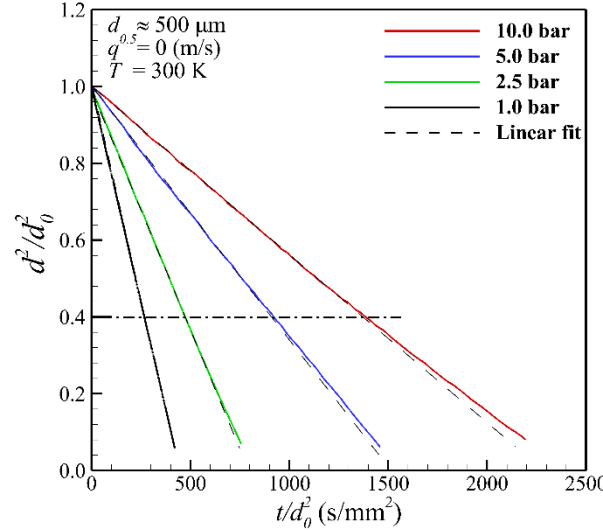


Figure 2-7. Time history for the normalized squared diameter of butanol droplet evaporation for various ambient pressure at the stagnant condition.

2.4.3 Effect of turbulence on butanol droplet evaporation

A single butanol droplet with a diameter of 500 μm is exposed to a turbulent environment with varying intensities up to 1.5 m/s at different ambient pressures (up to 10.0 bar). Figures 2-8 present the temporal variation of the normalized butanol droplet squared diameter for different turbulence intensities (up to 1.5 m/s) at two different ambient pressure conditions of 1.0 and 10.0 bar, respectively. As can be seen, increasing turbulence intensity accelerates the evaporation process and shortens the droplet lifetime at both ambient pressure conditions. Turbulence increases the rate of mass transfer from the droplet surface while simultaneously increasing the rate of heat transfer to the droplet—the latter stems from both an increase in the convective heat transfer coefficient and a somewhat lower surface temperature which improves the driving gradient. Both heat and mass transfer phenomena work together to re-establish a steady-state evaporation process that is much faster than the conditional equivalent in a stagnant environment. The d^2 -law deviation seen

in a quiescent atmosphere at elevated ambient pressure (Fig. 2-7) is also observed at the later stage of the droplet lifetime under turbulent flow conditions.

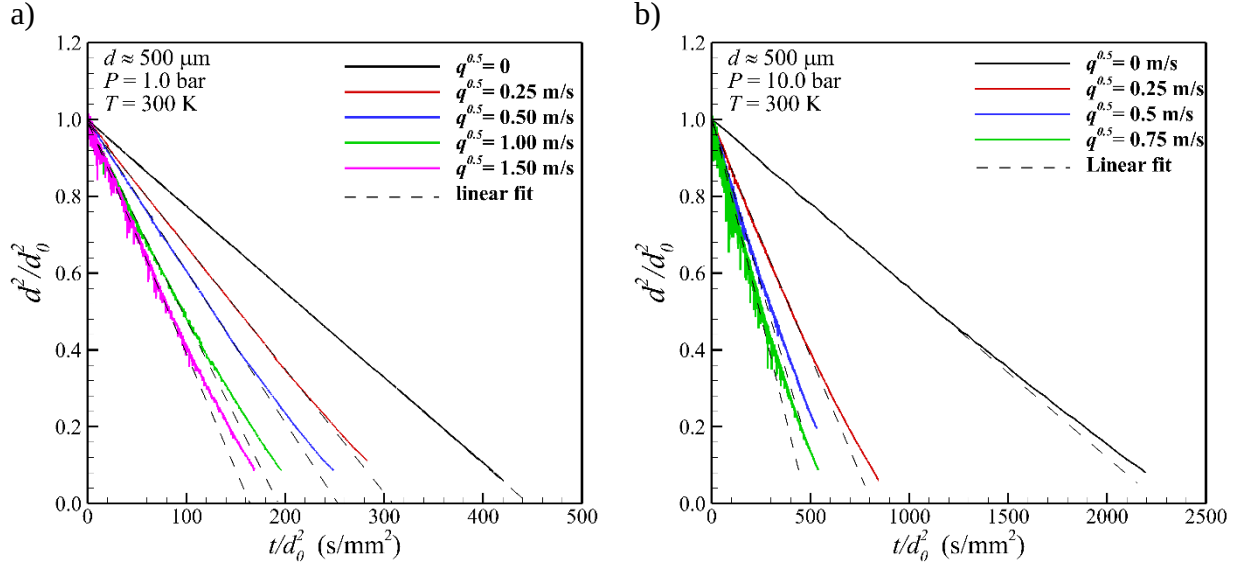


Figure 2-8. Time history of butanol droplet evaporation for various turbulence intensities at a) $P = 1.0$ bar, and b) $P = 10.0$ bar.

Fig. 2-9 is a presentation of the variation of normalized vaporization rate as a function of the turbulence intensity for different ambient pressure. The turbulent vaporization rate of the butanol droplet is normalized by its corresponding value in stagnant conditions, K_0 . It should be noted that each point is the average of ten tests and in all cases the uncertainty in the mean (95% confidence interval) is found to be less than 5%. Note that the highest fan speed at which a droplet can be reliably anchored to the suspending fiber decreases with ambient pressure; this is caused by a reduction in the liquid fuel surface tension coupled with the aerodynamic force. Nonetheless, this figure shows that the normalized vaporization rate is enhanced with turbulence at any explored ambient pressure. Additionally, Fig. 2-9 reveals that the enhancement in the butanol droplet vaporization rate is more pronounced at low levels of turbulence intensity. As this figure shows, the effect of turbulence becomes relatively less at high turbulence intensity. It is also interesting

to notice that this transition in the effectiveness of turbulence depends on the ambient pressure where it occurs much sooner as the ambient pressure increases.

The fact that the effectiveness of turbulence is lessened at higher intensities can be attributed to the main role of turbulence, which consists of improving the mass diffusion from the droplet surface to the surroundings. Hence, the turbulence effect on the vaporization process is linked to the vapor production rate, and increasing the turbulence level beyond a certain point in an environment with very poor diffusive potential (high pressure) may not yield the expected increase in evaporation rate. This transition in the effect of turbulence was witnessed for ethanol droplet at atmospheric pressure [55]. More importantly, Fig. 2-9 reveals that the effectiveness of turbulence intensifies with increasing ambient pressure, which is in line with published data of hydrocarbon fuels [69]. As shown in Fig. 2-7, high pressure severely oppresses the mass diffusion, resulting in a significant reduction in the vaporization rate. Under these circumstances, turbulence has more propensity to promote mass transfer by enhancing the mixing of the liquid and the gas phase. Therefore, turbulence is more influential at higher pressure conditions.

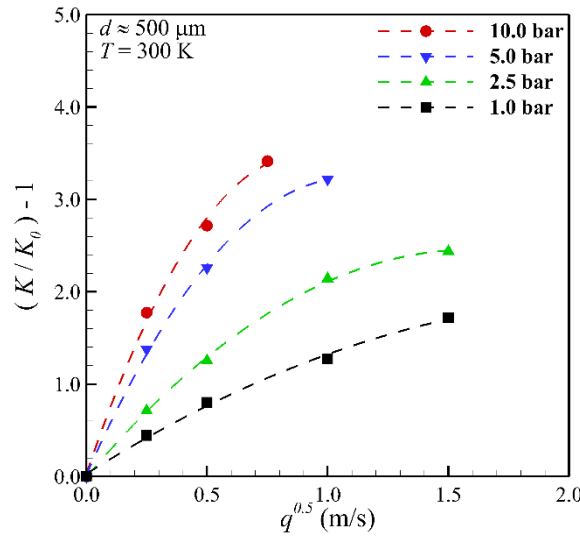


Figure 2-9. Butanol normalized evaporation rate as a function of turbulence intensity for different ambient pressures. K_0 is the droplet vaporization rate at zero rpm (no-flow).

2.4.4 Comparison with hydrocarbon fuels

Verwey and Birouk [56] investigated the effect of turbulence intensity on the vaporization of heptane and decane droplets at various ambient pressure and temperature conditions. The turbulent evaporation data for droplets with similar initial diameters ($d_0 = 500 \pm 50 \mu\text{m}$) at room temperature and different ambient pressure conditions are extracted from [56] and compared with the present butanol data. This comparison is shown in Fig. 2-10 as a function of turbulence intensity for the 1.0 bar pressure condition. This figure indicates that the vaporization rate of butanol is positioned between heptane and decane, with a closer resemblance to decane ($K_{Decane} < K_{Butanol} < K_{Heptane}$). A similar pattern exists at the other examined pressure conditions.

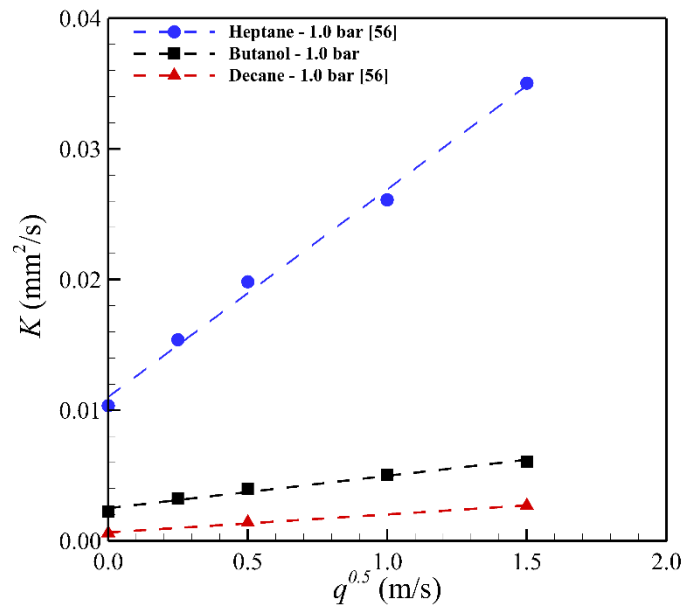


Figure 2-10. Comparison of droplet vaporization rate between butanol and hydrocarbon droplets.

Fig. 2-11 compares the butanol droplet vaporization rate with that of heptane and decane droplets as a function of ambient pressure under quiescent and turbulent conditions. As expected, the vaporization rate drops with increasing ambient pressure for all cases. Fig. 2-11 also reveals that

the trend of the droplet vaporization reduction with increasing pressure is almost identical for all fuels. This drop in the droplet vaporization rate is more noticeable when ambient pressure increases from standard up to 5.0 bar, which is in accordance with the experimental findings of Birouk and Fabbro [63].

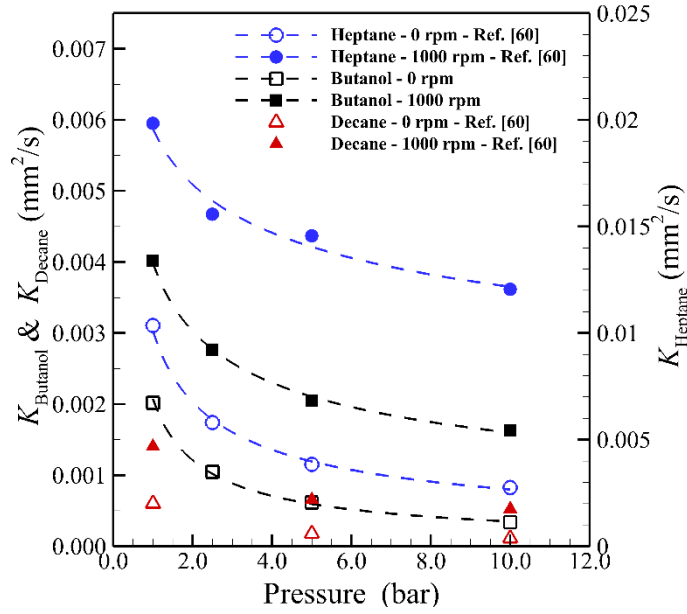


Figure 2-11. Variation of the droplet vaporization rate of butanol, heptane and decane fuels as a function of ambient pressure in quiescent and typical turbulent atmosphere, $q^{0.5} = 0.5$ m/s.

In Fig. 2-12, the normalized vaporization rates of butanol, heptane, and decane droplets are illustrated as functions of turbulence intensity at various ambient pressures. This figure depicts that the influence of turbulence on enhancing the vaporization rate is comparatively less pronounced for butanol in comparison to the other two fuels, heptane and decane.

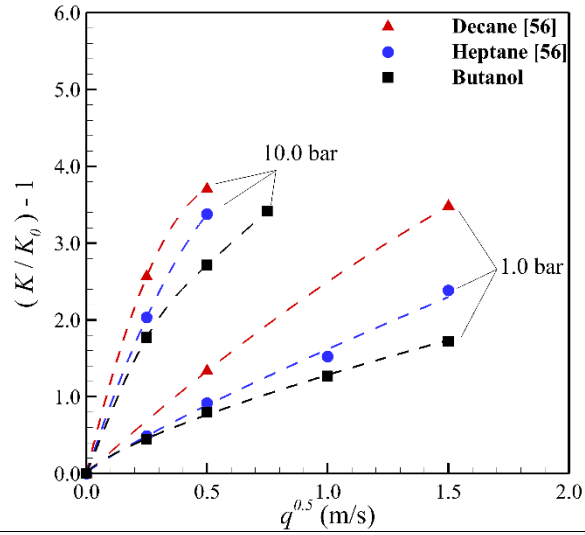


Figure 2-12. Variation of the droplet normalized vaporization rate of butanol and alkane fuels as a function of turbulence intensity for different ambient pressures.

There is an argument in the literature about the effect of fuel type on droplet evaporation under turbulence conditions. Some studies concluded that the effect of turbulence is more significant for less volatile fuels [58, 70, 71]. This is attributed to the slow evaporation process of the less volatile fuels, which benefits greatly from turbulence in dispersing the vapor away from the droplet surface and, consequently, enhancing the fuel vapor concentration gradient and thereby improving the vaporization rate [70]. In fact, this conclusion was based on alkane fuel droplets at standard ambient pressure conditions.

However, the findings depicted in Fig. 2-12 reveal that this conclusion does not always hold true. Despite butanol being considered less volatile compared to heptane (see vapor pressures in Table 2-3), its vaporization rate appears to be less influenced by turbulence intensity. This is in line with the experimental results of Verwey and Birouk [56]. They showed that the effect of turbulence is more pronounced for heptane (which is more volatile) than decane for small droplets ($d < 300 \mu\text{m}$) at elevated pressure conditions ($P > 2.5 \text{ bar}$).

Patel and Sahu [72] concluded that fuels which have higher vapor mass diffusivity are less affected by the ambient turbulent flow during the vaporization process. This is attributed to the decrease in the contribution of turbulence to mass dispersion as molecular diffusivity increases. Following the methodology of Patel and Sahu [72], the mass diffusivity coefficient under stagnant conditions is employed for comparison in the present study. For the calculation of the fuel vapor mass diffusivity coefficient in nitrogen (D_{Fuel-N_2}), the Fuller method is used [73]. Also, the ambient temperature is used for the calculation of D_{Fuel-N_2} as opposed to the droplet surface temperature, T_s , which is not readily available. Table 2-3 presents the physical properties of these fuels. As can be seen, butanol has the highest vapor mass diffusivity in nitrogen followed by heptane and decane. According to the conclusion of Patel and Sahu [72], it is expected that the higher the mass diffusivity of a fuel is, the less effect turbulence would exert on the vaporization rate, which is consistent with the findings in Fig. 2-12.

Table 2-3. Physical properties of fuels at atmospheric pressure and room temperature.

Fuel	Molecular Weight (kg/Kmol) from [73]	Density (kg/m³)	Vapor Pressure at 300 K (kPa)	^AVapor mass diffusivity in N₂ (m²/s) D_{Fuel-N_2} (T = 300 K)
Butanol (C ₄ H ₉ OH)	74.123	806 [49]	1.02 [74]	9.32×10^{-6}
Heptane (C ₇ H ₁₆)	100.204	684	6.70 [75]	7.33×10^{-6}
Decane (C ₁₀ H ₂₂)	142.285	730	0.13 [76]	6.06×10^{-6}

^A Calculated based on the Fuller equation [73]

2.4.5 Correlations

Two published comprehensive approaches were proposed to predict the turbulent vaporization rate of conventional/hydrocarbon fuels at standard ambient conditions [69, 70]. The first approach uses a Damköhler number [70] and the second uses a turbulent Reynolds number [69]. While the application of these correlations to elucidate the impact of turbulence on droplet vaporization has been studied in the context of hydrocarbon fuels [56, 77] and light alcohols [78], their application to high alcohols has not been yet verified.

The vaporization Damköhler number, Da_v , is defined as the ratio of the turbulent flow characteristic time scale, t_{flow} , to the vaporization time scale, t_{vap} , which is expressed as follows:

$$Da_v = \frac{t_{flow}}{t_{vap}} \quad (2-6)$$

$$t_{flow} = \frac{d_0}{q^{0.5}} \quad (2-7)$$

$$t_{vap} = \frac{r_0}{V_r} \quad (2-8)$$

Considering that the droplet lifetime follows the d^2 -law, and using the liquid-vapor continuity at the droplet surface [68], the radial velocity can be calculated as follows [54]:

$$\rho_v V_r = \rho_l \left(\frac{dr}{dt} \right) = \frac{\rho_l K_0}{4d_0} \quad (2-9)$$

Using Eqs. (2-7) – (2-9), the Damköhler number can be written as:

$$Da_v = \frac{1}{2} \left(\frac{\rho_l}{\rho_v} \frac{K_0}{d_0 q^{0.5}} \right) \quad (2-10)$$

Two further assumptions are implicit in the development of this correlation. The first is that the droplet diameter is set to its initial diameter, and the second assumption is that $T_s \approx T_\infty$ for the purposes of calculating the vapor density ρ_v . This approximation is acceptable for slowly evaporating fuels such as decane and butanol, while a reasonable estimate of surface temperature is recommended for fuels with higher vapor pressures including heptane and ethanol. The droplet normalized vaporization rate of butanol, heptane and decane is plotted versus the Damköhler number in the Fig. 2-13, and a correlation in the form of Eq. (2-11) is derived. The coefficients obtained in [54] are used here, yielding satisfactory results.

$$\frac{K}{K_0} = 1.0 + 0.0948 Da_v^{-0.765} \quad (2-11)$$

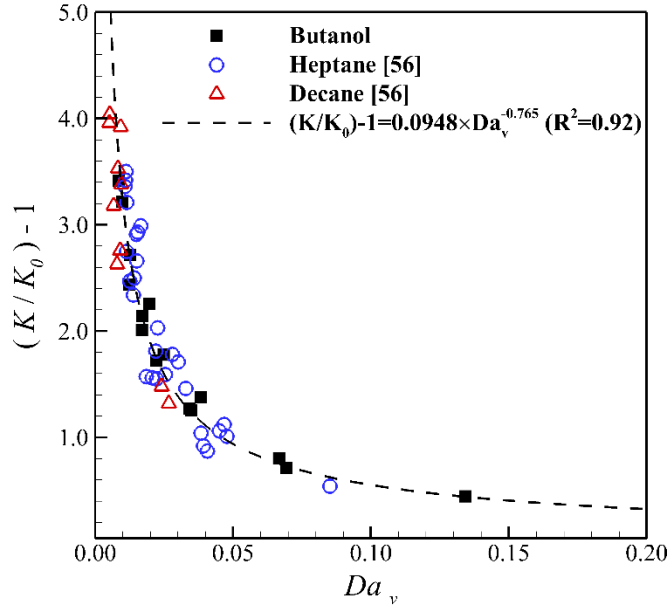


Figure 2-13. Droplet normalized vaporization rate versus Damköhler number.

Eq. (2-12) proposed by Verwey and Birouk [56] uses Reynolds ($Re_{t,d_0} = q^{0.5} d_0 / \nu$) and Schmidt ($Sc = \nu / D_{AB}$) numbers, where ν is the kinematic viscosity of the ambient nitrogen and D_{AB} is the mass diffusivity coefficient of the binary nitrogen-fuel vapor system. The best fit line suggested in [56] is:

$$\frac{K}{K_0} = 1.0 + 0.0439 Re_{t,L}^{0.66} Sc^{1.16} \left(\frac{T_\infty}{T_0} \right)^{-1.42} \left(\frac{P_\infty}{P_0} \right)^{-0.19} \left(\frac{L}{d_0} \right)^{-0.53} \quad (2-12)$$

Fig. 2-14 clearly demonstrates that Eq. (2-12) can predict the turbulent vaporization rate of a butanol droplet, similar to alkane fuels. The coefficient of determination for the best fit line is 0.90, which is comparable to the findings reported in Verwey and Birouk [56] for alkane droplets. Evidently, the addition of butanol data does not significantly alter the form of the trend line in either Eq. (2-11) or Eq. (2-12)

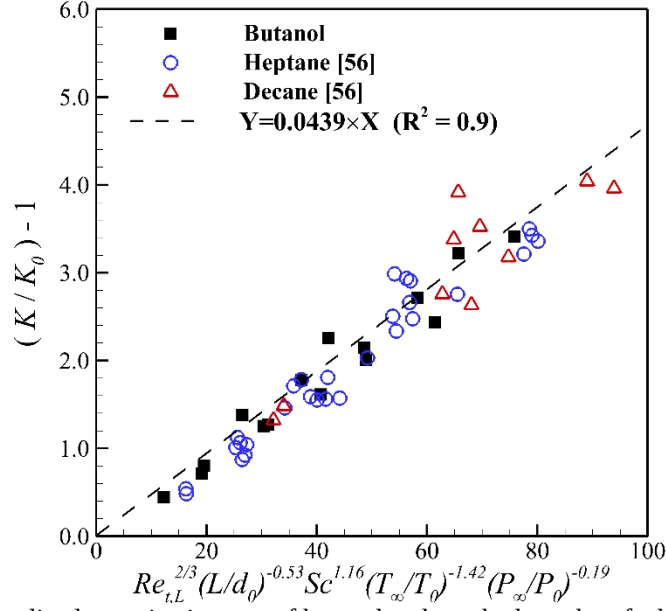


Figure 2-14. Droplet normalized vaporization rate of butanol and two hydrocarbon fuels from [56] as a function of the Reynolds correlation.

2.5 Concluding remarks

This study endeavored to explore the vaporization characteristics of butanol droplets, with the ultimate objective of identifying a potential alternative fuel for future combustion CI engines. A fan-stirred spherical chamber was used for the droplet vaporization tests. It was shown that this setup can create a controllable isotropic and homogenous turbulent flow field with a nearly zero mean velocity at various fan speeds and ambient pressure conditions. Turbulent flow characteristics, such as turbulence intensity and integral length scale, were measured and their relationships with ambient pressure and fan speeds are specified. The main findings are summarized below.

- The experimental results under stagnant conditions showed that the butanol droplet vaporization rate reduces with increasing ambient pressure, mainly due to the suppression of the fuel vapor mass fraction at the droplet surface. Experimental results under turbulent conditions revealed that the vaporization rate is improved by turbulence at low levels of

turbulence intensity. However, the effect of turbulence is attenuated at high levels of turbulence intensity.

- Plots of d^2 vs. time exhibited a d^2 deviation, and the severity of this deviation appeared to increase with ambient pressure and turbulence intensity. However, the majority of the droplet's lifetime followed the quasi-linear vaporization behavior, confirming that the d^2 -law is still valid in all explored conditions.
- A comparison of the vaporization behavior of butanol droplets with heptane and decane droplets, as investigated in reference [56], has yielded several intriguing observations. Firstly, the vaporization rate of butanol is found to fall between the vaporization rates of heptane and decane, with closer proximity to the latter. Secondly, results reveal that the influence of turbulence on the improvement of the vaporization rate of different fuel types is primarily dependent on the vapor mass diffusivity of the fuel in relation to the ambient conditions. It confirms the finding of Patel and Sahu [72] and shows that vaporization of fuels with higher mass diffusivity are less responsive to turbulence.
- Finally, published vaporization Damköhler and turbulent Reynolds number correlations, which were developed for alkane fuels, were tested and found able to predict the butanol vaporization rate.

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Chapter 3: Experimental investigation of the effect of droplet size on the vaporization of butanol in turbulent environments at elevated pressure

3.1 Abstract

This paper presents an experimental study of the effect of droplet size on the vaporization rate of butanol fuel under turbulent flow conditions at elevated pressure and room temperature. The butanol droplet is suspended at the intersection of two micro-fibers in the center of a spherical vessel. The initial size of the butanol droplet is varied in the range between 300 and 700 μm . A controlled turbulent flow field, characterized by quasi-zero mean velocity and turbulence intensity of up to 1.5 m/s, was generated by eight axial fans. The findings reveal an improvement in the vaporization rate of butanol droplet as the droplet size increases. This improvement is more pronounced under conditions of elevated pressure and turbulence intensity. The results show that turbulence begins to influence the vaporization process when the droplet diameter exceeds the Kolmogorov length scale. Butanol droplet vaporization rate is found to lie between heptane and decane, leaning towards decane under all explored test conditions. The results reveal that the vaporization rate of hydrocarbon fuels is more sensitive to the droplet size variations than butanol. Turbulence is found to exert greater impact on the vaporization of fuels that have lower gas-phase mass diffusivity and higher thermal diffusivity. Finally, the previously proposed correlations, expressed in terms of Damköhler and turbulent Reynolds numbers, are assessed and found capable of predicting the vaporization of butanol droplet over a wide range size.

3.2 Introduction

Presently, approximately 84% of the global energy consumption is still derived from fossil fuels [1]. About 30% of this energy is used in the transportation sector [2]. Combustion of fossil fuels inevitably results in the emission of harmful gases into the atmosphere which gives rise to significant environmental concerns. Moreover, increasing energy demand, combined with fluctuating oil prices and uncertainties in the long-term availability of oil, further complicates the energy landscape [3]. Consequently, the quest for alternative fuels for use in internal combustion engines has recently gained more attention.

Among all alternative fuels under scrutiny, alcoholic fuels attract significant attention due to their diverse range of sources and potential for clean combustion [4]. The efficacy of light alcoholic fuels, such as ethanol, has been well established in spark ignition engines and has found application in the transportation sector [5, 6]. On the other hand, higher alcoholic fuels, such as butanol, have several advantages over light alcohols, making them more favorable candidates for compression ignition (CI) engines. Compared with light alcohols, butanol has higher calorific value [7], lower latent heat of vaporization [8], higher cetane number [9], and superior material compatibility with engines' components [10]. It was reported that butanol-fueled CI engines can operate with reduced NO_x emissions, acceptable performance, and often require only minor engine modifications [11].

While butanol production is relatively more expensive compared to ethanol, the increasing demand for, and interest in, butanol are expanding agricultural and industrial activities [12]. It has recently been asserted that advancements in production technology have led to a gradual reduction in the cost of butanol [13]. Consequently, there has been a significant increase in the number of published studies exploring the utilization of butanol in CI engines (e.g., [14, 15]). The expectation is that

butanol will continue to gain prominence and attract even more attention for use in internal combustion engines in the foreseeable future [16].

In CI engines, liquid fuel is injected into the combustion chamber as a cloud of droplets, which must evaporate rapidly and completely to create a combustible mixture with air [17]. Understanding this evaporation process enables engineers to optimize fuel injection systems by enhancing atomization and improving air mixing. Moreover, the evaporation process of fuel droplets significantly impacts the combustion efficiency and emission of pollutants [18]. Therefore, a comprehensive understanding of droplet evaporation is crucial for optimizing fuel injection systems, combustion efficiency, and emissions control in CI engines.

Owing to the heterogeneous nature of the atomization process, a wide range of droplet sizes coexist within a combustor, spanning from a few micrometers up to 500 μm [19]. Each distinct droplet size shows unique vaporization characteristics, encompassing diverse transient heating periods and evaporation rates [20]. Moreover, these droplets are subjected to intense turbulence and high-pressure conditions within a combustion chamber [21]. Consequently, it is important to elucidate the interrelationships among the aforementioned parameters. The influence of droplet size on the burning rate has been studied [22]. Larger droplets exhibit an enhanced propensity for soot generation during the combustion process [23]. This phenomenon significantly impacts both heat and mass transfer, and subsequently leads to alterations in the burning rate [24, 25]. However, these studies often utilized excessively large and unrealistic droplets. Moreover, due to the absence of soot in the evaporation process, droplet combustion findings cannot be generalized to droplet vaporization.

A literature review reveals that there are limited studies on the effect of droplet size on the vaporization process. Abou Al-Sood and Birouk [26] conducted a computational simulation for a

droplet evaporating in a turbulent flow field under elevated ambient pressure and temperature conditions. Their findings indicated that, as the initial droplet diameter increases, the droplet wet-bulb temperature of the droplet increases, which leads to an increase in the vaporization rate. Pati et al. [27] depicted that, for water droplet lifetime, the prediction of both diffusion-controlled and kinetic models depends on the droplet size. Khan et al. [20] experimentally investigated the effect of droplet size on the transient heating and vaporization rate of kerosene droplets at different ambient pressures under stagnant conditions. They demonstrated that increasing the droplet size improves the vaporization rate, especially at elevated pressure. Verwey and Birouk [28, 29] further investigated the effect of droplet size on the vaporization rate of heptane and decane droplets under turbulent conditions at elevated temperature and pressure conditions. They confirmed that increasing the droplet size enhances the vaporization rate, which becomes increasingly pronounced as ambient turbulence intensity and pressure rise. They also demonstrated that the influence of droplet size on the vaporization rate diminishes notably as the ambient temperature increases. They argued that the common belief that turbulence has a greater impact on the vaporization rate of less volatile fuels does not always hold, particularly for small droplets.

The aforementioned literature on the effect of droplet size was focused only on alkanes. Moreover, numerical studies conducted on butanol have relied on data from water or ethanol for validation due to the lack of appropriate experimental data. While the authors of the present study have endeavored to furnish experimental data on the vaporization rate of butanol droplets with a fixed initial diameter, d_0 , of 500 μm [30], as mentioned earlier, the reliability of numerical models is also contingent on droplets size [27]. The present study experimentally investigates the effect of droplets size on the vaporization rate of butanol in turbulent flow conditions at elevated ambient pressure.

3.3 Experimental setup and Methodology

The experimental setup is depicted in Fig. 3-1. It consists of a spherical chamber with a volume of 29 liters, constructed from stainless steel to withstand elevated pressure. It is equipped with four pairs of co-axial fans to generate a homogenous isotropic turbulent flow field in the central region of the chamber. Additionally, it features two sets of quartz windows, serving multiple purposes such as facilitating particle image velocimetry (PIV) measurements, imaging of droplets vaporization process, and enabling physical access to the chamber's interior. Moreover, the setup includes ten accessory ports designed to accommodate various inputs, including a fuel injector, a frame for holding droplets, a heater, pressure gauges and transducers, thermocouples, as well as outlet and safety valves. As can be seen in Fig. 3-1b, two 14 μm silicon carbide fibers, crossing at a 90-degree angle and positioned in the central region of the chamber, were used to suspend the droplet. These micro fibers are secured onto a thin steel frame. The two fibers are affixed onto the holders using epoxy and kept under slight tension to avoid breakage. The frame is then fastened to the top of the chamber. This cross-fiber technique, which has been employed in previous works by this group (e.g.,[28-30]), promotes droplet sphericity and supports a wide range of initial diameters while minimizing conductive heat transfer. For the generation and release of a droplet onto the fiber, a hand-operated fuel injector was utilized. This injection system consists of a leadscrew-driven piston, a retractable barrel, a steel needle, and a capillary tube with an inner and an outer diameter of 40 μm and 60 μm , respectively.

3.4 Result and discussion

To examine the impact of droplet size on the vaporization rate of butanol droplets, three initial diameters were selected: 300, 500, and 700 μm . The evaporation process was carried out at different ambient pressures ranging from 1 to 10 bar. The flow surrounding the droplet was varied

from a stagnant to a turbulent regime characterized by a turbulence intensity of up to 1.5 m/s. All experiments were conducted at room temperature. The results of PIV tests are presented in Section 3.4.1. The effect of butanol droplet size on the vaporization rate is presented in Section 3.4.2. In Section 3.4.3, the effectiveness of turbulence on butanol droplet vaporization rate is evaluated, and the relationship between droplets size, the Kolmogorov length scale, and turbulence effectiveness is explored. A comparison is made between the vaporization data of butanol and alkanes (heptane and decane) in Section 3.4.4. Furthermore, the underlying causes of the disparate vaporization rates exhibited between these fuels are examined. Finally, in Section 3.4.5, the validity of two commonly used correlations for predicting the droplet vaporization rate under turbulent conditions is assessed using the present data.

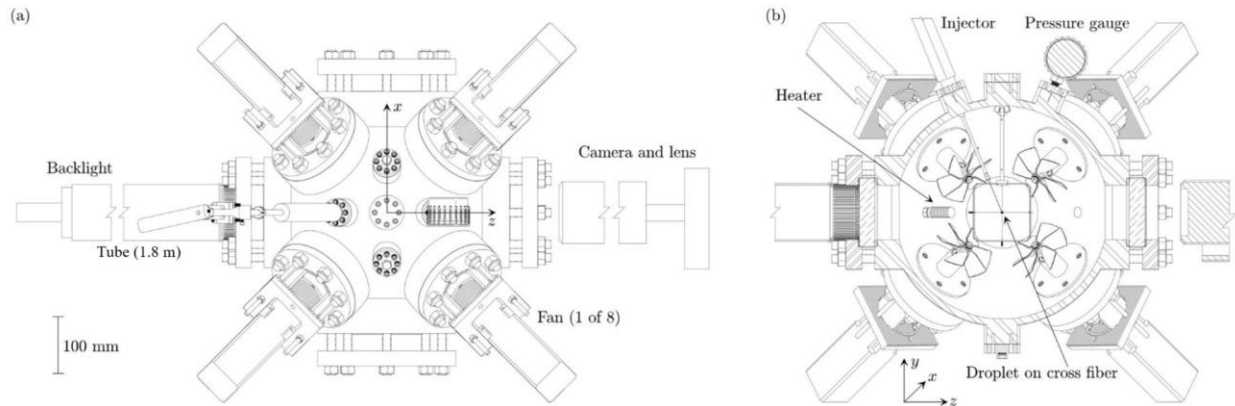


Figure 3-1. A schematic of a) top, and b) cutaway view of the spherical chamber (the cross fiber is exaggerated to make it visible) with related instrumentation.

The experimental methodology consisted of four stages. In the first one, the turbulent flow field in the chamber was documented using a Dantec Dynamics 2D-PIV system, incorporating a Dual Power Nd:YAG laser (135 mJ double pulse) and a FlowSense EO 4M camera. Olive oil micro-droplets, generated by a LaVision aerosol generator, were employed for seeding the flow. DynamicStudio software was used for control, synchronization, data acquisition, and raw image cross-correlation.

The second stage involved preparing the ambient conditions. In this step, the chamber was filled with nitrogen gas and maintained at a temperature of 300 ± 1 K. To achieve this, a compact cartridge heater with fins was employed, and the gas flow temperature was monitored by a K-type thermocouple positioned 180 degrees opposite to the heater. Additionally, the chamber's pressure, P , was adjusted to meet the desired target by introducing dry nitrogen from a commercial cylinder. Throughout the test, a transducer was used to closely monitor and maintain the pressure within $\pm 1\%$ of the specified value. Different turbulence intensity conditions at negligible mean velocity in the central region of the chamber were achieved. These axial fans were driven by independent servo drivers, and their rotational speed was precisely maintained within $\pm 1\%$ of the designated RPM.

The third stage of the experiment involved creating and suspending individual butanol droplets onto the intersection point of the two microfibers. Droplets with an initial diameter of 300 μm , 500 μm , or 700 μm were successfully formed. During this step, the injector was inserted into the chamber to create a droplet, and once the desired size is reached, the droplet was transferred onto the fiber. Subsequently, the barrel was quickly retracted to avoid interference with the flow field around the droplet.

The final stage of the experiment involved imaging and computing the vaporization process, as illustrated in Fig. 3-2. This figure shows images of a butanol droplet at different instances during its evaporation along with the corresponding temporal normalized diameter profile. It is worth mentioning that the horizontal microfiber in the subfigures of Fig. 3-2 is not visible because it is positioned along the camera axis direction. The evaporation process was recorded using a Fastec IL5Q camera paired with a Questar QM-100 long-distance microscope. This setup is capable of 24 fps with a spatial resolution of 1.08 $\mu\text{m}/\text{px}$ at a shutter speed of 200 μs . To enhance the

brightness of the captured images, a halogen lamp with a 250 W power output was employed as a backlight source. To eliminate any thermal impact this lamp might have on the droplet vaporization process, a 1.8-meter-long tube was placed between the lamp and the port window of the chamber. Droplet recorded images were processed using an in-house MATLAB code. This code initially determines d_0 by equating the planar area of the droplet image to that of a corresponding circle, and the vaporization rate, K , is then calculated as the slope of the linear portion of the temporal evolution of d^2 (as depicted in Fig. 3-2). To ensure consistency and avoid capturing transient conditions at the outset, as well as the potential influence of the fibers at the end of the process, the calculation of K is conducted within the droplet lifetime corresponding to $0.95 \geq d^2/d_0^2 \geq 0.4$, as can be seen by the red dashed dot line in Fig. 3-2. This approach accounts for approximately a 75% reduction in the droplet's volume, and the coefficient of determination of the best-fit line, R^2 , consistently exceeds 0.99.

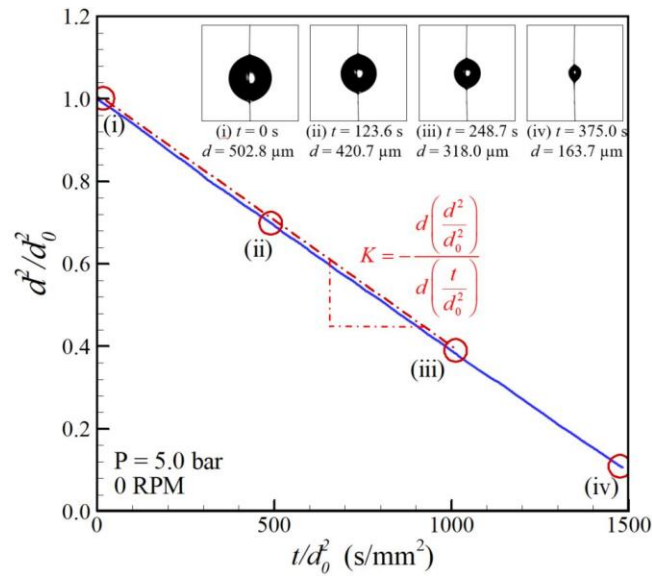


Figure 3-2. Temporal evolution of the normalized diameter, along with some images, of a 502.8 μm butanol droplet evaporating in a quiescent environment at 5.0 bar

In the present study, the estimation of the droplet vaporization rate was carried out by repeating each experiment at least four times and applying a 95% confidence interval to estimate the sampling error. The maximum uncertainty associated with the average vaporization rate at any given test condition is less than 5%. Systematic error involved in the determination of droplet size originates from the camera calibration and the droplet edge detection algorithm. The camera calibration involved the measurement of a known object's diameter, with an estimated associated uncertainty of 1%. Droplet edge detection is assessed through a comparison of two different thresholds (Otsu and an artificially high value) which yielded a difference of less than 2% in the calculation of d_0 .

3.4.1 Turbulence Characterization

To examine The turbulent flow field within the chamber has been comprehensively analyzed using PIV and previously reported elsewhere [30]. Since the present study employed the same experimental setup and test conditions, only a concise summary of the results is presented here. The variations of U_{rms}/V_{rms} and $q^{0.5}/q_{avg}^{0.5}$ are depicted in Fig. 3-3 for three different ambient pressures; where U_{rms} and V_{rms} are the root mean square values of the respective velocity fluctuations, $q^{0.5}$ denotes the turbulence intensity, defined as the square root of turbulence kinetic energy. The turbulence intensity is calculated by assuming that the Reynolds normal stress along z-coordinate is best approximated as an average of the two resolvable counterparts (i.e., $q^{0.5} = (\sqrt{3}/2)\sqrt{U_{rms}^2 + V_{rms}^2}$), and $q_{avg}^{0.5}$ is the average turbulence intensity, calculated within a 10 mm diameter circle at the chamber's center.

Fig. 3-3 illustrates high levels of isotropy (quantified by $U_{rms}/V_{rms} \approx 1$) and homogeneity ($q^{0.5}/q_{avg}^{0.5} \approx 1$) inside the chamber. The variations of U_{rms}/V_{rms} and $q^{0.5}/q_{avg}^{0.5}$ along the

horizontal axis ($y = 0$ mm) fall in the range between 0.9 and 1.1 within a spherical volume of 40 mm diameter at the center of the chamber. Fig. 3-3 also displays comparable patterns for fan speeds of both 200 and 3000 RPM (which are, respectively, the lowest and highest turbulence levels), suggesting a consistent level of isotropy and homogeneity across the entire range of fan speeds examined in this study.

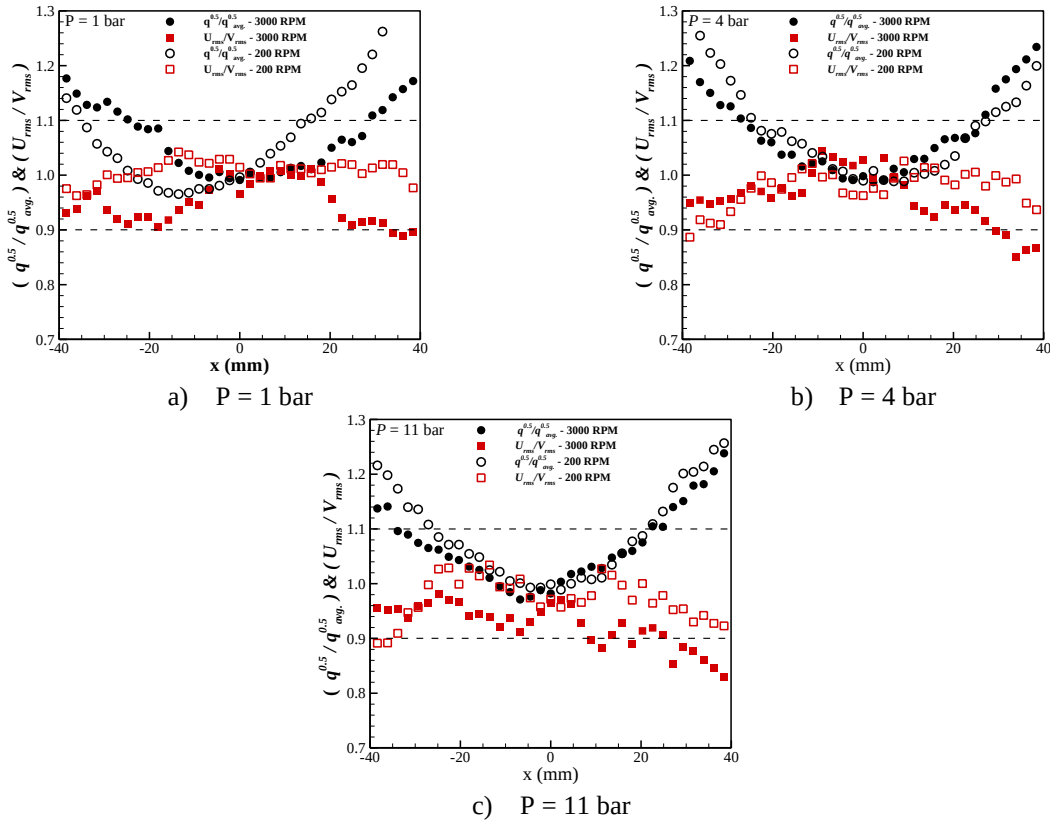


Figure 3-3. Isotropy and homogeneity of turbulence for the lowest and highest fan speeds along the horizontal axis for three different ambient pressures: a) 1 bar, b) 4 bar, and c) 11 bar

The PIV results indicate that the mean velocity components are negligible compared to their RMS counterparts. While the mean velocity components remain approximately constant regardless of fans speed, there is a linear increase in turbulence intensity with fans speed. This increase can be quantified as $q^{0.5} = 0.0005 \times N$, where N is the fan speed in RPM, and $q^{0.5}$ is expressed in m/s.

The integral length scale, L , is determined through numerical integration of the spatial correlation coefficient. Since the correlation does not approach zero, a combined approach recommended by

Verwey and Birouk [31] is utilized. This approach yields an average integral length scale of ~ 26 mm, which remains constant regardless of fans speed or pressure.

The Kolmogorov length scale, η , cannot be directly resolved and is therefore computed using the methodology outlined in [30]:

$$\eta \approx L \text{Re}_{t,L}^{-3/4} \approx C_\varepsilon^{-1/4} L \left(\frac{q^{0.5} L}{\nu} \right)^{-3/4} \quad (3-1)$$

where C_ε is the proportionality constant, which is assumed to be 0.5 [31], and ν is the kinematic viscosity. The computed Kolmogorov length scale falls between 10 and 700 μm , depending on the turbulence intensity and pressure.

Most importantly, the PIV results confirmed that the addition of different components to the chamber, such as the frame, heater, and injector, did not result in noticeable changes to the turbulence characteristics. Therefore, it can be concluded that the droplet evaporation tests were conducted under conditions of homogeneous isotropic turbulence (HIT) with nearly zero mean velocity. A summary of the test conditions and turbulence flow field characteristics is provided in Table 3-1.

Table 3-1. Summary of the test conditions and turbulence characteristics.

d_o (μm)	T (K)	P (bar)	N (rpm)	$q^{0.5}$ (m/s)	L (mm)	η (μm)
300, 500, 700	300.0	1.0 - 10.0	0 – 3000	0 – 1.5	26	10 – 700

3.4.2 Effect of droplet size

Fig. 3-4 illustrates the temporal variation of the (normalized) square of the droplet diameter under both quiescent ($q^{0.5} = 0$ m/s – solid lines) and turbulent ($q^{0.5} = 1.5$ m/s – dashed lines) conditions for different droplet sizes at atmospheric pressure. The findings demonstrate that an increase in

droplet size positively influences the vaporization rate, with this effect becoming more prominent in the presence of turbulent flow.

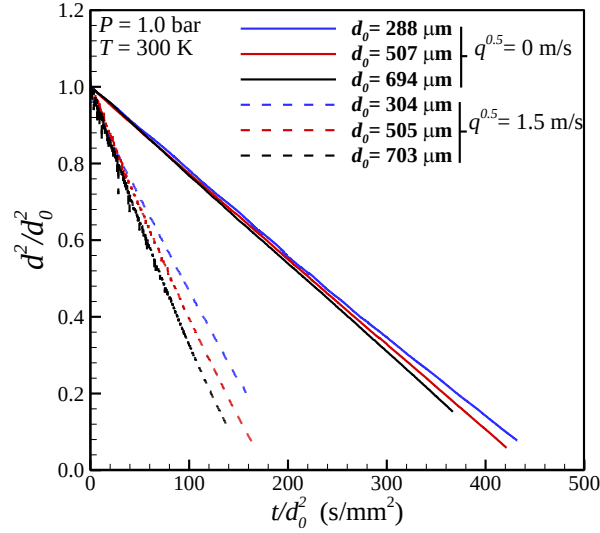


Figure 3-4. Time history of butanol droplet vaporization for different droplet sizes in quiescent and turbulent environments.

The vaporization rates of butanol droplets are presented under atmospheric pressure conditions (Fig. 3-5a) and at 10 bar pressure (Fig. 3-5b) for a variety of turbulence intensity conditions. In quiescent conditions, the droplet size exhibits negligible impact on the vaporization rate at atmospheric pressure (Fig. 3-5a). In contrast, Fig. 3-5b shows that, in the same quiescent conditions, an increase in droplet size results in an increased vaporization rate at higher pressures. This is consistent with the experimental findings reported by Verwey and Birouk [28] for heptane and decane, as well as the study conducted by Khan et al. [20] for kerosene. This is attributed to the heightened impact of natural convection on the vaporization rate of larger droplets in high-pressure environments. Natural convection is characterized by the Grashof number, Gr , where $Gr \sim d^3 P^2$. Raising the pressure from 1 to 10 bar results in a two-order-of-magnitude increase in the Grashof number. Gogos et al. [32] demonstrated that an increase in the Grashof number due to pressure can significantly change the vaporization rate under normal gravity conditions. Therefore,

larger droplets subjected to higher pressures would experience greater benefits from natural convection in quiescent conditions. This phenomenon enhances vapor mass diffusion, which leads to an increase in the vaporization rate.

More importantly, these two figures clearly demonstrate that, in the presence of a turbulent flow, increasing the droplet size enhances the vaporization rate, which is more pronounced at higher turbulence intensity levels. This observed trend remains consistent across all examined ambient pressure conditions. This corroborates the findings of Verwey and Birouk [28].

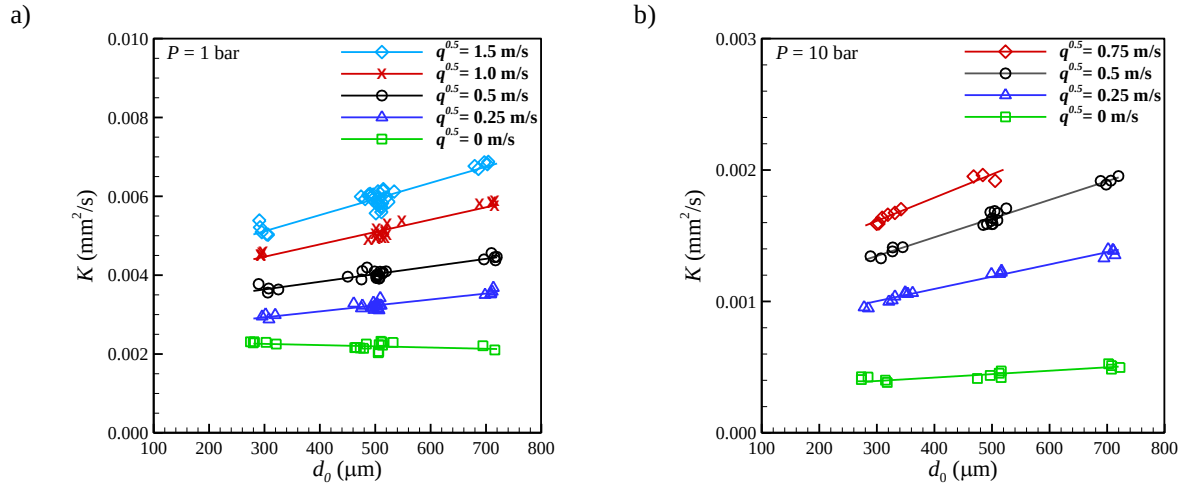


Figure 3-5. Butanol vaporization rate as a function of droplet size at a) 1 bar, and b) 10 bar

3.4.3 Relation between droplet size and turbulence effectiveness

To investigate the effect of turbulence on the vaporization rate, K is normalized by K_0 , which is the vaporization rate at the stagnant condition and corresponding pressure. This ratio (K/K_0) is termed the turbulence effectiveness. Fig. 3-6 elucidates the relation between K/K_0 and the initial droplet diameter under different ambient pressures subjected to moderate turbulence conditions ($q^{0.5} = 0.5$ m/s). This figure exhibits a consistent slope for all pressure conditions, indicating that the rate of increase in K/K_0 with respect to d_0 is independent of pressure. A similar trend is also observed for the other investigated turbulence intensity conditions. Verwey and Birouk [29]

previously demonstrated that the relationship between droplet size and turbulence effectiveness is more prominent at higher pressures for heptane and decane droplets. It seems that the different conclusion here stems from the utilization of different fuel type. Additional insights into the distinctions in the characteristics between butanol and alkanes (i.e., heptane and decane) will be presented in the following section.

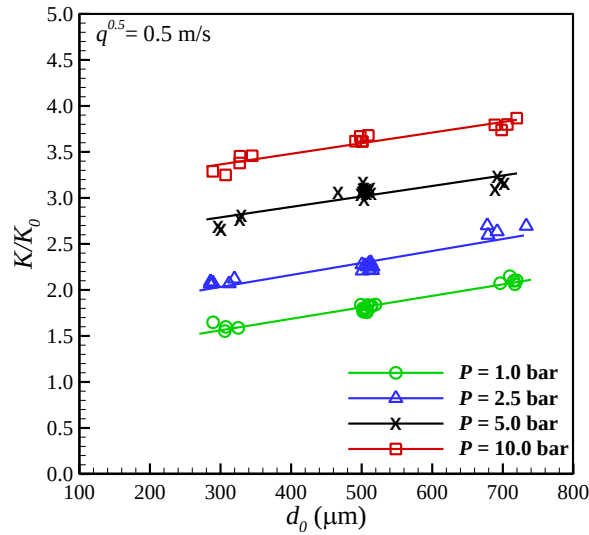


Figure 3-6. Turbulence effectiveness variation with the droplet initial diameter for 1000 RPM at different ambient pressures

So far, turbulence intensity has been utilized as a metric to assess the turbulent state surrounding the droplet. However, turbulent length scales can also have an impact on the vaporization rate. Relevant literature shows different conclusions. For instance, Eckartsberg and Kapat [33] stated that the energy contained in eddies smaller than the droplet diameter controls the evaporation rate. They claimed that the smallest eddies (on the order of η) dissipate quickly, so they do not significantly affect the evaporation process. Therefore, turbulence enhances the evaporation rate if droplets are at least higher than the Taylor microscale, λ . However, this theory is not confirmed by several recent studies [34]. Marti et al. [35] and Verwey and Birouk [28] demonstrated that turbulent flow significantly impacts the evaporation rate even when the droplet diameter is smaller

than the Taylor microscale. However, the aforementioned studies exclusively focused on hydrocarbon fuels, and no investigation has been conducted on other fuel types such as high alcohols (e.g., butanol).

In a manner similar to the analysis carried out in [28], Fig. 3-7 presents the normalized vaporization rate of butanol droplets of varying sizes, turbulence intensities, and pressure conditions, as a function of the ratio of the Kolmogorov length scale to the initial droplet diameter, η/d_0 . This figure shows that the influence of turbulence on the vaporization rate of butanol droplet becomes considerable when the droplet size is larger than the Kolmogorov length scale. This is in accordance with the experimental finding of Verwey and Birouk [29] for heptane and decane droplets, and a numerical study conducted by Dodd et al. [36] on heptane droplets.

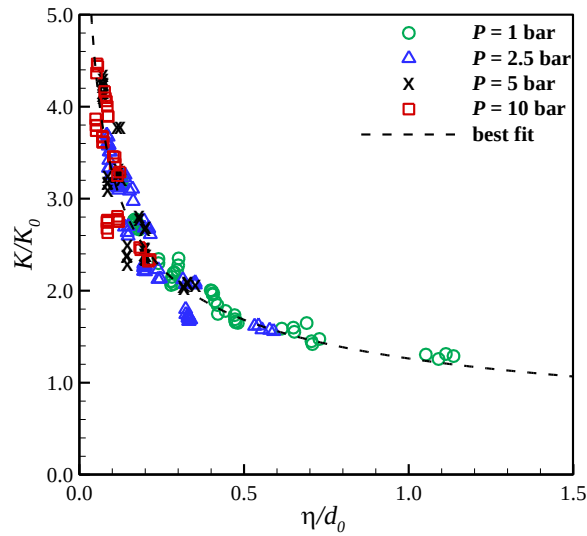


Figure 3-7. Turbulence effectiveness variation with the ratio of Kolmogorov length scale to the initial droplet diameter η/d_0 .

3.4.4 Comparison with hydrocarbons

To ensure the effective utilization of butanol fuel in combustion engines, it is crucial to comprehend its resemblance and distinction compared to the widely established alkanes/hydrocarbons. For this purpose, this section undertakes a comparative analysis of droplet

vaporization data for butanol, heptane, and decane, with different droplet sizes under diverse ambient pressure and turbulence conditions. Vaporization data for heptane and decane was obtained from the experimental study conducted by Verwey and Birouk [29], who employed the same apparatus. Consequently, the range of droplet sizes depicted in the following figures are not be identical.

Fig. 3-8a and Fig. 3-8b depict the variation of the vaporization rate with the droplet initial diameter for the three aforementioned fuels (heptane, decane, and butanol) under quiescent and turbulent ($q^{0.5} = 0.5$ m/s) conditions at an ambient pressure of 10 bar. Although the scatter in heptane data appears significant, the sampling/random errors are found to be 8% and 5% for stagnant conditions (Fig. 3-8a) and turbulent conditions (Fig. 3-8b), respectively. As clearly shown in these figures, heptane exhibits a notably higher vaporization rate compared to both butanol and decane. This difference is attributed to the higher volatility of heptane. As indicated in Table 3-3, heptane's vapor pressure (6.7 kPa) significantly exceeds that of butanol (1.02 kPa) and decane (0.13 kPa). These figures also demonstrate that, for all droplet sizes, the vaporization rate of butanol falls between that of heptane and decane, and exhibits a closeness to decane. Moreover, Fig. 3-8a reveals that the impact of droplet size on the vaporization rate under stagnant condition is more pronounced in the case of heptane and decane compared to butanol. The extent of this enhancement is presented in Table 3-2. For instance, when the droplet size increases from 300 μm to 600 μm under quiescent conditions, the vaporization rate of heptane and decane increases by 19.5% and 18.6%, respectively, while that of butanol is only 11.7%. A similar trend is also observed under stagnant condition for the other explored ambient pressure (2.5, and 5 bar). As mentioned earlier, increasing the droplet size improves the vaporization rate by enhancing the effect of natural convection around the droplet under quiescent conditions. This intensified convection aids in mass

diffusion, leading to improved vapor transfer from the droplet surface to the surrounding ambient. Consequently, it seems that the impact of droplet size on the vaporization rate under stagnant condition is more discernible for fuel types characterized by smaller mass diffusion coefficients, such as heptane and decane, as compared to butanol (the mass diffusion coefficients for these fuels can be found in Table 3-3).

As depicted in Fig. 3-8b and detailed in Table 3-2, the influence of droplet size on the vaporization rate enhancement becomes more pronounced with turbulence across all examined fuel types. Furthermore, although this enhancement is still greater for heptane and decane when compared to butanol, the difference between these fuels is smaller as compared to the stagnant conditions. This difference due to the presence of turbulence can be ascribed to the shift in the governing factor. While fuel mass diffusion prevails as the primary controlling parameter in stagnant conditions, its dominance wanes under turbulence. In other words, under turbulent conditions, forced convection takes center stage, displaying reduced sensitivity to the mass diffusion coefficients of these fuels, and thereby reducing the difference in the enhancement of evaporation between these fuels.

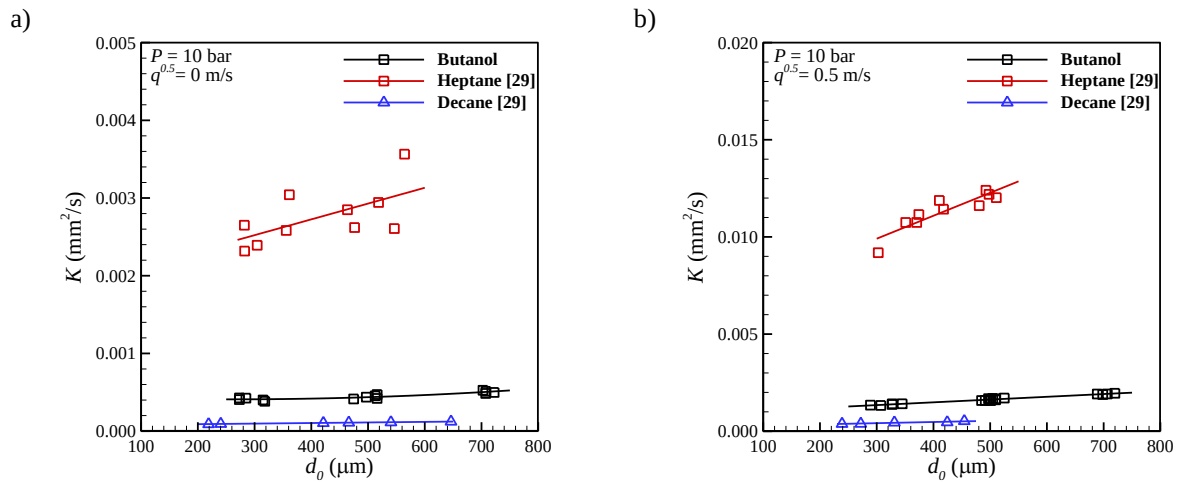


Figure 3-8. Variation of the droplet vaporization rate vs initial diameter under quiescent condition and at a) $P = 10$ bar, and b) $P = 10$ bar.

Table 3-2. Effect of droplet size variation on the vaporization rate enhancement under quiescent and $q^{0.5} = 0.5$ m/s at 10 Bar.

Fuel	P = 10 bar, $q^{0.5} = 0$ m/s		P = 10 bar, $q^{0.5} = 0.5$ m/s	
	Percent increase in K over a range of d_0 [μm]		Percent increase in K over a range of d_0 [μm]	
	300 – 450	300 – 600	300 – 450	300 – 600
Butanol (C ₄ H ₉ OH)	3.9%	11.7%	13.7%	24.1%
Heptane (C ₇ H ₁₆)	10.8%	19.5%*	15.2%	26.3%*
Decane (C ₁₀ H ₂₂)	10.2%	18.6%	17.9%	30.3%*

* Extrapolated from the best fit line.

To investigate the interplay between of the ambient pressure and the effectiveness of turbulence on the droplet vaporization rate of the abovementioned fuels, the variation of K/K_0 with the initial droplet size under different ambient pressure conditions at $q^{0.5}=0.5$ m/s is plotted in Fig. 3-9. Considering the fact that K_0 is slightly changed by the droplet size, especially at elevated pressure (as shown in Fig. 3-8a), the corresponding K_0 is employed for each individual droplet size instead of an average K_0 for all droplet sizes as in [29]. Fig. 3-9 reveals two important observations. First, it demonstrates that, while for heptane and decane, increasing the pressure greatly increases the importance of the effect of droplet size, the role of droplet size remains the same at all explored pressure levels for butanol droplet. For example, the lines representing butanol exhibit a consistent slope of 0.0012 independent of pressure, whereas for decane, this slope varies from 0.0009 to 0.0034 at 1 bar and 10 bar, respectively. Second, an increase in pressure leads to a greater separation between butanol and the other two fuels, indicating that turbulence effectiveness is less pronounced for butanol compared to the other fuels under elevated pressure conditions.

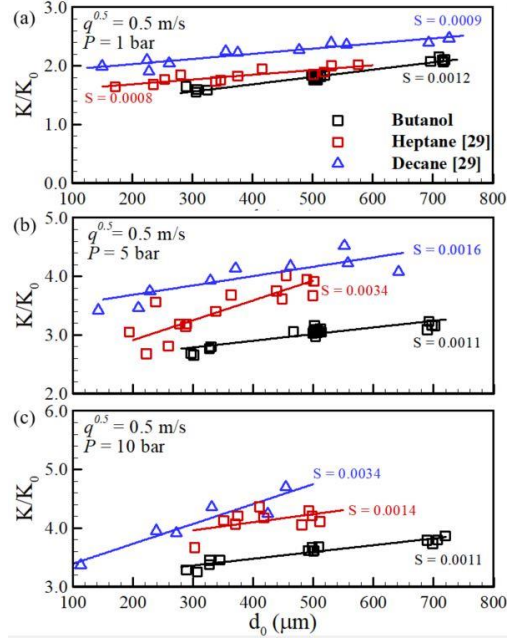


Figure 3-9. Variation of the turbulence effectiveness with the initial droplet size under turbulence condition (e.g., $q^{0.5} = 0.5 \text{ m/s}$) at a) 1 bar, b) 5 bar and c) 10 bar. The slope of each line is denoted by S .

To investigate the effect of turbulence intensity at different pressure conditions, Fig. 3-10a and Fig. 3-10b depict the vaporization behavior of these three fuels under two different turbulence conditions at 1 bar and 10 bar ambient pressure, respectively. It is observed that, as the ambient turbulence intensity increases, turbulence effectiveness (K/K_0) at different droplet diameters is less prominent for butanol compared to the other two fuels.

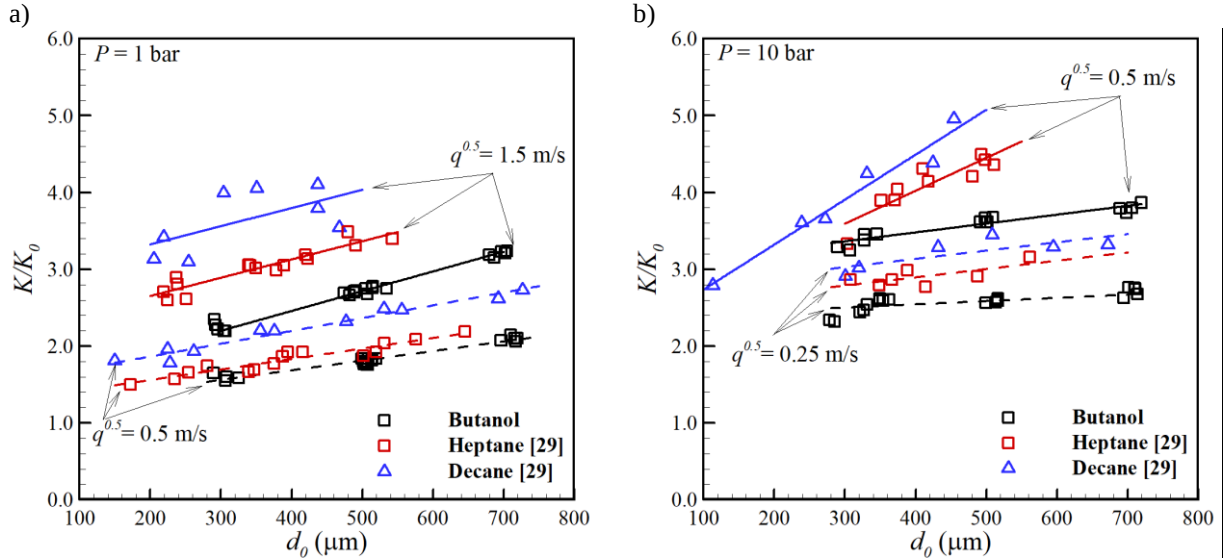


Figure 3-10. Variation of K/K_0 with the initial droplet size for two different turbulence conditions at a) 1 bar, and b) 10 bar.

Based on the observations in Figures 3-8 to 3-10, it can be concluded that the impact of increasing droplet size on the vaporization rate enhancement is less pronounced for butanol when compared to heptane and decane under all explored conditions. The effect of fuel type on the droplet vaporization rate has been studied in the literature, but different conclusions were reported. Several studies suggested that turbulence exerts a more pronounced impact on fuels with lower volatility [37-40]. On the other hand, Patel and Sahu [21] showed that fuels with higher mass diffusivity present the least favorable conditions for turbulence effectiveness. Furthermore, Verwey and Birouk [29] stated that low concentration gradient at the droplet surface is a key for turbulence enhancement of the evaporation rate. While all these studies primarily focused on the mass transfer process, it is important to also consider the role of heat transfer during the vaporization process. To arrive at a comprehensive conclusion, the present study presents a comparative analysis of these three fuels, taking into account some key parameters that impact droplet vaporization. The role of each parameter on the vaporization process of these fuels under turbulent conditions is theoretically examined to determine which parameter best characterizes the effect of fuel type on

droplet vaporization rate. These parameters include fuel volatility, surface concentration gradient, vapor fuel diffusivity, and thermal diffusivity.

- ***Volatility***

It is reported that turbulence is more effective for enhancing droplet vaporization rate for the less volatile fuels. This is due to the larger residence time of vapor fuel around the droplet surface, which is favorable for turbulence in the transfer of vapor and thereby improve the vaporization rate [40]. Vapor pressure serves as an indicator of fuel volatility [41], where fuels with higher volatility tend to vaporize more readily and consequently exhibit elevated vapor pressures. According to Table 3-3, the vapor pressure of butanol lies between that of heptane and decane. Therefore, based on vapor pressure, butanol is less volatile than heptane and more volatile than decane. Consequently, based on the concept of volatility, the effectiveness of turbulence on the vaporization rate should follow this order: decane > butanol > heptane.

- ***Surface concentration gradient***

Verwey and Birouk [29] suggested that using the concentration gradient (Eq. (2)) at the droplet surface may explain the reason for the disparity in the evaporation process between different fuel types.

$$\frac{dX_F}{dr} = -\frac{X_{Fs}}{r_s} \quad (3-2)$$

where, X_{Fs} represents the mole fraction of fuel vapor at the droplet surface, and it is determined using the Clausius–Clapeyron relation. The initial droplet radius r_0 is used as r_s . It should be noted that this is the theoretical gradient at the droplet surface, and it is derived for slowly evaporating droplets in a convection-free environment. Fig. 3-11 depicts the droplet normalized vaporization rate as a function of the fuel concentration gradient at different ambient pressure conditions. As

expected from thermodynamic equilibrium, increasing the ambient pressure suppresses the concentration gradient at the droplet surface, and hence promotes the role of turbulence on the vaporization process. Verwey and Birouk [29] concluded that fuels with lower surface concentration gradients are more influenced by turbulence during the vaporization process. Therefore, based on the concentration gradient, turbulence should be more effective following this order: decane > butanol > heptane.

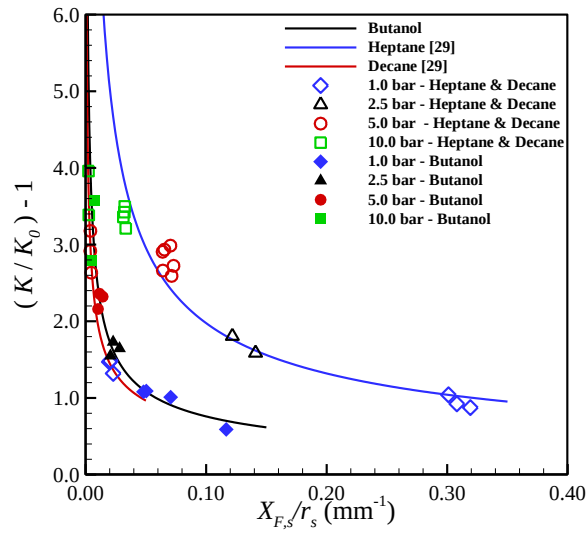


Figure 3-11. Relationship between the turbulent effectiveness and fuel concentration gradient at the surface of the droplet

- ***Vapor fuel diffusivity***

In accordance with the approach outlined by Patel and Sahu [21], the present study adopts the mass diffusivity coefficient under quiescent conditions for comparative analysis. The determination of the fuel vapor mass diffusivity coefficient in a nitrogen environment (D_{Fuel-N_2}) is obtained using Fuller method [42]. Notably, the ambient temperature is utilized for calculating D_{Fuel-N_2} due to the unavailability of the droplet surface temperature, T_s . Table 3-3 shows that butanol exhibits the highest vapor mass diffusivity in nitrogen, followed by heptane and then decane.

- **Thermal diffusivity**

While the influence of heat transfer is less pronounced in low-temperature ambient environments, it has been reported that conduction mode of heat transfer remains significant under these conditions [43]. Thermal diffusivity is defined as the ratio of the thermal conductivity to the heat capacity and density. In other words, it represents the competition between heat conduction and storage. The calculated thermal diffusivity for these fuels is very close, as tabulated in Table 3-3. It is recognized that turbulence can lower the droplet surface temperature, resulting in increased droplet heat transfer and, consequently, enhanced droplet evaporation [44]. Given that fuels with higher thermal diffusivity respond more swiftly to the heat transfer induced by turbulence, it is anticipated that turbulence will exert a more significant impact on the vaporization process of decane and heptane than butanol.

Table 3-3. Fuel thermophysical properties at atmospheric pressure and 300 K

Fuel	Molecular Weight (kg/Kmol) [42]	Liquid density (kg/m³)	Vapor Pressure (kPa)	^AVapor mass diffusivity in N₂ (m²/s) $D_{\text{Fuel-N}_2}$	Liquid thermal diffusivity (m²/s) α_{Fuel} [42]
Butanol (C ₄ H ₉ OH)	74.123	806 [45]	1.02 [46]	9.32×10^{-6}	7.9×10^{-5}
Heptane (C ₇ H ₁₆)	100.204	684	6.70 [47]	7.33×10^{-6}	8.0×10^{-5}
Decane (C ₁₀ H ₂₂)	142.285	730	0.13 [48]	6.06×10^{-6}	8.1×10^{-5}

^A Calculated based on the Fuller equation [42]

The abovementioned discussion has resulted in ranking the fuel properties as summarized in Table 3-4. This ranking reveals which fuel property serves as a good indicator of how turbulence affects the droplet vaporization rate. For instance, turbulence generally exerts a more pronounced influence on the vaporization rate of fuels of low volatility. Consequently, decane, being the fuel with the lowest volatility, is ranked top (1), followed by butanol (2), and then heptane (3), reflecting their order of volatility. The final column of Table 3-4 corresponds to the experimental observations illustrated in Figures 3-9 and 3-10. Analysis of the experimental data indicates that

turbulence has a more significant impact on the droplet vaporization rate for decane, followed by heptane, and finally butanol, across all explored test conditions.

Table 3-4. Order of the effectiveness of turbulence for improving the vaporization rate based on fuel property. The last column represents the order based on the present experimental results.

	Volatility	Surface concentration gradient	Vapor fuel diffusivity	Thermal diffusivity	Exp. results
Decane	1	1	1	1	<u>1</u>
Heptane	3	3	2	2	<u>2</u>
Butanol	2	2	3	3	<u>3</u>

Comparison of the ranking in Table 3-4 reveals that only vapor fuel diffusivity and thermal diffusivity align with the experimental results. Hence, it can be inferred that turbulence effectiveness on the vaporization rate is greater for fuels with the lowest vapor diffusivity and the highest thermal diffusivity.

Patel and Sahu [21] reported that vapor fuel mass diffusivity is a suitable parameter for categorizing the effect of flow turbulence on droplet vaporization in relation to fuel type. Mass diffusion is one of the controlling factors in the vaporization process and the contribution of turbulence to mass dispersion decreases for fuels with higher molecular diffusivity. This is why, as depicted in Figures 3-8 to 3-10, butanol vaporization rate is less affected by turbulence.

Furthermore, the present study demonstrates that thermal diffusivity serves as another valuable indicator. In terms of thermal diffusivity, the heat transfer process from the hotter region to the colder region in decane occurs at a higher rate compared to the other two fuels. Consequently, it is expected that decane would respond more quickly to the heat transfer induced by turbulence, resulting in a more pronounced impact of turbulence on its vaporization rate when compared to the other fuels. This explains why Figures 3-9 and 3-10 illustrate that turbulence has a greater influence on the vaporization rate of decane, followed by heptane and then butanol.

3.4.5 Correlations

Two comprehensive correlations commonly used for predicting the vaporization rate of fuel droplets in turbulent conditions are tested against butanol data. The first correlation employs the vaporization Damköhler number, Da_v , [40] and the second one relies mainly on the turbulent Reynolds number, $Re_{t,L}$ [49]:

$$\frac{K}{K_0} = 1.0 + 0.0948 Da_v^{-0.765} \quad (3-3)$$

$$\frac{K}{K_0} = 1.0 + 0.0439 Re_{t,L}^{0.66} Sc^{1.16} \left(\frac{T_\infty}{T_0} \right)^{-1.42} \left(\frac{P_\infty}{P_0} \right)^{-0.19} \left(\frac{L}{d_0} \right)^{-0.53} \quad (3-4)$$

In Equation (3-3), the Damköhler number is defined as the ratio of the characteristic time scale of the turbulent flow ($t_{flow} = d_0/q^{0.5}$) to the vaporization time scale ($t_{vap} = r_0/V_r$). V_r is the radial velocity and calculated using liquid-vapor continuity at the droplet surface as $V_r = \left(\frac{\rho_l}{\rho_v} \right) \left(\frac{K_0}{4d_0} \right)$ [30], where ρ_l and ρ_v are, respectively, the liquid and vapor densities. In Equation (3-4), the turbulent Reynolds number is computed as $Re_{t,d0} = q^{0.5}d_0/\nu$, and the Schmidt number is defined as the ratio of kinematic viscosity of the ambient nitrogen to the mass diffusivity coefficient of the nitrogen and butanol vapor ($Sc = \nu/D$).

While these correlations have been demonstrated to apply for different droplet sizes of hydrocarbons/alkanes [29], their application for butanol droplets has only been confirmed at 500 μm [30]. Thus, the present data of butanol is used to evaluate these correlations' applicability over a wide range of butanol droplet sizes. As shown in Fig. 3-12a and Fig. 3-12b, Eqs. (3-3)-(3-4) are clearly valid regardless of the droplet size and fuel type.

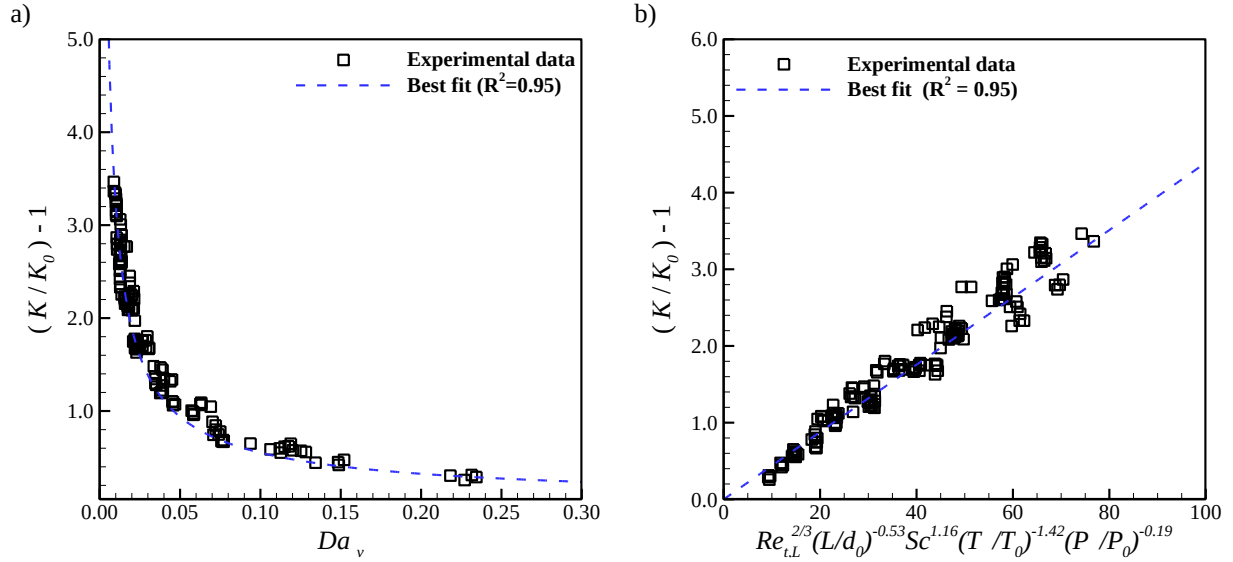


Figure 3-12. Turbulence effectiveness against a) the vaporization Damköhler number, and b) the Reynolds correlation.

3.5 Conclusions

The present study investigated the effects of butanol droplet size in turbulent environments at elevated pressure and room temperature. The vaporization data of butanol droplets are also compared with their hydrocarbon counterparts. The main findings are outlined below.

- 1) The results showed that, under atmospheric pressure, the vaporization rate increases with the droplet size mainly in the presence of turbulence. However, at elevated pressure, this increase is observed even under stagnant condition. This is attributed to the increased influence of natural convection at elevated pressure, especially for large droplets.
- 2) The vaporization rate of butanol droplet falls between that of heptane and decane, with a closer resemblance to the latter at all explored test conditions.
- 3) The influence of droplet size on the enhancement of the vaporization rate is more pronounced for heptane and decane across all examined conditions, and this difference is further accentuated with ambient pressure or turbulence intensity.

- 4) Contrary to the common belief that turbulence is more effective for the less volatile fuels, the present study found that turbulence influence on the droplet vaporization is greater for fuels with the lowest vapor diffusivity and the highest thermal diffusivity.

Lastly, published correlations commonly used for predicting droplet vaporization rates under turbulence conditions are found valid for butanol vaporization data at all explored test conditions.

3.6 References

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Chapter 4: Experimental study of butanol droplet combustion in a turbulent, elevated-pressure environment

4.1 Abstract

To assist in the search for clean liquid alternative fuels for future combustion engines, the combustion characteristics of butanol droplets were experimentally investigated. The experiments were conducted under varying flow turbulence intensity, $q^{0.5}$, (up to 0.5 m/s), pressure (up to 11 bar), and ambient compositions, including different levels of O_2 , CO_2 , and N_2 , at room temperature. A fan-stirred spherical chamber, equipped with four pairs of axial fans, was used to generate a controlled turbulent flow field with negligible mean velocity. A 500 μm butanol droplet was suspended on a single micro-fiber at the center of the chamber and ignited using a coil resistance wire. The combustion process, including the droplet time history and luminous flame structure, was recorded using two synchronized cameras. The findings revealed that increasing ambient pressure enhances the burning rate, K_b , while the effect of turbulence varies with pressure. At low pressure, turbulence has minimal impact, whereas at higher pressure, K_b increases with $q^{0.5}$, before declining due to temporary luminous extinction (TLE). Butanol exhibits a lower K_b than heptane; however, under high-pressure, high-turbulence conditions, their K_b values converge. Additionally, butanol droplet combustion is influenced by O_2 and CO_2 concentrations. Oxygen improves K_b by delaying TLE, while CO_2 reduces K_b by lowering flame temperature and thermal conductivity of the ambient mixture.

4.2 Introduction

Presently, the transportation sector accounts for 25% of the global energy consumption, primarily relying on internal combustion engines powered by fossil fuels [1]. Overreliance on fossil fuels can deplete reserves, escalate prices and, more importantly, cause significant environmental and health concerns [2]. To address these challenges, there is increasing interest in the use of bio-alcohols, particularly butanol. As a long-chain alcohol-based fuel, butanol offers several advantages over lighter alcohols like ethanol, especially for use in compression ignition engines (CIEs). Its main benefits include excellent miscibility with diesel, higher energy content, greater cetane number, and lower corrosiveness [3]. Butanol is traditionally considered an expensive fuel due to its production through fermentation, which is inefficient due to by-products that reduce the yield. However, growing demand has led researchers to explore alternative chemical production methods [4]. As a result, recent technological advancements have steadily reduced the cost of butanol [5] and it is anticipated to emerge as a promising and sustainable alternative liquid fuel in the near future [6].

In CIEs, liquid fuel is directly injected into the cylinder, followed by primary and secondary spray break up. In the spray downstream region, droplets undergo heating and vaporization due to thermal interaction with the surrounding hot gases and combustion by products. Ignition occurs when the necessary temperature and equivalence ratio conditions are met, initiating the combustion of individual droplets at the leading edge of the spray [7]. Understanding single droplet combustion can be essential for developing reliable spray combustion models and provides valuable insights into fundamental spray combustion processes.

While CIEs are known for their high efficiency, their emissions, particularly NO_x and soot, present significant challenges [8]. One approach that researchers have developed to enhance diesel engine

performance and reduce emissions consists of increasing the oxygen content in the combustion chamber. Higher oxygen levels promote more complete oxidation of fuel, resulting in more efficient combustion [7]. Ghany et al. [9] observed that while increasing oxygen concentration improves combustion and decreases soot emissions, it also results in elevated NO_x emissions due to the rise in combustion temperature. A potential solution to mitigate this issue is through exhaust gas recirculation (EGR) [8]. EGR functions by returning a portion of the exhaust gases to the combustion chamber, which helps to lower combustion temperatures and thus reduce NO_x emissions. The predominant components found in the exhaust of CIEs are CO_2 , N_2 , O_2 , and water vapor [10]. Therefore, investigating how different concentrations of these gases affect the combustion behavior of a single droplet can provide valuable insights for optimizing the design of future CIEs, with a particular focus on emission reduction.

Wu et al. [11] demonstrated that increasing the oxygen concentration reduces the flame standoff distance from the droplet surface, which significantly enhances the burning rate under atmospheric pressure conditions. Li et al. [12] confirmed that increasing oxygen concentration promotes droplet combustion for other fuel types, including iso-butanol. Zhang et al. [13] numerically demonstrated that reducing the oxygen concentration in the environment to 17% decreases the gas density and specific heat, which subsequently lowers the burning rate of a heptane droplet. However, they did not clarify whether the droplet is combustible under this low-oxygen concentration. The limit of oxygen concentration (LOC) required for complete droplet combustion is a debatable topic and conflicting results were reported in the literature. It was reported that, under normal gravity conditions, the LOC is restricted to 18% for alkane droplets [14]. On the other hand, the LOC is reported as 12% for methanol and 15% for heptane under microgravity conditions [15]. To the best of our knowledge, the LOC of butanol fuel has not been investigated in the literature.

Published findings regarding the impact of CO_2 composition on the burning rate of a single droplet are contradictory. For instance, Shaw and Wei [16] found that increasing the concentration of CO_2 reduced the burning rate of heptane droplet. Similar results were reported by Hicks et al. [17], who investigated the burning of methanol droplets. In contrast, Dzik et al. [18] found that the burning rate of heptane droplet increased with higher CO_2 concentration. They also reported that, under atmospheric pressure conditions, droplet ignition can occur in the presence of up to 46% CO_2 dilution in standard air (21% O_2 & 79% N_2).

While most of the reviewed literature was conducted under a quiescent environment, droplets in CIEs are typically subjected to intense turbulence [19]. Droplet burning in turbulent environments, which is a practical scenario, is among the least commonly discussed topics in the literature. Published relevant studies present inconsistent results regarding the effect of turbulent flow on the burning rate. For instance, Ohta et al. [20] was the first to study droplet burning rates using porous spheres in a fluctuating turbulent environment without mean velocity. They found that turbulent flow can significantly improve the burning rate at atmospheric pressure. A similar conclusion was reported by Agoston et al. [21], who experimentally investigated droplet burning rates in a forced convective turbulent flow field. They also reported that beyond a certain threshold of air stream velocity, referred to as the extinction velocity, the burning rate decreased due to turbulence, as the flame could no longer be maintained around the droplet. On the other hand, Birouk et al. [22, 23] using different apparatus showed that zero-mean turbulent flow field has little effect on the burning rate under atmospheric conditions. Patel et al. [24] reported that the burning rate decreases with increasing zero-mean turbulent flow at atmospheric pressure. It is important to note that these studies primarily focused on large droplets (beyond 1 mm) while employing thermally conductive suspension methods or porous spheres. In a recent study, the present authors have made an effort

to clarify some of the previously discussed controversial topics [25]. It was found that turbulence has little to no effect on the burning rate of heptane droplets at lower pressures, while K_b exhibited improvement at elevated pressure conditions. The findings revealed that a combination of elevated pressure and oxygen enrichment significantly enhances droplet burning rate. However, some aspects remain unanswered, including:

- Effects of turbulence and pressure on the combustion of an alcohol-based fuel droplet
- Similarities and differences between the combustion of alkane and alcohol-based fuel droplets
- Effect of ambient O_2 concentration on droplet combustion and the required LOC
- Impact of CO_2 concentration on droplet combustion in different oxygen environments

To address these questions, the present study investigates the combustion behavior of a single butanol droplet in varying pressure environments (up to 11 bar), turbulent flow fields ($q^{0.5}$ varies up to 0.5 m/s), and different ambient gas composition of N_2 , O_2 , and CO_2 .

4.3 Experimental Approach

Droplet combustion tests were performed in a fan-stirred spherical chamber, as described in [25]. A comprehensive description of the experimental apparatus is provided in Section 4.3.1. Section 4.3.2 outlines the experimental methodology, including procedural considerations and an analysis of the uncertainties associated with the measurements. Finally, Section 4.3.3 details the particle image velocimetry (PIV) procedures employed to characterize the turbulent flow field.

4.3.1 Experimental Apparatus

As depicted in Fig. 4-1, the experimental apparatus is a spherical chamber with a 29 L capacity, fabricated from stainless steel to resist high-pressure conditions. This chamber is equipped with ten auxiliary ports that support various equipment, including a fuel injector, a droplet holding frame, an ignitor, pressure sensors, transducers, thermocouples, and valves. The setup also incorporates four quartz windows, serving multiple roles, including PIV measurements, capturing images of droplet combustion, and allowing access to the chamber's interior. More importantly, the setup is equipped with eight fans positioned in pairs along the same axis, which generate a homogeneous isotropic turbulent flow in the central area of the chamber.

As illustrated in Fig. 4-1a, a single, horizontal 14 μm CG Nicalon fiber, chosen for its low thermal conductivity, is positioned in the center of the chamber to suspend the droplet. It is known that fiber tethering can increase burning rates through increasing the liquid-gas interfacial area and conducting heat [26], but this effect diminishes as the fiber diameter decreases. It is found that, for the droplet to fiber diameter in the range employed in the present study ($\frac{d_0}{d_f} \sim 35$, where d_0 and d_f are the droplet and fiber diameter, respectively), the effect of fiber on the burning rate becomes negligible [27]. In addition, the droplet evaporation rate in hot environments is found to be linearly correlated with both the square of the fiber diameter, d_f^2 , and the fiber's thermal conductivity, k_f [28, 29]. In the present experiment, $k_f d_f^2 = 4.5 \times 10^{-4} \left(\text{W} \cdot \mu \frac{\text{m}}{\text{K}} \right)$ is well below the recommended threshold [29]. Hence, the effect of the employed horizontal CG Nicalon fiber on the droplet burning rate can be considered negligible. The secure placement of small droplets on this fiber is achieved by adding a small, spherical epoxy node. The fiber is connected to a thin steel frame,

fastened with epoxy, and kept under slight tension to prevent it from breaking. This frame is then suspended from the top of the chamber.

A manually operated injector was used to produce and release droplets onto the fibers. This mechanism comprises a leadscrew-actuated piston, a sliding barrel, a steel needle, and a capillary tube with inner and outer diameters of 40 μm and 60 μm , respectively. The ignitor consists of a small coil of 27-gauge Kanthal A1 resistance wire which pneumatically moves to and from the droplet to initiate the combustion process.

The experiment was monitored using two cameras, as shown in Fig. 4-1b. The droplet's size reduction was monitored with a backlit IDT XS5-M-1 camera in conjunction with a Questar QM 100 long-distance microscope, providing a magnification of 5.5. The luminous part of the flame was recorded from a 90-degree plane using a Fastec IL5Q camera equipped with a Nikon 60 mm lens. Both cameras capture images in 8-bit grayscale at a steady frame rate of 350 fps and a shutter speed of 200 μs . Backlighting for the droplet was provided by a 250 W halogen lamp.

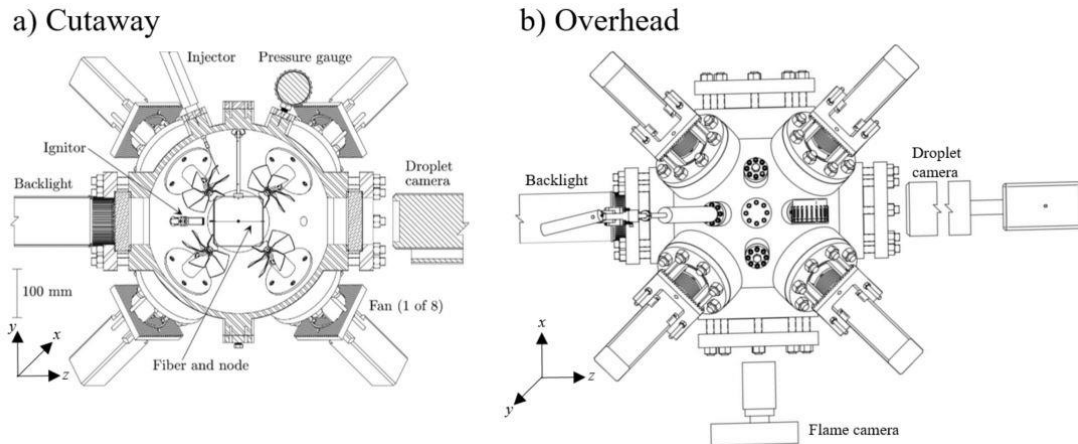


Figure 4-1. Cutaway (a) and Overhead (b) schematics of the spherical combustion chamber. (Normal gravity is in the opposite direction of y-axis in (a))

4.3.2 Experimental methodology

To perform droplet combustion experiments, the chamber was first evacuated and then pressurized with the desired gas composition. Pressure is carefully monitored with a gauge, keeping it within $\pm 1\%$ of the target value. After setting the desired pressure, fans were activated to create the necessary turbulent flow field. The rotational speed of the fans is measured with a digital stroboscope and controlled within $\pm 1\%$ of the desired RPM. Then, droplet was introduced into the chamber via the injection system and placed on the node of the fiber. The initial size of the droplet was made intentionally larger than the target diameter (d_0) to allow for the injector retraction and the warmup of the ignition wire. When the droplet's size neared d_0 during evaporation, it was quickly set alight by the ignitor, which is briefly positioned less than 0.5 mm away from the droplet surface. The residence time and power for the coil were adjusted according to the ambient pressure and turbulence levels. A series of experiments conducted under both atmospheric and higher pressure conditions validated the independence of the burning rate on these parameters, showing less than a 2.0% variation in burning rate even when the residence time was reduced from its maximum value required for ignition to its minimum value, and the power was increased from the required minimum to its maximum possible limit.

The signal to activate the ignitor also triggers two cameras, with one capturing the temporal droplet size and the other recording the surrounding flame shape. The captured images from droplet size reduction were processed using an in-house MATLAB code. The code first determines the initial droplet diameter, d_0 , by comparing the planar area of the droplet image to that of an equivalent circle. The algorithm pre-processes the images by cropping irrelevant portions, applying thresholding to create a binary representation, and then using morphological techniques to remove support fiber while preserving the droplet's integrity. The droplet diameter is then calculated based

on the number of foreground pixels, camera magnification, and pixel pitch. The initial droplet diameter is recorded just before the coil reaches the droplet surface. A test is only considered valid if the initial droplet diameter falls within the range of $500 \pm 25 \text{ } \mu\text{m}$. K_b was determined by measuring the slope of the linear segment of the droplet's squared diameter (d^2) over time.

To maintain consistency and eliminate the effects of transient conditions at the beginning, as well as the influence of the node toward the end of the process, the calculation of K_b is restricted to the range $0.75 > (d^2/d_0^2) > 0.25$. Consequently, for a test to be valid, the droplet should be ignited and the wire must retract from the droplet before (d^2/d_0^2) reaches 0.75, and the flame must remain around the droplet until (d^2/d_0^2) reaches 0.25. This span corresponds to a 52% reduction in the volume of the burning droplet. It was found that using the wider range ($0.9 > (d^2/d_0^2) > 0.2$) results in no more than a 2.5% change in the burning rate for linear cases, whereas for non-linear cases, the error increased to approximately 10%. However, by consistently fitting the burning rate line across all test cases, the data becomes more suitable for meaningful comparisons. Moreover, K_b is determined by conducting each experiment no fewer than four times and the sampling error, estimated using a 95% confidence interval, is visually represented by error bars in the relevant figures. To verify consistency in the experimental outcomes, certain sampling tests under stagnant conditions at varying pressures are repeated both at the beginning and end of each testing day.

Systematic error in droplet size measurement arises from droplet non-sphericity, camera calibration and the droplet edge detection algorithm. Regarding droplet sphericity, the fiber-node technique employed in this study preserves a high degree of sphericity. As shown in Fig. 4-6, the droplet images demonstrate near-spherical shapes, and the calculated circularity values, given by $C = 4A_s\pi/P^2$ (where $C = 1$ represents a perfect circle), consistently remain above 90%. For calibration, both droplet and flame cameras are referenced against a ball bearing with a known

diameter. After repeated calibrations and considering the uncertainty in the ball bearing's dimensions, the scale factor uncertainty is less than 1%. For edge detection, two methods—Otsu and manual—are compared. Otsu's method calculates an optimal threshold by maximizing the variance between foreground and background pixels, ensuring a reliable binary representation of the droplet edge. To evaluate the potential error, each image is also processed with a higher, user-defined threshold (e.g., 0.95 in normalized intensity), which retains nearly all edge pixels. This systematic approach ensures that the edge detection algorithm is consistent across all images, and in no case does the thresholding method change the initial droplet diameter by more than 2%.

4.3.3 Particle image velocimetry

A Dantec Dynamics 2D-Particle Image Velocimetry (PIV) system was utilized to characterize the turbulent flow field within the chamber. It features a 135 mJ double pulse Dual Power Nd:YAG laser and a FlowSense EO 4M camera. Olive oil micro-droplets, produced by a LaVision aerosol generator, were used to seed the flow. Control, synchronization, data acquisition, and cross-correlation of raw images were managed by Dantec DynamicStudio software. PIV flow characterizations were performed with the frame droplet suspending system installed and both the injector and coil retracted, meaning that the results represent the stationary turbulent flow field present before the formation of droplets and ignition. Due to the dimensions and position of the windows and the spatial constraints of the PIV system, the turbulent flow was captured over a 90 mm × 90 mm field of view, with 2000 image pairs acquired for each test condition. Interrogation areas were set to 32 × 32 pixels with 50% overlap.

The flow key statistics obtained from the PIV analysis included the orthogonal mean velocities, $\langle U \rangle$ and $\langle V \rangle$, and their corresponding root-mean-square (RMS) velocities, $\sqrt{\langle u'^2 \rangle}$ and $\sqrt{\langle v'^2 \rangle}$, where the angled brackets denote temporal averaging. The mean velocities were designed to be

approximately zero, and the uncertainty in the RMS velocities, resulting from sampling error, was estimated at 4% based on a 95% confidence interval

4.4 Result and discussion

To investigate the combustion characteristics of butanol droplets, an initial droplet diameter of 500 μm was chosen. The combustion experiments were performed under varying ambient pressures, spanning from atmospheric pressure (1 bar) to elevated pressure conditions (11 bar). It should be noted that the term 'elevated pressure' does not refer here to real engine conditions; rather, it is used to indicate that the experiment was conducted at ambient pressures elevated above atmospheric pressure. The surrounding airflow conditions were modified from a stationary state to a turbulent regime, with turbulence intensity reaching up to 0.5 m/s. All experiments were carried out at room temperature. The PIV test results are discussed in Section 4.4.1. In Section 4.4.2, the combustion behavior of a single butanol droplet under varying turbulence intensity and pressure conditions is investigated, and the underlying reasons for the observed variations in K_b are discussed. This analysis sets the groundwork for a deeper exploration of how turbulence and pressure affect the combustion process. To explore the possibility of using butanol as a fuel, Section 4.4.3 provides a comparative analysis of its combustion characteristics with those of heptane. To understand the role of O_2 and CO_2 concentrations on the combustion characteristics of butanol droplets, Section 4.4.4 examines how variations in O_2 levels influence K_b , while Section 4.4.5 explores the impact of CO_2 variations on K_b under different pressure and turbulence condition.

4.4.1 Flow Characterization

The flow field generated by the fans has been systematically characterized at various fan speeds and pressure levels. The flow characterization demonstrates that the setup is capable of producing

nearly zero-mean flow and high turbulence levels while maintaining isotropy and homogeneity. For brevity, Fig. 4-2 illustrates the case with the highest explored pressure (11 bar) and turbulence intensity ($q^{0.5} = 0.5$ m/s) as a representative example, with similar trends observed across all other tested conditions. It is important to emphasize that the results in Fig. 4-2 were obtained in the presence of all components used in the experiments, including the droplet suspension frame assembly, fuel injector, and ignition system. Although the injector and ignitor were retracted, the influence of the frame is noticeable in Fig. 4-2 in the blue region at the top and the light blue line near $x = 10$ mm. The vectors depict the mean velocity, which is notably low at the center of the chamber. The heat map in this figure shows the variation in turbulence intensity, $q^{0.5}$, and displays a highly symmetric distribution with little variation in the central region. The turbulence intensity is defined as the square root of turbulent kinetic energy, ($q^{0.5} = (1/\sqrt{2}) (\sqrt{\langle u'^2 \rangle + \langle v'^2 \rangle + \langle w'^2 \rangle})$), where the third component, $\langle w'^2 \rangle$ is assumed to be equivalent to the average of the other two resolvable components. To assess the isotropy and homogeneity of the field, statistics are averaged across the central region (10 mm diameter, depicted by the solid black circle) and in thin (1 mm thick) radial shells. The dashed-dot circle shown in Fig. 4-2 marks the location of the last radial shell that satisfies $\left| 1 - \sqrt{\langle u'^2 \rangle} / \sqrt{\langle v'^2 \rangle} \right| < 0.05$, indicating near-perfect isotropy from the center out to that location. Additionally, the dashed circle designates the last radial shell with an average $q^{0.5}$ value within 5% of the corresponding average value in the central region. As can be seen, both homogeneity and isotropic circles have sufficiently large diameters (greater than 20 mm), which is around 40 times the size of droplet.

To determine the integral length scale, L , numerical integration of the spatial correlation coefficient is carried out. Applying the method recommended in [30], the average integral length scale is

found to be approximately 26 mm, remaining constant across various fan speeds and pressure conditions. The Kolmogorov length scale, η , was found to range between 10 and 700 μm , assuming equilibrium between the dissipation rate and the production rate. Further details regarding these length scales are available in [31]. It is also observed that $q^{0.5}$ changes linearly with fans speed as $q^{0.5} = 0.0005 \times N$, where N represents the fan speed in RPM. It should be noted that although the turbulent flow field around the droplet has a zero-mean velocity, the presence of a flame enhances natural convection, which may influence the droplet surroundings.

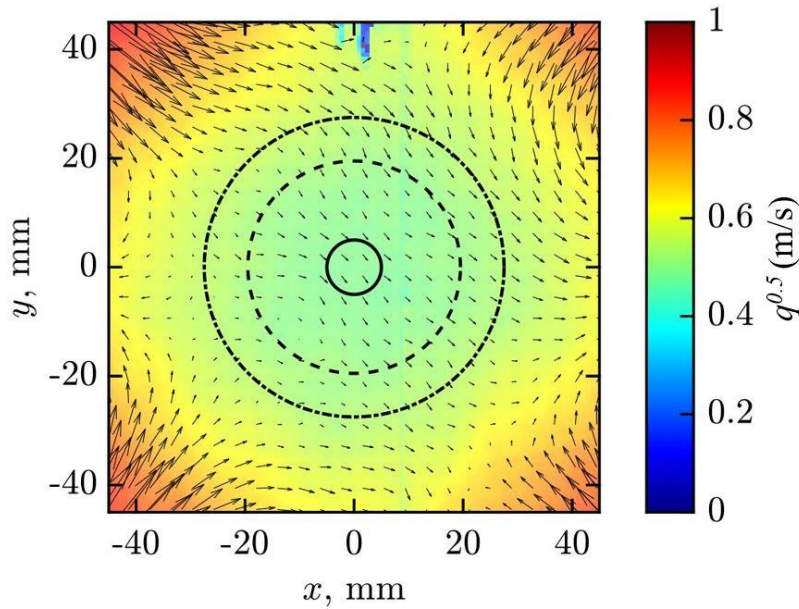


Figure 4-2. Heat map of $q^{0.5}$, with mean velocity vectors superimposed, for the test case involving the highest pressure and turbulent flow conditions ($P_\infty = 11$ bar, $q^{0.5} = 0.5$ m/s). The solid circle represents the spatial averaging region ($r = 5$ mm), the dashed circle marks the radius of homogeneity, and the dash-dot circle indicates the radius of isotropy. Normal gravity is in the opposite direction of y-axis.

4.4.2 Butanol droplet combustion

The combustion behavior of a 500 μm butanol droplet is investigated under a range of conditions, including turbulence intensity up to 0.5 m/s and ambient pressures up to 11 bar. These conditions resulted in a turbulent Reynolds, defined as $Re_t = (q^{0.5}d_0/\nu)$, where ν is the kinematic viscosity of air at 300 K, ranging up to 140. These conditions were chosen to facilitate comparison with

previous studies conducted by this group [25]. Fig. 4-3 illustrates how K_b varies with turbulence intensity with different ambient pressures. Several key observations emerge from this figure. Firstly, an increase in pressure consistently enhances K_b under all tested conditions. Under stagnant conditions, the increase is 32% at 6 bar and 48% at 11 bar. Secondly, while turbulence has minimal effect on K_b at atmospheric pressure, it initially enhances K_b and then reduces it beyond a certain turbulence level at elevated pressures. Thirdly, the error bars in this figure indicate that the variability between repeated runs increases significantly as turbulence level rises under high-pressure conditions. Each of these observations will be discussed in more detail in the subsequent figures.

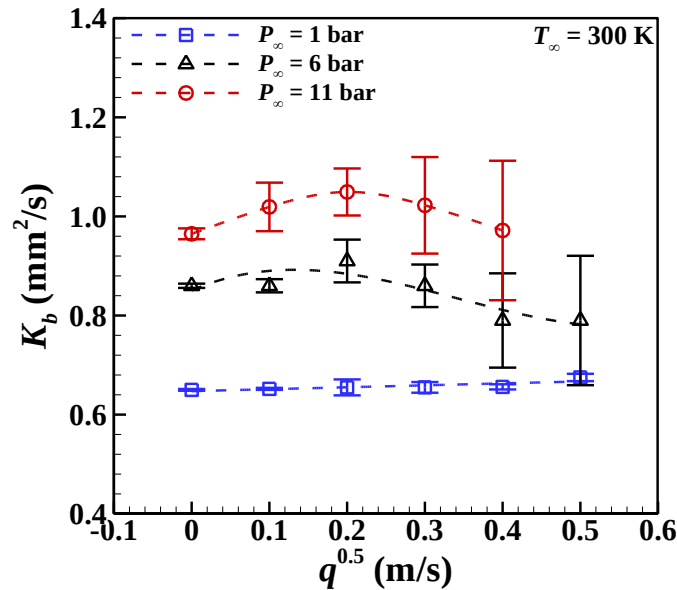


Figure 4-3. Average burning rate of butanol droplets under various pressure and turbulent flow field.

The effect of pressure on K_b is investigated in Fig. 4-4. The plot shows the time history of butanol droplet combustion in a quiescent environment under different pressure conditions. The dashed lines in the plot represent the upper and lower limits for the calculation of K_b and the circles indicate the points where the coil was retracted. As can be seen, the coil is sufficiently retracted

before the point at which the calculation of K_b begins. Fig. 4-4 also includes the flame average luminous zone (LZ) for each test. LZ images were generated using individual flame frames corresponding to the range $0.75 > d^2/d_0^2 > 0.25$. This selected range is the same as that used for the burning rate calculation. Frames were first binarized, then summed, and finally normalized by the total number of frames to obtain an average flame image. In this process, a pixel value of 1 indicates locations where the flame was present in all frames across all tests, while a value of 0 represents locations where no flame was observed in any frame. It should be noted that the two horizontal luminous regions appearing on both sides of the flame images result from interaction between the flame and the droplet's supporting fiber [32]. The yellow-orange coloration observed in flame images is attributed to soot radiation [33]. For high-alcohol fuels, such as butanol, the presence of oxygen promotes the formation of relatively stable carbon monoxide (CO), which reduces the availability of carbon for soot formation [34]. Consequently, under atmospheric pressure conditions, the flame becomes nearly invisible. This observation aligns with the experimental findings of Hoxie et al. [35], who reported that pure butanol droplets produced chemiluminescence too weak to be captured by a high-speed camera.

As indicated in Fig. 4-4, increasing the ambient pressure intensifies the LZ. This finding is consistent with the conclusion of Kadota et al. [36], who reported that higher pressure promotes soot particle growth, resulting in the formation of a visible flame. This observation can also be attributed to the increased gas density at higher pressures, which results in a greater availability of the oxidizer molecules per unit of volume. Consequently, the droplet experiences a more efficient and accelerated combustion process due to the enhanced oxidizer supply. Additionally, the flame images show that increasing pressure reduces the flame stand-off distance, defined as the distance between the droplet and the flame front. A reduced stand-off distance implies that the luminous

flame is closer to the droplet, which improves heat transfer to the droplet and further increases the burning rate.

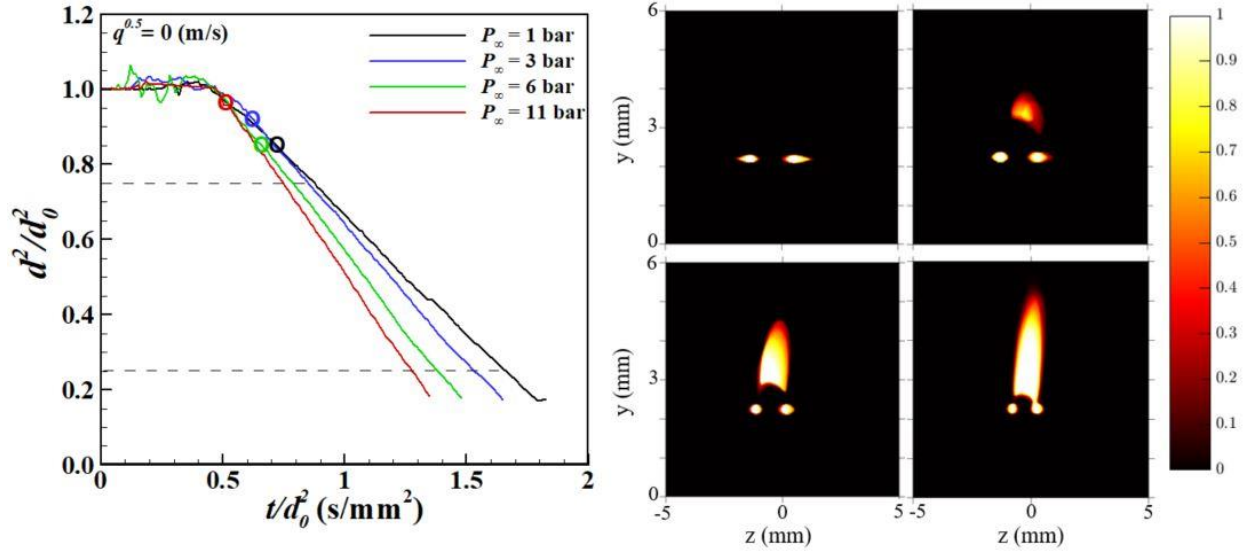


Figure 4-4. Temporal variations in normalized droplet size corresponding LZ of a butanol droplet burning in a stagnant environment under varying pressure conditions.

Fig. 4-3 showed that K_b exhibits improvement followed by reduction at higher pressures, whereas it remained relatively constant under atmospheric pressure conditions. To elucidate the differences between these two scenarios, the average LZ are analyzed in Fig. 4-5 for various turbulent intensities at an ambient pressure of 11 bar. To minimize the impact of random variations, the flame shapes are derived by averaging images from four tests conducted under each fixed condition. These figures demonstrate the impact of turbulence by altering the LZ and, consequently, the droplet burning rate. In the absence of turbulence (stagnant conditions), the LZ exhibits an upward shape driven by natural convection [37]. However, as turbulence is introduced, the relative influence of natural convection weakens, and becomes almost unnoticeable at $q^{0.5} = 0.4$ m/s as can be witnessed in Fig. 4-5e. Combining the information from Fig. 4-3 and Fig. 4-5, it can be concluded that introducing turbulence to a certain extent reduces the flame stand-off

distance. This facilitates the formation of a radial shell around the droplet, which improves heat transfer and consequently enhances the burning rate. However, further increases in the turbulence level beyond this point diminishes the likelihood of forming a strong flame around the droplet, thus weakening the burning rate, as illustrated in Fig. 4-3.

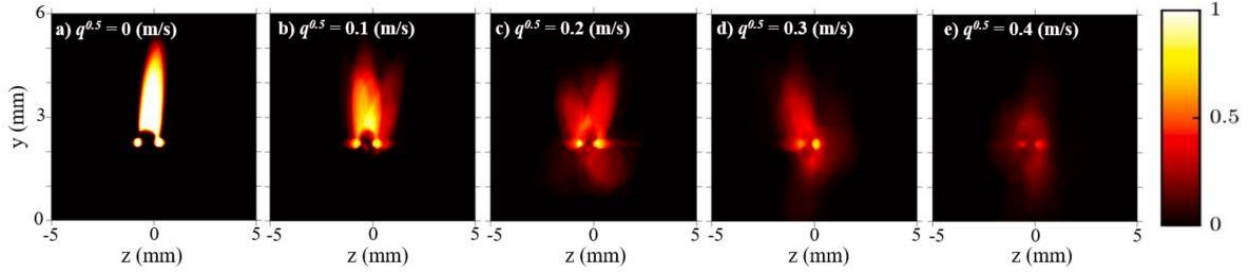


Figure 4-5. Averaged LZ at different levels of turbulence intensity for butanol droplet at 11 bar.

If turbulence initially improves K_b , the question arises as to why K_b drops at higher turbulence levels. The answer lies in phenomena that occur exclusively at elevated turbulence intensities. To illustrate this, Fig. 4-6 presents the time history of butanol droplet combustion at a high turbulence intensity $q^{0.5} = 0.4$ m/s, under 6 bar pressure. This condition corresponds to the point where a reduction in K_b is observed in Fig. 4-3. The combustion process depicted in Figure 4-6a exhibits a non-linear profile, distinct from what is observed in Fig. 4-4. In Fig. 4-6a, point (i) represents the location where the coil is retracted, and K_b is determined between points (ii) and (vi). There is a notable change in the slope of the profile extending between points (iii) and (v). Corresponding flame images reveal that this section ((iii) to (v)) aligns with periods when the luminous flame temporarily disappears and reappears. This phenomenon, referred to as temporary luminous extinction (TLE), is responsible for the significant reduction in the burning rate (as shown in Fig. 4-3). TLE was also observed in previous experiments, and it is concluded that this represents a 'cool flame' region, arising due to low-temperature chemical reactions triggered by the extinction of the visible hot flame [15, 38].

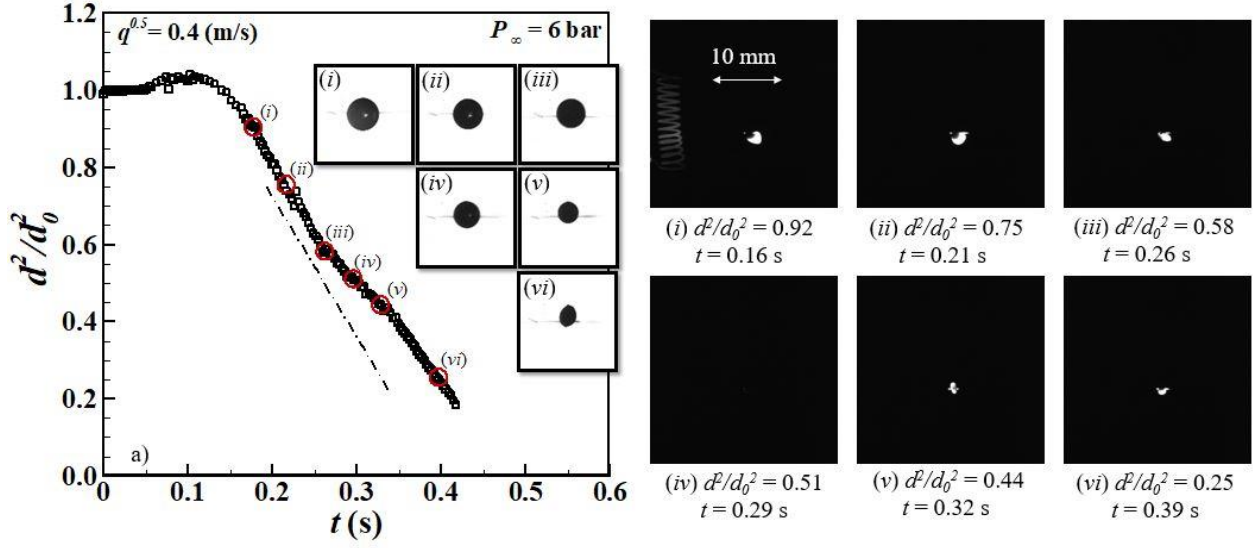


Figure 4-6. a) Example of TLE occurrence in the temporal variation of normalized droplet diameter. The droplet and flame images for the indicated conditions are provided in (i) to (vi).

The duration of TLE depicted in Fig. 4-6 constitutes approximately 21% of the total combustion process, spanning from the point where the coil is retracted (i) to the end point for calculating K_b (vi). Fig. 4-7 presents the variation of K_b , alongside the average duration of TLE, and the frequency (f) of TLE occurrence, to establish a relationship between these parameters. It is important to note that f is calculated based on the number of tests exhibiting TLE divided by the total number of tests at each condition. Fig. 4-7 reveals that turbulence can enhance the burning rate as long as the flame is maintained around the droplet. Beyond a certain point, the occurrence of TLE leads to a reduction in the burning rate. Additionally, further increases in turbulence levels beyond that point results in longer average duration of TLE, which, in turn, increases run-to-run variability and consequently enlarges the error bars.

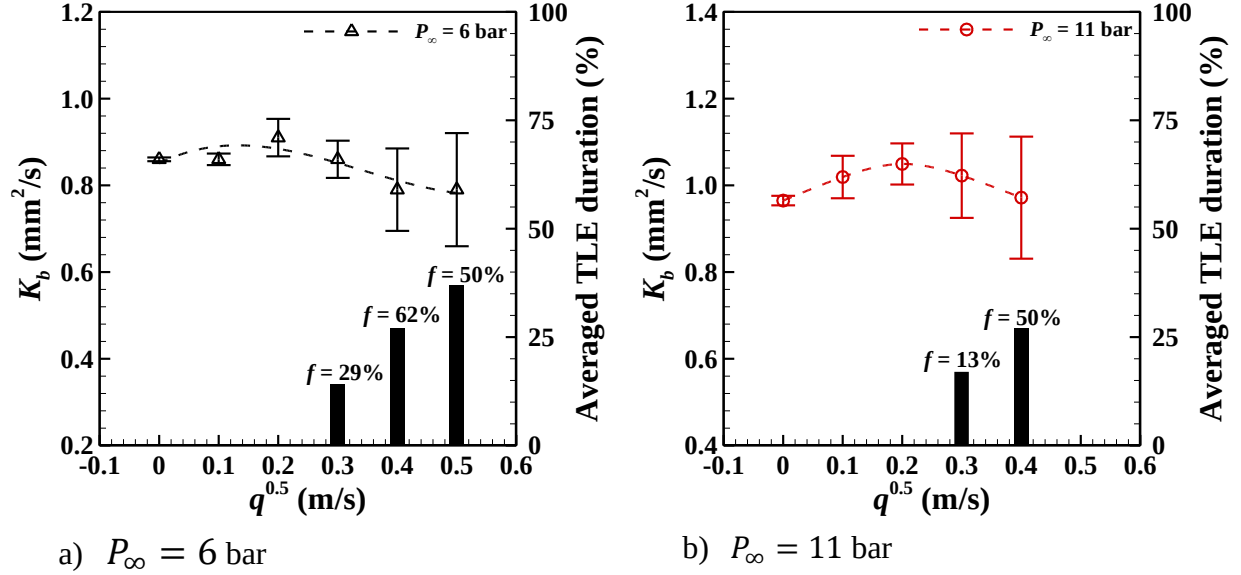


Figure 4-7. Variation of the burning rate with turbulence intensity at a) 6 bar, and b) 11 bar. The bars represent the average duration of TLE, and f denotes the frequency of TLE occurrence. For example, at $q^{0.5} = 0.3$ m/s and $P_\infty = 6$ bar, TLE was observed in 2 out of 7 tests, resulting in $f = 29\%$.

Thus far, the discussion has been focused on pressure conditions higher than atmospheric, where turbulent flow significantly influences K_b . To understand why turbulence has a minimal effect on K_b at atmospheric pressure, the LZ for different turbulence level under atmospheric pressure condition is shown in Fig. 4-8. As observed in this figure, the luminous flame is very weak, and only radiation from the fiber is visible. Consequently, turbulence has less favorable conditions to cause significant changes in K_b under atmospheric pressure condition. This can also be attributed to the stronger influence of fuel molecular diffusivity, combined with Stefan (blowing) flow which prevail over the vapor diffusion induced by turbulence [39].

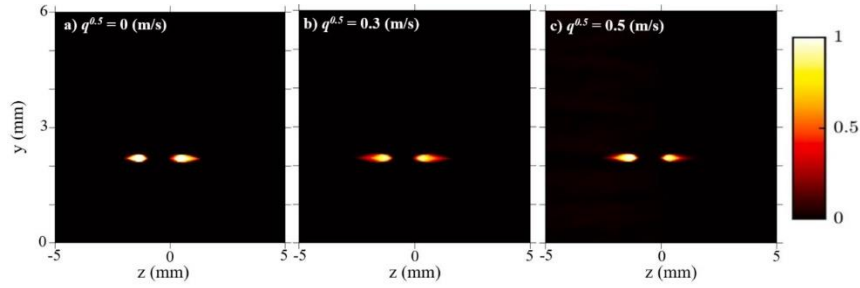


Figure 4-8. Averaged LZ at different levels of turbulence intensity at 1 bar.

4.4.3 Comparison with heptane

To evaluate the possibility of using butanol as a fuel in combustion engines, it is essential to analyze how its combustion properties compare with those of conventional alkanes and hydrocarbons. This section offers a comparative assessment of the combustion behavior between butanol and heptane, examining their performance under different pressure and turbulence test conditions. Heptane was selected for this comparison due to the availability of experimental data obtained under test comparable conditions and using the same apparatus. A previous study by this group examined the combustion behavior of heptane droplets with initial diameters of 500 μm at room temperature over a similar range of ambient pressure and turbulence conditions [25]. As a simple hydrocarbon with significantly higher volatility than butanol, heptane provides a useful reference for assessing how fuel volatility influences droplet combustion characteristics, particularly in relation to the effect of turbulence. Fig. 4-9 presents the variation of K_b with turbulence intensity under different pressure conditions for both butanol and heptane, along with their averaged LZ for two test cases.

Fig. 4-9 illustrates that, under stagnant conditions, the burning rate of heptane is higher than that of butanol, and the difference is 17% at 1 bar and 26% at 11 bar. This finding corroborates that of LZ presented in Fig. 4-9b and c, where the luminous flame surrounding the heptane droplet is both

longer and closer to the droplet surface, implying enhanced heat transfer toward the droplet. The observed difference between their burning rates can be supported by differences in fuel properties. For instance, the density of butanol (806 kg/m³) is higher than that of heptane (684 kg/m³), which, according to classical models, leads to a reduction in the burning rate, as K_b is predicted to scale inversely with density [40]. Additionally, butanol has a smaller heating value (LHV) and a higher enthalpy of vaporization compared to heptane [41]. These characteristics reduce the transfer number, thereby a lower K_b [16]. Another possible reason is the greater combustion enthalpy of heptane, which leads to higher flame temperatures and consequently greater heat transfer to the droplet [12].

Fig. 4-9a illustrates that the change in the burning rate is more pronounced for heptane, which has a larger luminous flame. This suggests that fuels with larger luminous flames are more affected by a turbulent environment. The maximum difference in K_b is 24%, occurring at 11 bar and $q^{0.5} = 0.1$ m/s. Interestingly, this figure reveals that the burning rates of both fuels become comparable at elevated turbulence intensities and pressures; conditions that resemble real engine applications. Although further investigation is required for different fuels, this finding suggests that under engine-like conditions (high pressure and intense turbulence), the burning rate of a droplet becomes largely independent of fuel type. While Fig. 4-9d and e show that the luminous flame is brighter in the case of heptane, it does not result in a significant difference in the burning rate under elevated turbulence intensity and pressure conditions.

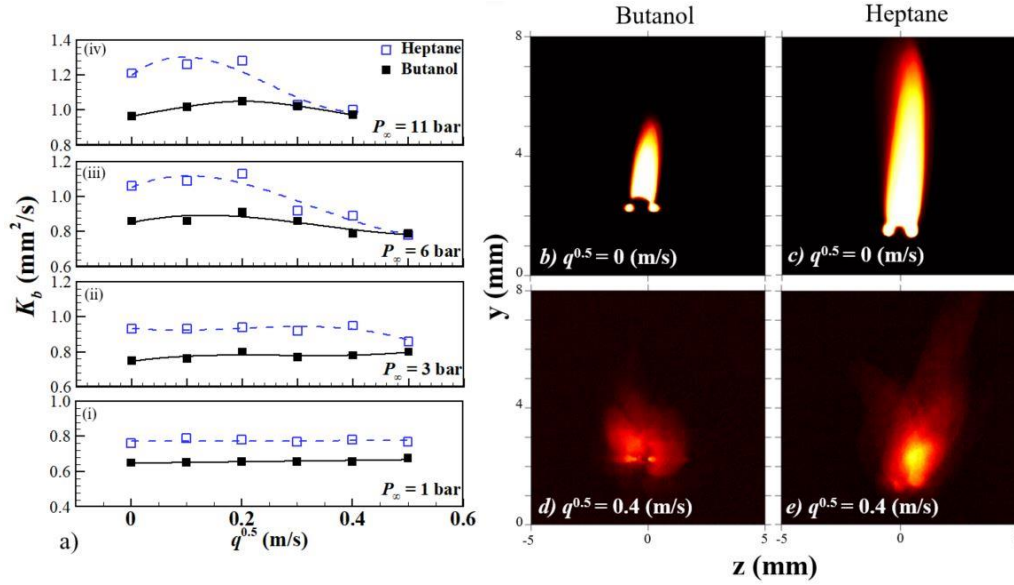


Figure 4-9. Comparison of the combustion behavior between butanol and heptane droplets

4.4.4 Effect of oxygen

Thus far, the discussion has centered on data obtained with ambient standard air, which consist of 21% oxygen and 79% nitrogen. This section explores the impact of oxygen variation on the combustion behavior of butanol droplets. Fig. 4-10 presents the variation of K_b as a function of turbulence intensity for different oxygen concentrations for two ambient pressures. It should be noted that the remainder of the chamber is filled with nitrogen. Reducing the oxygen level in the in the droplet's surroundings reveals that $x_{O_2} = 18\%$ represents the LOC necessary for the complete burning of the butanol droplet. This finding is consistent with the conclusions of Williams et al. [14]. Our experiments showed that, at $x_{O_2} = 18\%$, droplet combustion does not occur under elevated turbulence intensity conditions (i.e., for $q^{0.5} > 0.3$ m/s).

Fig. 4-10 illustrates that increasing the oxygen level enhances K_b across all explored conditions. According to Fig. 4-10a, under atmospheric conditions, increasing oxygen concentration from 18% to 21%, improves K_b by 8% while increasing oxygen concentration from 18% to 30%,

improves K_b by 35%. Fig. 4-10a and b also indicate that the effect of oxygen enrichment becomes more pronounced at elevated turbulence intensity and pressure. To investigate the reason for this improvement, Fig. 4-11 presents images of LZ for various oxygen levels under stagnant conditions at 11 bar. This figure reveals that increasing the oxygen concentration, similar to increasing pressure, reduces the flame stand-off distance. This improves heat transfer to the droplet, and thereby enhances the burning rate. This observation is consistent with the findings reported by Wu et al. [11]. Comparing Fig. 4-10a and b shows that while turbulence has a negligible impact on K_b for different level of oxygen at atmospheric pressure, its influence becomes significant under 11 bar. Different scenarios emerge under 11 bar. That is, at a low oxygen concentration of $x_{O_2} = 18\%$, turbulence begins to suppress K_b at low levels of turbulence intensity ($q^{0.5} \sim 0.1$ m/s). In contrast, increasing the oxygen concentration to $x_{O_2} = 21\%$ shifts this suppression to higher levels of turbulence intensity ($q^{0.5} \sim 0.3$ m/s). As discussed in Section 3.2, the primary cause of the reduction in K_b is the occurrence of TLE. Fig. 4-10b also depicts the average duration of TLE, and the frequency (f) of TLE occurrence. It is found that no TLE occurred in oxygen-rich environment ($x_{O_2} \geq 25\%$). This figure also indicates that lower oxygen levels increase both the frequency and the duration of TLE. Consequently, in oxygen-deficient environments, such as those found in fuel-rich or combustion products-diluent regions of a flame, turbulence is unlikely to enhance the burning rate and may lead to rapid flame extinction. Conversely, higher oxygen levels allow a burning droplet to withstand turbulence before TLE occurs, and hence its K_b improves.

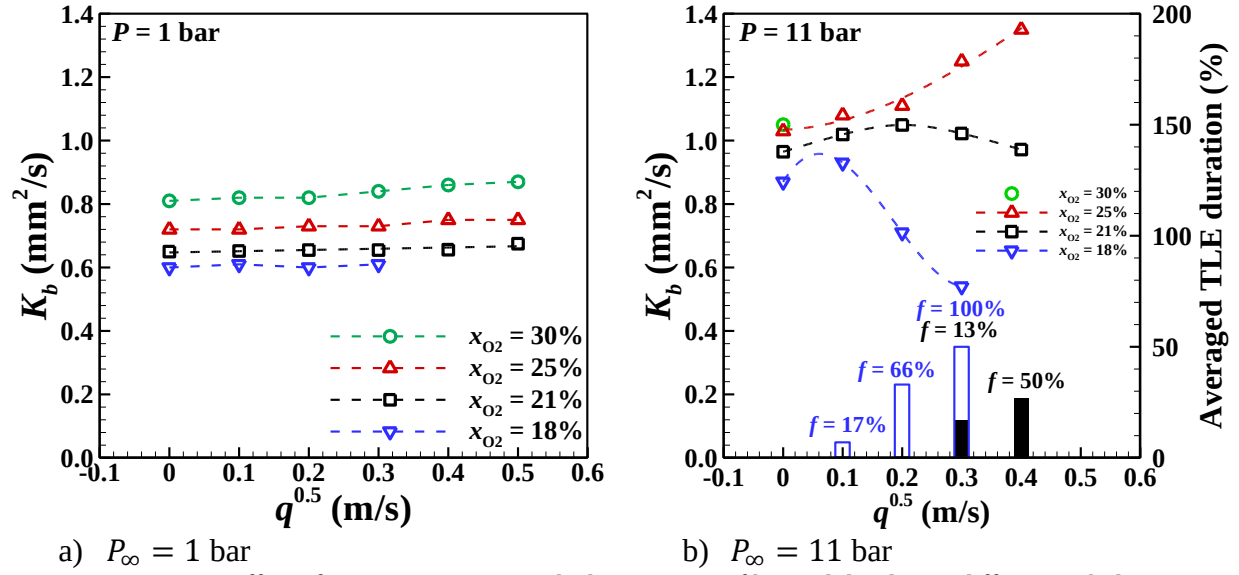


Figure 4-10. Effect of oxygen variation on the burning rate of butanol droplets in different turbulent environments at a) 1 bar, and b) 11 bar. The bars represent the average duration and frequency of TLE occurrence (blue and black bars correspond to 18% and 21% oxygen concentration, respectively). Repeated fiber breakage at $x_{O_2} = 30\%$ and 11 bar prevented turbulent tests at this condition.

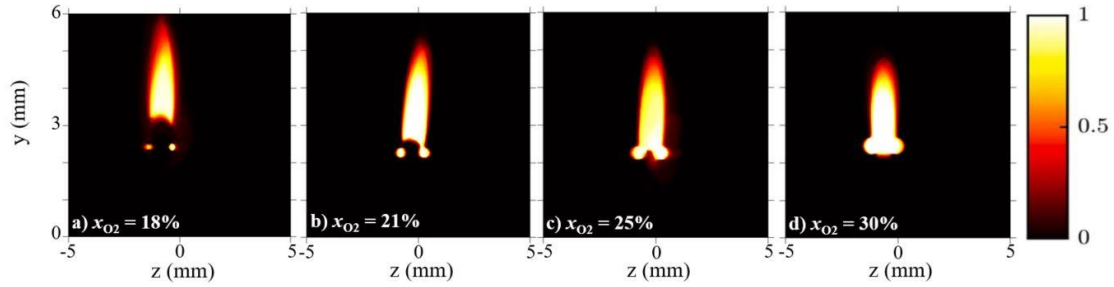


Figure 4-11. Averaged LZ at different levels of oxygen concentration for the stagnant environment at 11 bar.

Fig. 4-12 illustrates the variations of K_b with oxygen concentration. Earlier studies have demonstrated that K_b increases approximately linearly with oxygen concentration [12, 14, 42, 43], with findings from Wu et al. [11] suggesting a steeper increase at higher oxygen levels. However, Fig. 4-12a indicates that this trend is only valid at low ambient pressures (up to ~ 3 bar) under stagnant conditions. As shown in Fig. 4-12a and b, increasing ambient pressure with the presence of a turbulent flow field alters the expected linear trend, resulting in improvement in K_b but with a reduced rate as oxygen concentration increases. As previously mentioned, both oxygen

concentration and ambient pressure influence K_b by reducing the flame stand-off distance and consequently increasing heat transfer, thereby enhancing K_b . However, at higher pressures, the combined effects of oxygen concentration and ambient pressure evidently result in diminishing impact. It is seen that increasing pressure up to 6 and 11 bar reduces the impact of additional oxygen, as the stagnant burning rate is only marginally improved with an increase of background oxygen concentration from 25 to 30%. As noted in Section 3.2, the higher gas density at elevated pressures results in a greater availability of oxidizer molecules per unit volume. Consequently, the combustion process becomes highly efficient and any additional increase in oxygen concentration may not lead to further improvement. Moreover, at elevated pressure, heat loss mechanisms such as thermal radiation and conductive heat transfer become more significant, reducing the amount of heat available to sustain combustion. This leads to a diminished improvement in the burning rate at elevated oxygen levels. Although further investigation at higher oxygen concentrations is required, the present study suggests that beyond a certain threshold, oxygen concentration has a lessened effect on improving the burning rate, especially under elevated pressure conditions and intense turbulence environments.

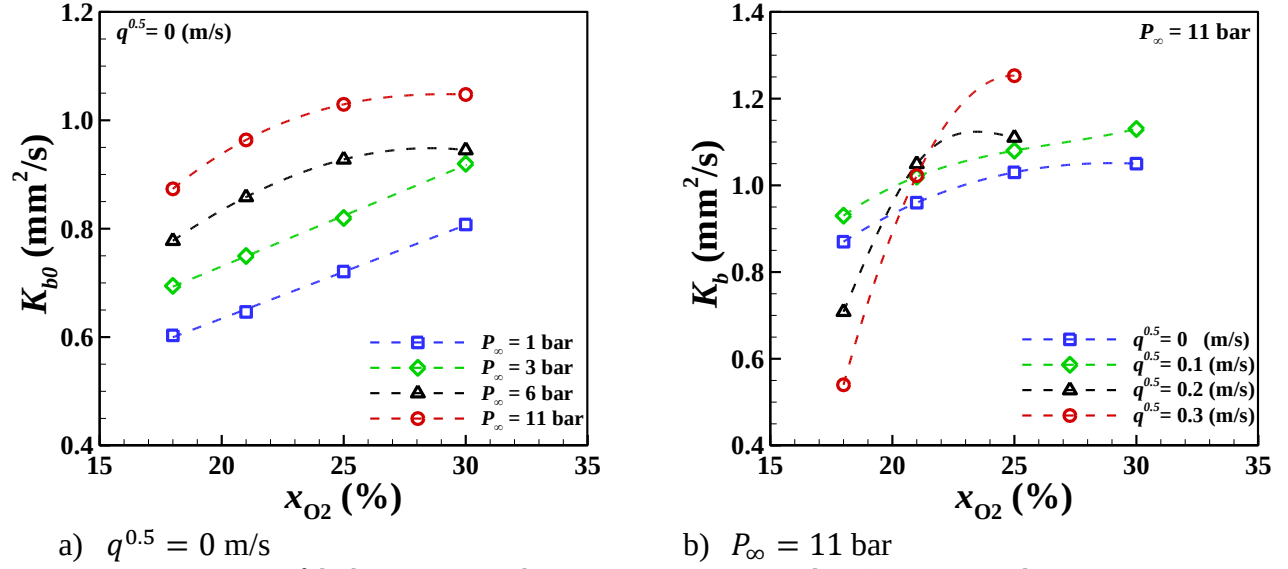


Figure 4-12. Variation of the burning rate with oxygen concentration under: a) stagnant conditions at various pressure levels, and b) 11 bar at different turbulence intensities.

4.4.5 Effect of Carbon dioxide

The effect of CO_2 addition on the combustion behavior of butanol droplets is investigated by varying CO_2 concentration under two conditions: one with 21% oxygen, representative of standard air, and the other with a reduced oxygen level of 18%, simulating an oxygen-deficient environment. In both scenarios, the rest of the chamber content is filled by nitrogen. The maximum CO_2 concentration allowing droplet ignition is 41%, which aligns closely with a previously reported finding [18]. Fig. 4-13 illustrates the impact of CO_2 on the burning rate of butanol droplets under atmospheric pressure conditions over a wide range of turbulence intensity. This figure shows that the presence of CO_2 leads to a reduction in K_b . This can be attributed to the fact that the presence of CO_2 lowers the overall thermal conductivity of the surrounding gas mixture [17], thereby reducing heat transfer from the flame to the droplet, and consequently lowers K_b . Additionally, Fig. 4-13 shows that changing CO_2 concentration from 20% to 41% does not significantly affect K_b under atmospheric pressure conditions. According to this figure, under stagnant condition), the presence of 20% CO_2 reduces K_b by 9%. However, increasing CO_2 level

up to 41% does not lead to further change in K_b . This observation aligns with the findings of Nakaya et al. [44, 45], where the difference in K_b for 30% and 60% CO_2 concentration was less than 0.5% under microgravity conditions.

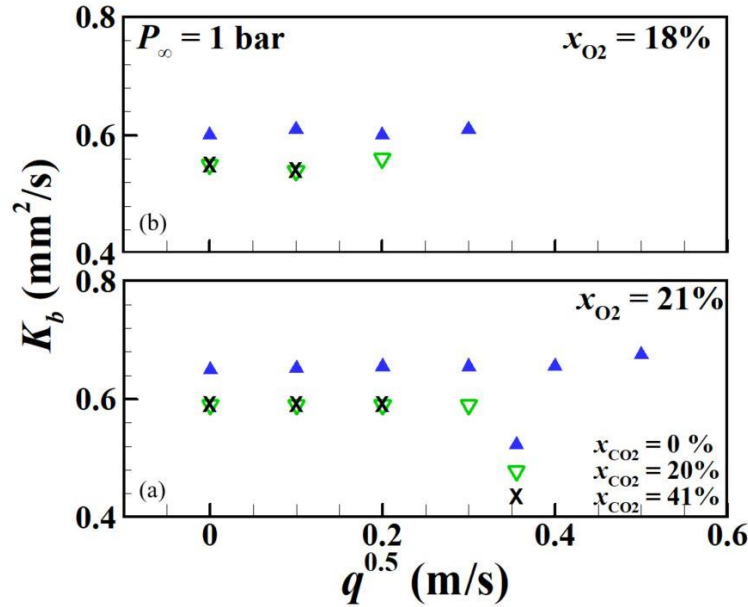


Figure 4-13. Effect of CO_2 addition on the butanol droplet burning rate under atmospheric pressure at different turbulent intensities for a) $x_{O_2} = 21\%$, and b) $x_{O_2} = 18\%$, with the remainder filled by nitrogen.

So far, the discussion has focused on atmospheric pressure conditions. To investigate the effect of CO_2 at elevated pressures, experiments were repeated over the same range of pressures and turbulence levels as in the previous sections. It is observed that, under 11 bar pressure, ignition of the butanol droplet was not possible, even at a 20% CO_2 concentration, and thus, the results are obtained only up to 6 bar. It is found that the suppression effect of CO_2 on K_b persists at elevated pressures of 3 and 6 bar, which are not shown here for brevity. Fig. 4-14a and b show the averaged LZ for the burning droplet at 6 bar pressure for 0% and 20% CO_2 concentrations, respectively. This figure clearly demonstrates that the addition of CO_2 increases the flame stand-off distance and reduces the likelihood of a strong flame forming around the droplet, which consequently

lowers K_b . This observation also confirms the conclusions of published studies indicating that the presence of CO_2 reduces flame temperature [17, 44].

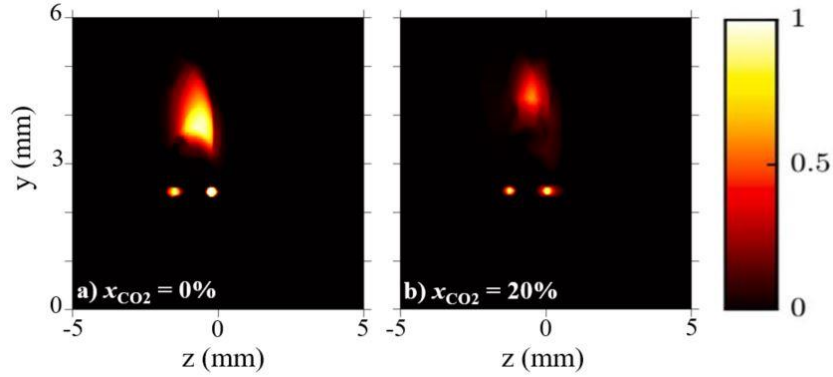


Figure 4-14. The averaged LZ at 6 bar and stagnant conditions for different CO_2 concentrations: a) $x_{CO_2} = 0\%$, and b) $x_{CO_2} = 20\%$.

4.5 Conclusions

The combustion behavior of individual butanol droplets over a range of ambient pressures (up to 11 bar) and turbulence intensities (up to 0.5 m/s) is experimentally investigated. In addition, the combustion performance of butanol droplets was compared with that of heptane, a conventional hydrocarbon fuel. Moreover, variations in the ambient concentrations of O_2 and CO_2 were introduced to evaluate their influence on the burning rate, K_b . The key findings are summarized below.

- Aside from the tests including TLE, temporal evolution of the square of droplet diameter exhibited a quasi-linear trend across all the conditions studied, confirming the validity of d^2 -law.
- Increasing ambient pressure enhances K_b via inducing more oxidizer and reducing the flame stand-off distance, which increases heat transfer toward the droplet.
- The effect of turbulence on K_b varies under different pressure conditions. At low pressures (up to 3 bar), turbulence has a negligible impact on K_b , which can be attributed to the weak

luminous zone flame shape (LZ) around the droplet and the predominance of the vapor transport radial velocity over turbulence induced vapor diffusion. However, at elevated pressures, K_b initially increases with $q^{0.5}$, due to the dominance of turbulent flow and also the formation of a strong radial flame shell around the droplet which enhances droplet heat transfer. Beyond a certain level, further increases in $q^{0.5}$ leads to a decline in K_b , which is attributed to the onset of temporary luminous extinction, TLE. As TLE becomes more frequent and prolonged with increasing $q^{0.5}$, K_b continues to decrease, reaching a point where droplet ignition becomes increasingly difficult.

- K_b of butanol droplets is smaller than that of heptane over all explored pressures in a quiescent environment. However, the difference decreases when turbulent flow is introduced, until K_b becomes comparable at higher turbulence intensities. Based on this, it is suggested that K_b may become independent of fuel type under high pressure and intense turbulence conditions. However, further studies using different fuels are required to verify this claim.
- The limit of oxygen concentration (LOC) required for butanol combustion is found to be 18%, and this oxygen-deficient environment suppresses K_b . Increasing the oxygen level beyond the LOC improves K_b , though this improvement is found to be nonlinear under elevated pressure conditions. It is also observed that the addition of oxygen in the presence of turbulent flow delays the occurrence of TLE. In other words, it helps maintain the flame around the droplet at higher turbulence levels, which, as a result, improves heat transfer and shifts the peak of K_b to higher levels of turbulent flow.
- The maximum CO_2 concentration that allows complete burning of butanol droplets is found to be 41%. The presence of CO_2 is shown to reduce K_b , primarily due to a decrease in the

thermal conductivity of the ambient mixture and flame temperature. Consistent with findings reported in [44], K_b remains unaffected as the CO_2 concentration increases from 20% to 41%.

All in all, turbulence is found as an effective mechanism for improving K_b of butanol droplet in elevated pressure environments and oxygen-rich conditions. However, turbulence is detrimental at oxygen-deficient ambient conditions. This information could be useful when utilizing EGR with butanol in CIEs. Moreover, while butanol shows lower K_b than heptane under stagnant conditions, both fuels exhibit comparable burning characteristics in highly turbulent flow field at elevated pressure conditions. Nevertheless, further studies involving other fuels in addition to alkanes and alcohols under more realistic test conditions that involve higher pressure and temperature are necessary to gain further insights into the interplay between K_b and fuel chemistry.

4.6 References

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Chapter 5: Effect of Ambient Gas Composition on Butanol Droplet Vaporization in Turbulent High-pressure Environments

5.1 Abstract

The present work systematically investigated how ambient conditions influence the evaporation characteristics of butanol droplets. Experiments were conducted in a spherical chamber capable of generating isotropic, homogeneous turbulence with negligible mean flow, using four pairs of axial fans to generate turbulence intensity up to 3.0 m/s. The investigation involved varying ambient pressure, up to 10 bar, and gas compositions, including pure and binary mixtures of N_2 , O_2 , and CO_2 , all at room temperature. Single butanol droplets of 500 μm in diameter were delicately positioned in the center of the chamber onto the intersection of two or four micro-fibers and observed throughout the evaporation process using a high-speed camera with precise magnification. Results demonstrated that the normalized squared diameter of the droplets exhibited a linear decline with time, consistent with the classical d^2 -law. More importantly, the evaporation rate was found to be highly sensitive to ambient gas composition under stagnant conditions, with CO_2 reducing the evaporation rate by 26% compared to N_2 , while O_2 caused only a slight decrease. However the presence of a turbulent flow field with intensities up to 3.0 m/s reduced these disparities by nearly half. In binary gas mixtures, the evaporation rate was found to be intermediate between those of the corresponding pure gases, with a tendency to follow the characteristics of the heavier component. It was found that the presence of turbulence and elevated pressure reduced the effect of ambient gas by diminishing the role of molecular diffusion. The

effectiveness of turbulence increased with both pressure and turbulence intensity and was more pronounced in heavier ambient gases.

5.2 Introduction

The Compression ignition engines (CIEs) have long served as a cornerstone of the transportation sector and continue to be regarded as a viable option for the future, primarily due to their superior fuel efficiency and durability. Currently, the majority of CIEs rely on conventional diesel fuels derived from crude oil [1]. Projections suggest that fossil fuels will remain a dominant energy source, a trend that not only hastens the exhaustion of these finite resources but also drives up the price of petroleum. Moreover, the widespread consumption of fossil fuels presents major environmental concerns, such as global warming and the steady increase in average global temperatures, largely attributed to elevated CO_2 levels [2]. In response to these concerns, researchers are actively investigating alternative liquid fuels that can serve as sustainable replacements for conventional diesel in CIEs [3].

In recent years, bio-alcohols have emerged as a promising category of alternative fuels for CIEs [4]. Although lower alcohols such as methanol and ethanol have been successfully implemented in spark ignition (SI) engines [5], they are inappropriate for use in CIEs. This limitation stems from several unfavorable properties, including low lubricity, low heating value, poor miscibility with diesel, high latent heat of vaporization, and a significantly high auto-ignition temperature [6]. In contrast, higher alcohols such as butanol, offer more favorable characteristics for CIE applications due to their longer carbon chains, higher energy content, greater cetane number, and better miscibility with diesel fuel [7]. There is extensive research on butanol usage in CIEs, which has been summarized in recent review studies [8, 9]. These studies suggest that butanol can be

efficiently employed in CIEs with minor engine modifications, leading to notable reductions in nitrogen oxide (NO_x) and smoke emissions.

CIEs are known for their inherently high thermal efficiency, primarily due to their elevated compression ratios, which enable more efficient energy conversion compared to SI engines [10]. Moreover, enriching the intake air with additional O_2 has been suggested as a promising approach to enhance combustion performance and lower overall emissions in CIEs [11].

However, these advantages come with the drawback of elevated in-cylinder temperatures, which promote the formation of NO_x and soot emissions [12]. To reduce NO_x emissions, a common approach involves recirculating a portion of the combustion product back into the cylinder. This technique, known as exhaust gas recirculation (EGR), is an efficient, readily adaptable, and reliable technology with several advantages. EGR introduces CO_2 into the combustion process, which raises the specific heat capacity of the in-cylinder gases. This, in turn, lowers the cylinder and flame temperatures, enhances flame radiation, and suppresses soot formation [13, 14]. Finally, the shorter ignition delay associated with EGR reduces the premixed combustion fraction, resulting in a lower rate of heat release and consequently less NO_x generation [15]. The recirculated gases consist mainly of CO_2 , nitrogen (N_2), and oxygen (O_2) [16]. Under oxygen-enriched conditions or EGR, the gas composition surrounding fuel droplets differs significantly from that of inert environments like pure nitrogen, which in turn alters the droplet's vaporization process [17]. As a result, understanding how variations in ambient composition influence fuel droplet evaporation has become increasingly important.

Gaining insight into the evaporation characteristics of individual fuel droplets is essential for a wide range of engineering systems, especially in CIEs utilizing direct in-cylinder fuel injection.

Because combustion efficiency strongly depends on how fuel vapor is distributed both spatially and temporally within the chamber, reliable prediction of droplet vaporization is a key element in improving engine modeling and performance optimization [17]. In practical spray combustion systems, liquid fuel is broken down into numerous fine droplets, each of which must undergo vaporization before combustion can occur—making the evaporation process a critical precursor to ignition. Due to the intricate and highly dynamic behavior of spray phenomena, direct experimental analysis is often difficult. Consequently, simplified single droplet experiments are commonly used to investigate the core physical processes that govern spray evaporation [18].

A review of existing literature revealed the existence of a limited studies that have systematically examined the vaporization characteristics of single fuel droplets under diverse ambient gas compositions and different conclusions have been reported. Yi et al. [17] developed a numerical model to investigate the effect of ambient gas composition on diesel droplet evaporation. Their results showed that adding O_2 to N_2 ambience consistently enhances the vaporization rate. In contrast, the effect of CO_2 is more complex, while low concentrations (up to 10%) can promote the vaporization rate, higher CO_2 levels suppress it. However, Markadeh and Ghassemi [19] reported a different conclusion regarding the role of O_2 in the vaporization rate of diesel droplet. They observed that increasing O_2 initially enhances the vaporization rate, but further enrichment reduces it, due to the competing effects of thermal conductivity, thermal diffusivity, and mass diffusivity in the N_2 – O_2 mixture.

Additionally, they found that EGR has a negligible effect on diesel droplet evaporation. Kelly et al. [20] reported that the evaporation rate of methanol droplet is reduced as the molecular weight of the ambient gas increases. Karn et al. [21] showed that polar ambient gases improve the

vaporization rate of water droplets. Mazumder et al. [22] found that the evaporation rate of ethanol decreased in less viscous ambient gases.

It is important to mention that all the aforementioned studies were numerical. In one of the few experimental studies conducted in this area, Radhakrishnan et al. [23] investigated the evaporation of water droplets in different ambient gas compositions. Their results showed that the evaporation rate decreases when the droplet is exposed to a heavier ambient gas. Yang et al. [24] also experimentally investigated the effect of O_2 concentration on evaporation rate of hydrocarbon droplets in a weakly convective flow. They demonstrated that the evaporation rate of heptane or hexadecane droplets increased when the ambient gas composition was changed from an oxygen-free CO_2 – N_2 mixture to a hot gas flow containing 21% O_2 . Table 5-1 provides a summary of published studies along with their respective test conditions.

Table 5-1. A summary of published studies on the effect of ambient composition on single droplet evaporation.

Authors	Type	Fuel	d_0 (μm)	P (bar)	T (K)	Condition	Ambient composition
Yang et al. [24] (2001)	Exp.	Heptane, hexadecane	700	1.0	750	Laminar ($U =$ 0.6 m/s)	Air, O_2
Yi et al. [17] (2014)	Num.	Diesel	NA	10.0	700	Stagnant	O_2 , N_2 , CO_2
Markadeh et al. [19] (2018)	Num.	Deisel	20	30.0	700	Stagnant	O_2 , N_2 , H_2O
Kelly et al. [20] (2018)	Num	methanol	NA	6.0	300	Stagnant	Air, Ar, He
Radhakrishnan et al. [23] (2019)	Exp.	Water	1000	1.0	300	Stagnant	O_2 , N_2 , CO_2 , Ar, SF_6
Karn et al. [21] (2021)	Num.	Water	NA	1.0	310	Stagnant	Air, $C_2H_2F_4$
Mazumder et al. [22] (2023)	Num.	Ethanol	1200	1.0	500	Laminar ($Re =$ 100)	O_2 , N_2 , CO_2 , Ar

As summarized in Table 5-1, the majority of previous investigations on droplet evaporation have been numerical. Due to the limited availability of experimental data under appropriate ambient conditions, several of these studies validated their models using measurements obtained under ambient conditions composed solely of nitrogen. Furthermore, most of the existing experimental and numerical efforts have been conducted under quiescent or weakly laminar flow conditions,

which do not represent turbulent environments encountered in practical combustion systems [25]. While some investigations have examined the evaporation behavior of light alcohols, the literature reveals a lack of studies focused on higher alcohols such as butanol. In light of these research gaps, the present study aims to experimentally investigate the combined effects of turbulence intensity, ambient gas composition, and ambient pressure on the evaporation behavior of butanol droplets. The present study makes mainly two key contributions. First, it provides new experimental data on butanol droplet evaporation under systematically varied ambient pressures (up to 10 bar), turbulence intensities (up to 3.0 m/s), and gas compositions, including pure and binary mixtures of N_2 , O_2 , and CO_2 . Second, it investigates how turbulence and elevated pressure affect the sensitivity of the evaporation rate to gas composition, offering insights that are directly relevant to practical combustion scenarios such as exhaust gas recirculation (EGR).

5.3 Experimental apparatus

All experiments were conducted in a custom-designed, stainless-steel spherical chamber with a volume of 29 liters, capable of withstanding elevated pressures. The chamber is equipped with eight axial fans, arranged in four opposing pairs to ensure the generation of a homogeneous and isotropic turbulent field with negligible mean velocity. Two sets of optical-grade quartz windows were installed to facilitate high-resolution imaging, visualization, particle image velocimetry (PIV) measurements, and physical access to the chamber.

The droplet vaporization process was monitored using a high-speed Fastec IL5Q imaging system coupled to a Questar QM-100 long-focus microscope, offering a spatial resolution of 1.08 $\mu\text{m}/\text{pixel}$. Images were captured at a constant frame rate of 24 frames per second with a 200 μs shutter speed. Uniform illumination was achieved using a 250 W halogen lamp positioned as a

backlighting source. To prevent thermal interference with the evaporation process, the lamp's light was directed through a 1.8-meter metal tube, minimizing radiative heat transfer to the droplet.

The turbulent flow field inside the chamber was characterized using a Dantec Dynamics 2D Particle Image Velocimetry (PIV) system, comprising a Dual Power laser and a FlowSense camera. DynamicStudio software was employed for system control, synchronization, image acquisition, and cross-correlation. PIV measurements were conducted over a 90×90 mm field of view, with a spatial resolution defined by 32×32 pixel interrogation windows and 50% overlap. For each test condition, 2000 image pairs were recorded at a frequency of 10 Hz, which was verified to ensure statistical convergence of the turbulence quantities.

The droplet injection system, is mounted at the chamber's upper section to utilize gravitational assistance during droplet release. The system comprises a threaded rod driven piston, a sliding barrel, and a 30-gauge stainless steel needle. To enable the generation of small droplets, a polycarbonate micro-capillary tube with an inner diameter of $40 \mu\text{m}$ and outer diameter of $60 \mu\text{m}$ is inserted into the needle and fixed in place using cold weld epoxy. To suspend the droplet at the center of the chamber while preserving its spherical shape and minimizing conductive heat losses, a cross-fiber suspension technique was utilized. Under low-turbulence conditions, the system comprised two $14 \mu\text{m}$ silicon carbide (SiC) fibers positioned orthogonally at 90 degrees and mounted on a square aluminum frame. However, in highly turbulent environments, this configuration proved insufficient to support the droplet. Therefore, two additional fibers were incorporated into the support frame, forming a radially symmetric arrangement as illustrated in [26]. The fibers are secured to the frame with cold weld adhesive and maintained under light tension to prevent deformation or breakage. The suspended fibers intersect at the chamber's geometric center, providing stable support for the droplet while occupying less than 1% of the

droplet's volume, thus ensuring minimal influence on size or shape. This frame is mounted vertically via a single rod connected to the chamber roof.

A finned cartridge heater was installed on the chamber wall to regulate the internal temperature during experiments. This heating element maintained the nominal chamber temperature at 300 ± 1 K. To ensure a uniform temperature distribution, two thermocouples were employed: a K-type thermocouple placed 180 degrees opposite the heater and an internal thermocouple embedded within the heater itself.

5.3.1 Methodology and uncertainties

Prior to each experiment, the chamber was evacuated to approximately 0.1 bar using a vacuum pump to eliminate residual moisture and impurities. The pressure control system employed two pressure gauges: one low-range gauge to verify near-vacuum conditions, ensuring the chamber was fully purged before gas introduction; and another high-range gauge used to accurately adjust and monitor elevated pressure conditions during testing. Following purging, the chamber was pressurized to the desired composition using high-purity gases from commercial cylinders. Chamber pressure was closely regulated and maintained within $\pm 1\%$ of the target pressure. After reaching the target temperature of 300 ± 1 K, the heater was turned off and tests start when the heater temperature has cooled down to the target temperature. For the temperature measurement, combined uncertainties from the thermocouple (± 2.2 K) and the ADC module (± 1.2 K) yield a conservative total uncertainty of ± 3.4 K. Once the desired ambient pressure, ambient composition, and temperature were achieved, axial fans driven by independent servo motors were activated to generate a turbulent flow field within the chamber. Fan rotation speeds were regulated with high accuracy, maintaining deviations within $\pm 1\%$ of the set RPM. After stabilizing the flow field, a single butanol droplet with a 500 ± 25 μm initial diameter was generated and placed on the cross

section of the fibers. After droplet placement, the injector was retracted immediately to avoid disturbing the surrounding flow and interfering the images. Then the evaporation process was recorded and the image sequences were analyzed via a custom-developed MATLAB code. The initial diameter (d_0) was determined by matching the pixel area of the droplet image to a circle. The vaporization rate (K) was determined based on the well-established d^2 -law, which states that the square of the droplet diameter decreases linearly with time. Accordingly, K was obtained as the slope of the linear decrease, extracted within the range $0.95 \geq (d/d_0)^2 \geq 0.25$, which corresponds to approximately 80% reduction in volume. This range was selected to exclude any early transient and end-of-life nonlinearities. The coefficient of determination (R^2) for the linear fit consistently exceeded 0.99 across all tests. To evaluate the droplet sphericity, the circularity is calculated as $C = (4A_s\pi/P^2)$ where A_s is the projected area and P is the perimeter. A value of $C \approx 1$ corresponds to a perfect circle. In this study, C was consistently above 90 percent, indicating that deviations from perfect sphericity is negligible. To assess repeatability, each test condition was repeated at least four times. A 95% confidence interval was applied to estimate the uncertainty in the vaporization rate, which remained below 5% for all conditions. Systematic errors in droplet size measurement arose from camera calibration and edge detection. Camera magnification was calibrated using a reference sphere with a defined size, resulting in an estimated uncertainty of 1%. Edge detection accuracy was evaluated by comparing Otsu and manual thresholding methods, with differences in d_0 remaining below 2%. The generated turbulent flow field was verified before and after each test using PIV measurements to confirm consistency. The turbulent RMS velocity components were derived from PIV data using custom MATLAB codes, with sampling uncertainty estimated at 4% (95% confidence level).

5.3.2 Test conditions

This study examines the evaporation characteristics of individual butanol droplets (99.9% purity) with an initial diameter of $500 \pm 25 \mu\text{m}$ under various ambient gas compositions. Experiments were conducted using O_2 , N_2 , and CO_2 as well as their mixtures as the surrounding gases, with absolute chamber pressures P_∞ , ranging up to 10 bar. A summary of the gas ambient conditions are provided in Table 5-2. The chamber temperature was held constant at $300 \pm 1 \text{ K}$. Droplet evaporation was evaluated under both quiescent and turbulent conditions, with fan speeds varying from 0 to 6000 RPM, corresponding to turbulence intensities between 0 and 3.0 m/s .

Table 5-2. Explored ambient gas compositions

Type	Case #	N_2	O_2	CO_2
Single gas	Case 1	100%	0	0
	Case 2	0	100%	0
	Case 3	0	0	100%
Binary gas	Case 4	50%	50%	0
	Case 5	50%	0	50%
	Case 6	0	50%	50%

5.4 Results and discussion

This study investigates the influence of ambient conditions on butanol droplet vaporization over a wide range of pressure (1–10 bar), turbulence intensity (0–3.0 m/s), and gas compositions including pure and binary mixtures of N_2 , O_2 , and CO_2 . Section 3.1 presents the characterization of the turbulent flow field based on PIV measurements to confirm isotropy and homogeneity. In Section 3.2, the effect of ambient gas composition on droplet lifetime and evaporation rate is examined under both stagnant and turbulent environments in various pressure environments. Finally, in Section 3.3, the turbulence effectiveness is quantified and compared against existing semi-empirical correlations to evaluate their applicability across the explored conditions.

5.4.1 Turbulence Characterization

As a representative case, Fig. 5-1 illustrates the PIV results acquired under an ambient pressure of 1 bar and a fan speed of 5000 RPM in a pure N_2 environment. This figure displays key features of the flow field, including the mean velocity vectors, a color map of turbulence intensity, $q^{0.5}$, and spatial variation in isotropy. The turbulence intensity, $q^{0.5}$, defined as the square root of the turbulent kinetic energy, is computed using the relation $q^{0.5} = \sqrt{3} \left(\sqrt{U_{rms}^2 + V_{rms}^2} \right) / 2$, where U_{rms} and V_{rms} represent the root mean square of the velocity fluctuations in the horizontal and vertical directions, respectively. Regions highlighted in white correspond to areas where the deviation from isotropy, measured by $|1 - U_{rms}/V_{rms}|$, exceeds 10%. The results indicate that the setup is capable of generating a turbulent flow field with a high degree of isotropy, as the $|1 - U_{rms}/V_{rms}|$ remains within $\pm 10\%$ of unity across the center. Furthermore, the flow demonstrates a high level of homogeneity within the central region (marked by the black circle), where the variation in $q^{0.5}$ relative to its local average remains below 5%.

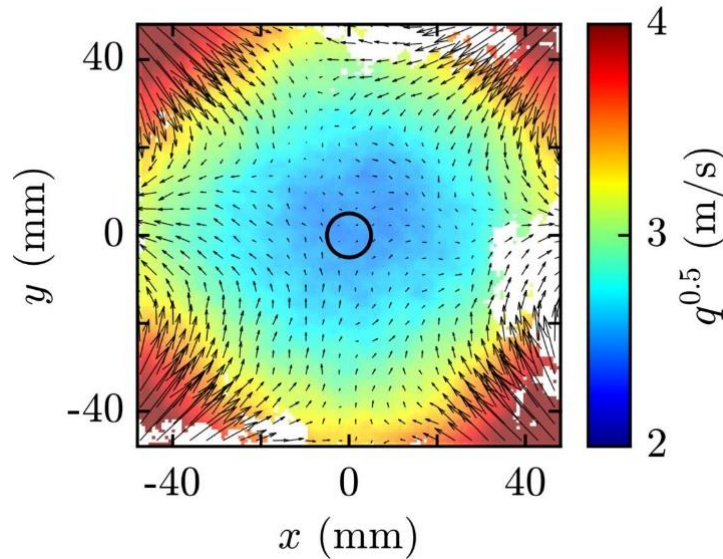


Figure 5-1. The 2D map of $q^{0.5}$ with the mean velocity vectors at 1 bar and 5000 RPM in N_2 environment. Areas highlighted in white indicate regions where flow anisotropy exceeds 10%. The black circle marks the 10 mm diameter used for spatial averaging.

Fig. 5-1 corresponds to the test conducted in a pure N_2 environment. However, since the objective of this study is to examine the influence of ambient composition on droplet evaporation, it is essential to characterize the turbulent flow field in other environment as well. Accordingly, PIV tests were also performed in CO_2 environment, and the corresponding results are summarized in Table 5-3. Table 5-3 presents the averaged turbulence statistics and length scales obtained from various PIV measurements at different pressure levels and fan speeds for two pure ambient compositions (N_2 and CO_2). The overbar notation denotes a circular spatial average centered in the center of the chamber, within a 5 mm radius, as indicated by the solid black circle in Fig. 5-1. The selected size for spatial averaging is sufficiently large and is approximately 10 times the droplet size. Consistent with prior studies, Table 5-3 confirms a linear relationship between turbulence intensity and fan speed, N , approximated by $q^{0.5} \sim 0.0005 \times N$. Table 5-3 also indicates that a high level of isotropy is consistently maintained within the central region, regardless of the ambient pressure, fan speed, or gas composition (where $|1 - U_{rms}/V_{rms}|$ remains below 3%). Additionally, Table 5-3 shows that the mean planar velocity ($\sqrt{U^2 + V^2}$) remains negligible compared to $q^{0.5}$, supporting the capability of the setup to generate nearly zero mean velocity turbulent flow field.

Using the methodology outlined in [27], the integral length scale, L , is calculated approximately 25.8 mm and exhibits negligible variation across different ambient compositions, pressures, and fan speeds. This value aligns with those typically observed in practical combustor systems [28]. The Kolmogorov length scale, η , is estimated based on the assumption of equilibrium between turbulence production and dissipation, using the relation $\eta \approx C_\epsilon^{-1/4} L (q^{0.5} L / \nu)^{-3/4}$. Here, ν represents the kinematic viscosity of the ambient gas, and C_ϵ is a proportionality constant, which was shown by Verwey and Birouk [27] to approach a value of approximately 0.5 for the current

setup. As presented in Table 5-3, η is smaller in CO_2 , compared to N_2 , which is due to the lower kinematic viscosity of CO_2 . Notably, the largest values of η , are observed at the lowest fan speed of 500 rpm ($q^{0.5} = 0.25 \text{ m/s}$) under 1 bar pressure, reaching approximately 340 μm for N_2 and 212 μm for CO_2 .

Table 5-3. Spatially averaged turbulence statistics for N_2 and CO_2 at 1 and 5 bar

Ambient	Pressure (bar)	Fan speed (rpm)	$\overline{q^{0.5}}$ (m/s)	$ 1 - U_{rms} / V_{rms} (\%)$	$\sqrt{U^2 + V^2}/q^{0.5}(\%)$	$\eta (\mu\text{m})$	$L (mm)$
N_2	1	5000	2.48	1.6	2.3	60.4	25.8
	5	2000	0.99	0.6	1.2	35.2	
CO_2	1	5000	2.46	3.0	3.8	37.6	25.8
	5	2000	0.99	0.9	3.5	22.4	

Although the PIV measurements presented here were conducted in an empty chamber, prior validation [29] has confirmed that the presence of experimental components such as the injector, heating element, and support frame does not alter the characteristics of the turbulent flow field. It should be mentioned that due to the 3D nature of the turbulent flow field and 2D of the PIV setup, the results were further validated by performing additional PIV velocity measurements at 90-degree with respect to the original layout to confirm the symmetrical nature of the flow field.

5.4.2 Effect of ambient composition

Fig. 5-2 depicts the temporal evolution of the normalized squared diameter of a butanol droplet at atmospheric pressure under both stagnant ($q^{0.5} = 0 \text{ m/s}$) and turbulent ($q^{0.5} = 2.5 \text{ m/s}$) conditions, for three distinct pure ambient gas compositions. Three key observations can be drawn from this figure. Firstly, under all investigated conditions, the droplet lifetime evolution exhibits an approximately linear trend, supporting the applicability of the classical d^2 -law for calculating the evaporation rate, K , within the following range: $0.95 < d^2/d_0^2 < 0.25$. Secondly, Fig. 5-2 showed that, at the same test conditions, the evaporation behavior in pure N_2 and pure O_2

environments appears nearly identical, whereas a noticeably prolonged droplet lifetime is observed in a pure CO_2 atmosphere. The suppressive effect of CO_2 on the droplet evaporation rate is consistent with previous studies [17, 22, 23] and can be attributed to multiple thermophysical properties, which are shown in Table 5-4. The primary contributing factor is the relatively high specific heat capacity of CO_2 , which enables it to absorb more thermal energy and thereby delaying heat transfer to the droplet surface in comparison to other ambient gases [30]. Additionally, the lower viscosity of CO_2 diminishes the overall enthalpy diffusion and further hindering both heat and mass transfer processes [17, 22]. Furthermore, according to Table 5-4, CO_2 has a lower thermal conductivity, which reduces the rate of heat conduction to the droplet and results in slower evaporation rate. Thirdly, the increase in droplet lifetime in a pure CO_2 environment becomes significantly more pronounced in a stagnant environment. While the difference in droplet lifetime between pure N_2 and pure CO_2 under turbulent conditions (e.g., $q^{0.5} = 2.5 \text{ m/s}$) is approximately 13%, this difference doubles to 26% under stagnant conditions. This observation can be attributed to the higher density of CO_2 , which reduces the density gradient between the ambient gas and the evaporating fuel vapor. Consequently, buoyancy-driven natural convection around the droplet is further suppressed in CO_2 [23], leading to a notable increase in droplet lifetime.

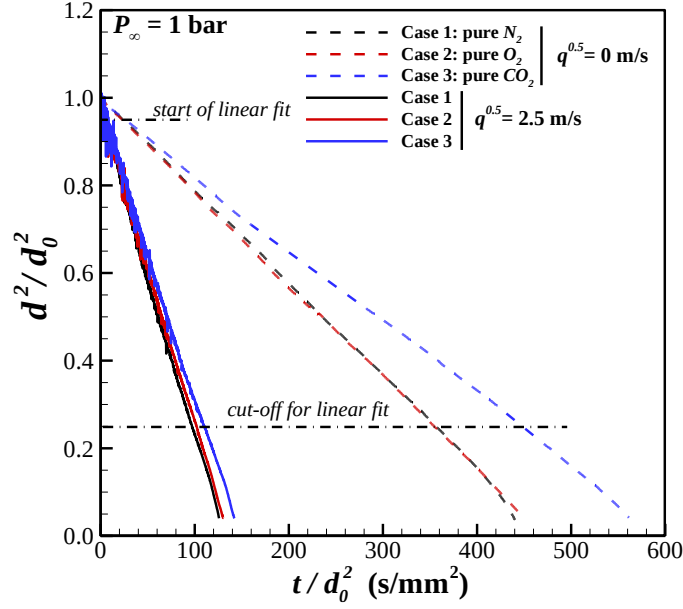


Figure 5-2. Lifetime history of a butanol droplet in different pure ambient compositions under stagnant and turbulent flow conditions.

Table 5-4. Thermophysical properties of different ambient composition at 1 bar and 300 K [31]

	N_2	O_2	CO_2
Density (kg/m^3)	1.292	1.13	1.775
Heat Capacity ($J/mol.K$)	29.18	29.39	37.25
Viscosity ($\mu poise$)	179.4	207.0	158.7
Thermal conductivity ($W/m.K$)	0.02646	0.02674	0.01724

To draw a more comprehensive conclusion, Figures 5-3a and 5-3b present the vaporization rate, K , of a butanol droplet across the entire range of investigated conditions, including pressures up to $P_\infty = 10.0$ bar and turbulent intensity up to $q^{0.5} = 3.0$ m/s. A clear trend observed in these figures is the decline in the number of valid data points with increasing pressure. While the evaporation rate can be obtained at turbulent intensities up to 3.0 m/s at 1 bar, it is only attainable up to 1.0 m/s at 10 bar. This reduction is primarily attributed to droplet detachment caused by the decrease in surface tension at elevated pressures [32]. Additionally, it is evident that under all tested conditions, the presence of pure CO_2 environment consistently results in one fewer data point compared to other ambient gases. This behavior can be attributed to the higher density of CO_2 , which further reduces the density difference between the liquid droplet and the surrounding

gas at elevated pressures, thereby promoting earlier droplet detachment [33]. Another contributing factor to the earlier droplet detachment in CO_2 , may be the smaller Kolmogorov length scale, η , as shown in Table 5-3. The associated eddies, which are responsible for droplet deformation and spray breakup [34], exhibit higher velocity gradients and thus generate stronger local shear stresses, increasing the likelihood of droplet detachment from the fiber.

Nevertheless, Figures 5-3a and 5-3b confirm that the observations at atmospheric pressure in Fig. 5-2 persist at higher pressure levels; where K remains largest in pure N_2 , intermediate in pure O_2 , and smallest in pure CO_2 . Increasing pressure in turbulent environment, however, diminishes these disparities. At 1 bar $q^{0.5} = 1.0$ m/s.

Figures 5-3a and 5-3b also indicate that turbulence mitigates the influence of ambient-gas composition on K . Under stagnant conditions, the difference in K between pure N_2 and CO_2 is 23% at 1 bar and is 31% at 2.5 bar. However, at the highest available turbulence intensity, these differences are reduced to 12% and 18% at 1 bar and 2.5 bar, respectively. The reason is that turbulence enhances mixing and accelerates heat and mass transfer around the droplet, thereby reducing the role of molecular diffusion, which is more sensitive to ambient gas properties. As a result, the disparities caused by differences in ambient gas composition become less pronounced under elevated turbulent conditions.

a)

b)

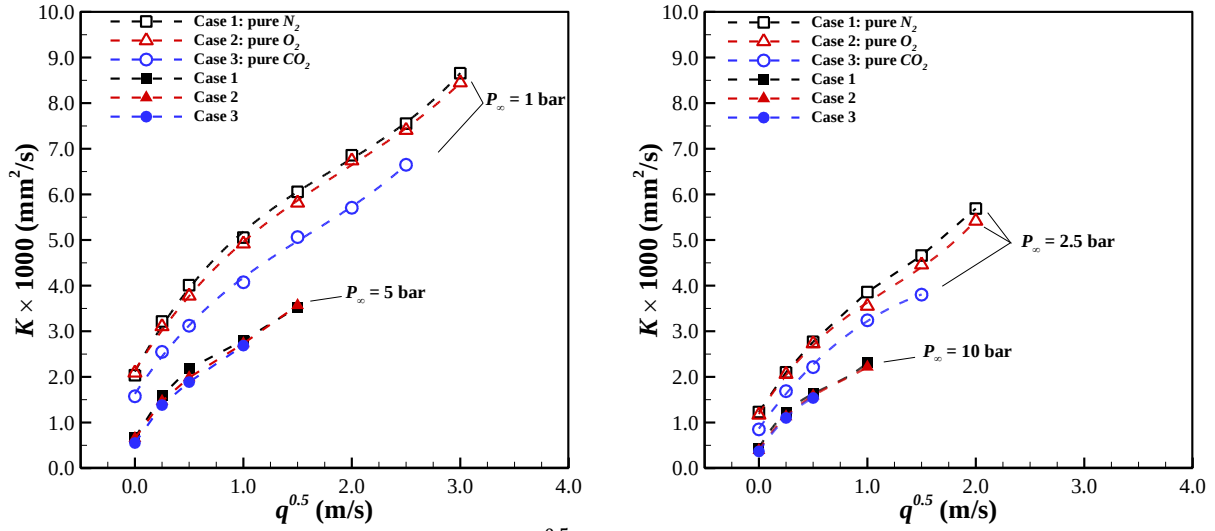


Figure 5-3. K as a function of $q^{0.5}$ at a) 1 and 5 bar, and b) 2.5 and 10 bar.

Thus far, the discussion has focused on droplet evaporation behavior in pure ambient environments. To investigate the combined effect of different ambient-gas compositions, Figures 5-4a and 5-4b present the evaporation rate of butanol droplets across all explored ambient compositions—including binary gas mixtures—at two different ambient pressures; 2.5 bar and 10.0 bar. In these figures, symbols represent the previously discussed pure ambient compositions, while various line styles indicate the evaporation rates in binary mixtures. The results show that the evaporation rate in 50–50 binary mixtures consistently falls between the rates observed for the corresponding pure gases. Notably, the value of K in these binary mixtures tends to be closer to that of the heavier pure component. This trend suggests that droplet evaporation behavior in equal binary mixtures is predominantly influenced by the heavier ambient species.

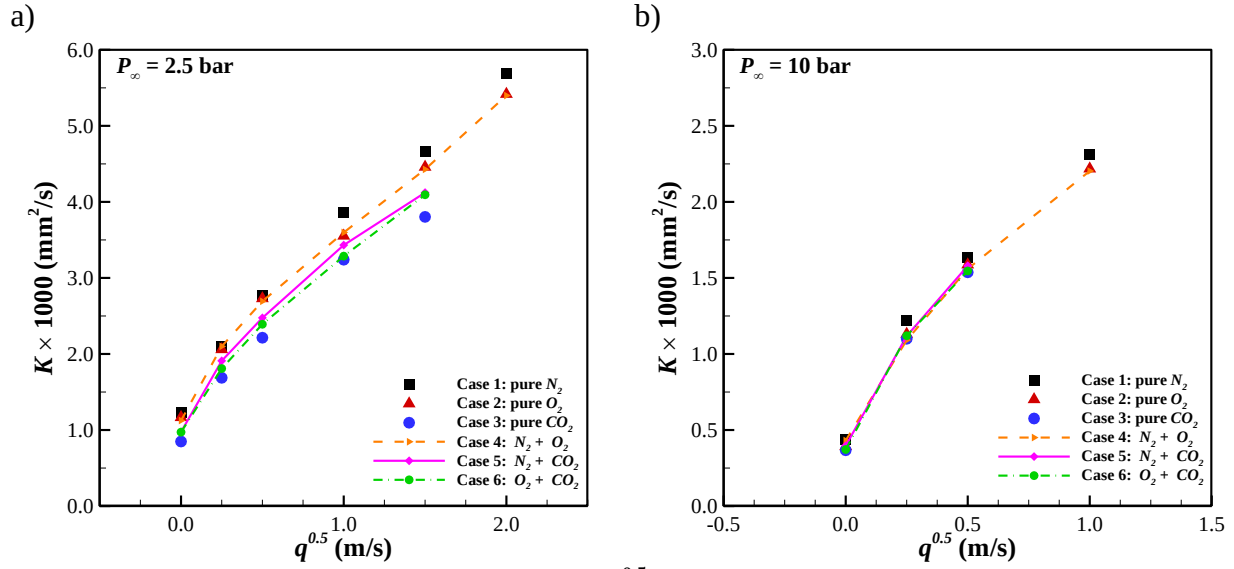


Figure 5-4. K as a function of $q^{0.5}$ at a) 2.5 bar and b) 10.0 bar.

To further investigate the effect of turbulence on butanol droplet evaporation rate under different ambient compositions, the value of K is normalized by K_0 , which represents the evaporation rate under stagnant environment for the corresponding ambient condition. This term is called turbulence effectiveness. The values of K presented herein are calculated from the average of a minimum of four separate experiments at the same test conditions. Fig. 5-5 confirms that turbulence effectiveness continues to increase for butanol droplet similar to what is observed for alkane fuels and ethanol [26]. Furthermore, this figure shows that higher pressures enhance the effectiveness of turbulence across all ambient compositions, consistent with previously reported data on hydrocarbon fuels [35] and butanol in N_2 environment [36]. Notably, this trend is observed consistently across all explored ambient compositions. This behavior arises because elevated pressure suppresses mass diffusion, which in turn reduces K . Under such conditions, turbulence plays a more dominant role by enhancing the interaction between the droplet and surrounding gas, thereby exerting a greater impact on the evaporation process. As demonstrated in Fig. 5-5, the impact of turbulence becomes more significant with a heavier ambient gas. As shown in this figure,

under pure ambient conditions, the effectiveness of turbulence is highest for CO_2 , followed by O_2 and then N_2 . For binary ambient mixtures, the effectiveness of turbulence is also greater in ambient mixtures containing CO_2 and O_2 , which have higher molecular weights. It should be noted that the same trend is observed across the other explored pressure conditions.

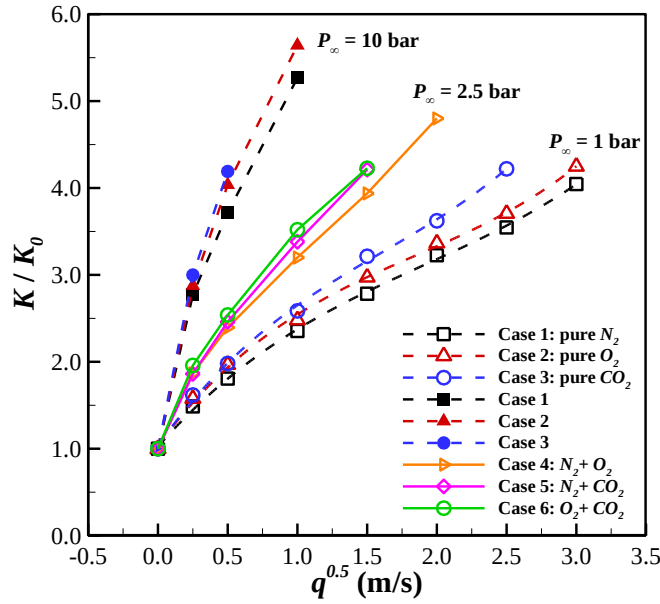


Figure 5-5. Butanol normalized evaporation rate a function of $q^{0.5}$ in different ambient compositions and various pressure levels

5.4.3 Correlations

Two semi-empirical correlations are available for predicting the normalized vaporization rate of a single droplet in turbulent flow. The first correlation uses the vaporization Damköhler number, Da_v , defined as the ratio of the characteristic time scale of the turbulent flow (t_{flow}) to that of droplet vaporization (t_{vap}). It is expressed as:

$$Da_v = \frac{t_{flow}}{t_{vap}} = \frac{d_0/q^{0.5}}{r_0/V_r} = \frac{d_0/q^{0.5}}{r_0/((\rho_l/\rho_v)(K_0/4d_0))} = \frac{1}{2} \left(\frac{\rho_l}{\rho_v} \right) \left(\frac{K_0}{d_0 q^{0.5}} \right) \quad (5-1)$$

where V_r denotes the radial velocity, which is determined based on the continuity of mass between the liquid and vapor phases at the droplet surface, and ρ_l and ρ_v are the liquid and vapor densities.

The second form of correlation is based on the turbulent Reynolds number and Schmidt number expressed as:

$$Re_{t,d_0} = \frac{q^{0.5} d_0}{v_g}, \quad Sc = \frac{v_g}{D_{AB}} \quad (5-2)$$

where v_g , refers to the kinematic viscosity of the surrounding gas and D_{AB} is the binary diffusion coefficient characterizing mass transfer between the ambient gas and the vaporized fuel. While it has been shown that these correlations hold true for butanol droplets with different sizes (from 300 to 700 μm) in turbulent (up to 1.5 m/s), elevated-pressure N_2 environment (1–10 bar) [37]. The present work extends that baseline by examining whether the same relationships remain valid for higher turbulent intensity levels (up to 3.0 m/s) and different ambient gases other than N_2 .

Figures 5-6a and 5-6b demonstrate that all data points collapse onto the relationships defined by Eqs. (5-3) and (5-4), regardless of the turbulence intensity level, ambient pressure or ambient composition, thereby confirming the validity of these correlations.

$$\frac{K}{K_0} = 1.0 + 0.0948 Da_v^{-0.763} \quad (5-3)$$

$$\frac{K}{K_0} = 1.0 + 0.0479 Re_{t,L}^{0.66} Sc^{1.16} \left(\frac{L}{d_0} \right)^{-0.53} \left(\frac{T_\infty}{T_0} \right)^{-1.42} \left(\frac{P_\infty}{P_0} \right)^{-0.19} \quad (5-4)$$

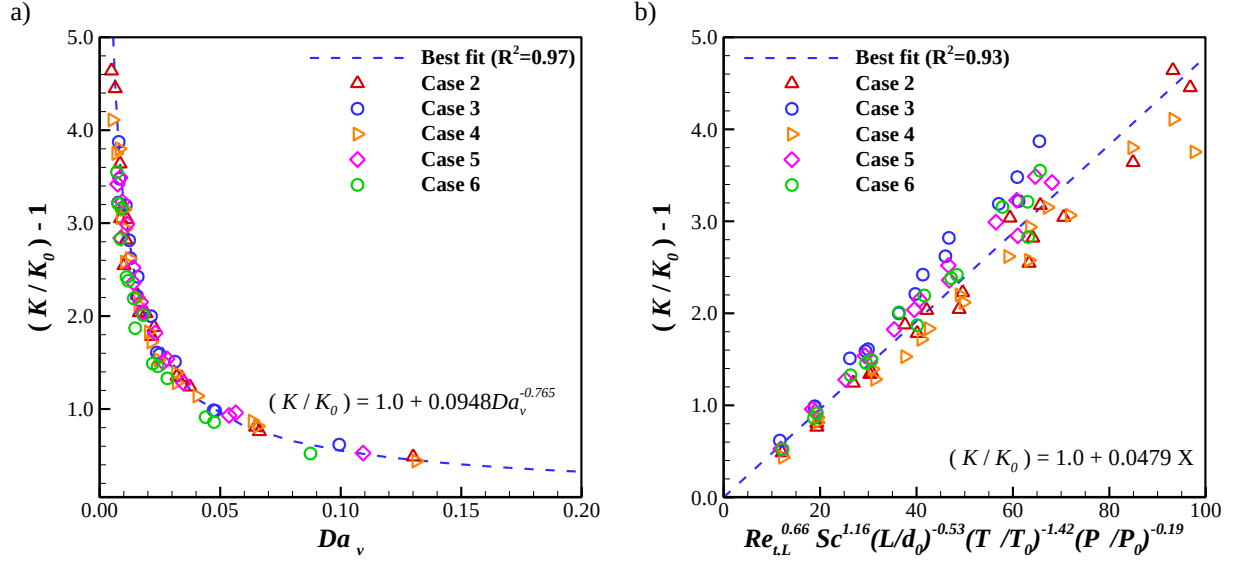


Figure 5-6. Turbulence effectiveness versus a) the vaporization Damköhler number, and b) the Reynolds – Schmidt correlation.

As illustrated in Fig. 5-6a, a clear trend emerges where smaller Damköhler numbers correspond to stronger turbulence influence on droplet evaporation. Larger Da_v , is generally associated with fuels possessing high volatility, due to their inherently short vaporization time scales and consequently less effective turbulence. On the other hand, Fig. 5-6b indicates that turbulence effectiveness increases linearly with turbulent Reynolds number.

5.5 Conclusions

This study experimentally examined the influence of ambient-gas composition on the vaporization behavior of single butanol droplets. Six ambient conditions were considered, comprising pure and binary mixtures of N_2 , O_2 , and CO_2 . Experiments were performed in a specially designed facility capable of generating an isotropic and homogeneous turbulence with near-zero mean velocity flow field. Key turbulence parameters, including turbulence intensity and length scales, were systematically characterized and correlated with ambient composition, pressure and fan speed. Throughout the experiments, the droplet diameter was maintained at 500 μm , while the ambient

turbulence and pressure were, respectively, varied up to 3.0 m/s and 10 bar at room temperature. The main conclusions are summarized below.

- The temporal evolution of the normalized droplet diameter exhibits an approximately linear trend, confirming that the classical d^2 -law remains valid across all tested conditions, regardless of ambient gas composition.
- The butanol droplet evaporation rate, K , is sensitive to the ambient-gas composition. In pure environments, K is significantly reduced in CO_2 and slightly decreased in O_2 compared to N_2 . This trend is explained by differences in thermophysical properties including specific heat capacity, thermal conductivity, and viscosity. In binary ambient mixtures, the evaporation rate was consistently observed to fall between the values corresponding to the respective pure gases. More specifically, the value of K in equal binary mixtures tended to be closer to that of the heavier constituent gas.
- The presence of turbulence is shown to reduce the sensitivity of K to ambient-gas composition by promoting convective heat and mass transfer while minimizing the role of molecular diffusion, which is more strongly influenced by the type of ambient species. Similarly, increasing the ambient pressure further diminishes the impact of composition on K by lowering vapor diffusivity.
- Turbulence effectiveness, K/K_0 , becomes more pronounced at elevated pressures and continues to increase with higher turbulence intensities. This effect is particularly notable in environments with heavier ambient gases.
- Finally, existing correlations based on the Damköhler and turbulent Reynolds number, were evaluated and shown to accurately predict the butanol vaporization rate across all tested ambient compositions, turbulence intensities and pressures.

All in all, the results of this study reveal that there exists a clear association between the flow nature, ambient pressure, and ambient gas composition on the evaporation behavior of butanol droplets. Under quiescent and low-pressure conditions, the ambient gas composition has a significant impact on the butanol droplet vaporization. However, this effect becomes less pronounced as ambient turbulence intensity and pressure increase. This finding is particularly useful for practical applications such as EGR strategies in compression ignition engines. It should be noted that this experiment was conducted under room temperature. Thus, further studies to include high ambient temperatures are recommended to better understand the interplay between thermal effects, turbulence, pressure and ambient composition on droplet vaporization. Moreover, this study considered only the effects of three main components of exhaust gases on the evaporation rate. Future investigations into the influence of other engine exhaust species, such as water vapor, unburned hydrocarbons, and carbon monoxide, can provide further insight into this topic.

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Chapter 6: Conclusions and recommendations for future research

A summary of the findings of this research is presented below, followed by some suggested future research directions.

6.1 Research summary and major findings

To assist in the search for clean alternative liquid fuels for future combustion engines, this study presents an experimental investigation of the evaporation and combustion characteristics of single butanol droplet in turbulent, high-pressure environments. To accomplish this, a homogeneous isentropic turbulence flow field with negligible mean velocity was generated in the central region of a high-pressure spherical chamber. Turbulent flow characteristics, such as turbulence intensity and integral length scale, were measured and their relationships with ambient pressure and fan speeds are specified. The following are the main key conclusions of this research.

6.1.1 Validity of d^2 -law

The results from both evaporation and combustion experiments confirm the general validity of the d^2 -law under all tested conditions. In the evaporation tests, plots of normalized droplet size versus time exhibited a quasi-linear relationship throughout most of the droplet's lifetime, despite noticeable deviations toward the end of the lifetime, which became more pronounced with increasing ambient pressure and turbulence intensity. Nevertheless, the linear portion of the droplet lifetime remains largely sufficient for calculating the vaporization rate according to the classical d^2 -law.

Similarly, in single-droplet combustion tests, the temporal evolution of the normalized square of the droplet diameter also exhibited a quasi-linear behavior under all explored conditions. Nonlinearity was observed in cases where temporary luminous extinction occurred. This observation suggests that the d^2 -law remains valid for droplet combustion, particularly when a flame is present around the droplet.

6.1.2 Effect of ambient turbulence and pressure

- *Droplet evaporation*

This study demonstrates that under stagnant conditions, higher ambient pressures lead to a reduction in the vaporization rate of butanol droplets, resulting in an extended droplet lifetime. Two primary mechanisms are responsible for this behavior. First, at low ambient temperatures and quiescent environment, droplet evaporation is predominantly governed by mass diffusion. Elevated pressure suppresses this diffusion by lowering the fuel vapor mass fraction near the droplet surface, thereby hindering the vaporization process. Second, increasing the ambient pressure raises the droplet surface temperature, which in turn reduces the temperature gradient between the droplet and its surroundings. This weakened temperature gradient diminishes the rate of heat transfer to the droplet, further contributing to the decline in the droplet's evaporation rate.

Under turbulent conditions, experimental findings demonstrated that turbulence significantly enhances the butanol droplet vaporization rate, leading to a reduction in droplet lifetime across all tested scenarios. Turbulence primarily promotes droplet vaporization by enhancing the transport of fuel vapor away from the droplet surface once it is generated. In addition, it intensifies convection around the droplet, thereby improving heat transfer toward droplet surface and ultimately increasing the rate of vapor production.

- ***Droplet combustion***

In the case of butanol droplet combustion, the results indicate that increasing ambient pressure (from 1 to 11 bar) enhances the burning rate across all examined conditions, including both stagnant and turbulent environments. This enhancement is accompanied by a more intense luminous flame, primarily due to pressure-induced soot formation and growth, which leads to a visibly brighter flame. The higher burning rate can be linked to the increased gas density at higher pressures, which raises the concentration of oxidizer molecules in the vicinity of the droplet, thereby promoting more efficient combustion. Furthermore, flame imaging reveals that elevated pressure reduces the flame stand-off distance—the distance between the droplet surface and the flame front. A shorter stand-off distance brings the flame closer to the droplet surface, enhancing heat transfer, and thus further accelerating the burning rate.

The influence of turbulence on the burning rate is strongly dependent on the ambient pressure conditions. At lower pressures (up to 3 bar), the presence of turbulence exerts minimal influence on the droplet burning rate. This limited effect can be attributed to two coupled mechanisms. First, the luminous visible flame formed around the droplet is very weak and poorly developed at low pressure. The absence of luminous flame reduces the heat transfer to the droplet, creating less favorable conditions for turbulence to induce significant changes in the burning rate. . Second, under these conditions, the transport of fuel vapor away from the droplet is primarily governed by molecular diffusion, which is further accelerated by the Stefan blowing effect — the outward radial flow generated by the continuous release of vapor during evaporation. Together, molecular diffusion and Stefan blowing dominate the vapor transport process, leaving little room for turbulence-enhanced diffusion to significantly alter the burning rate. In contrast, under higher pressure conditions, the droplet burning rate initially rises as the turbulence intensity increases.

This rise is attributed to both the strengthened role of turbulent mixing and the formation of a more defined radial flame shell, which facilitates improved heat transfer toward the droplet surface. However, as turbulence intensity continues to increase beyond a certain point, burning rate begins to decline. This reduction is linked to the emergence of temporary luminous extinction (TLE) events. As the frequency and duration of TLE increase with higher turbulence levels, the burning rate continues to fall, ultimately reaching conditions where droplet ignition becomes significantly challenging.

6.1.3 Effect of droplet size

This research shows that the effect of droplet diameter/size on the evaporation rate is highly dependent on both the ambient pressure and turbulence. Under quiescent conditions at atmospheric pressure, droplet size exhibits minimal influence on the evaporation rate. However, larger droplets exhibit higher evaporation rate at elevated pressures. This trend is primarily attributed to the enhanced role of natural convection, which becomes increasingly significant with large droplet sizes and elevated ambient pressures. As pressure increases, the associated rise in the Grashof number intensifies buoyancy-driven flow around the droplet, thereby promoting vapor mass diffusion and thus accelerating evaporation.

More importantly, in the presence of turbulence, the impact of droplet size becomes more pronounced across all tested pressure conditions. Larger droplets respond more effectively to turbulent eddies, leading to stronger mixing and improved heat and mass transfer at the droplet surface. This interaction between turbulence and droplet size results in a consistently higher vaporization rate for larger droplets, with the enhancement becoming increasingly significant as turbulence intensity rises.

6.1.4 Effect of fuel type

A comparative analysis of the vaporization behavior of butanol droplets with heptane and decane revealed that the vaporization rate of butanol consistently falls between those of these two fuels, with a closer resemblance to decane across all explored test conditions. Furthermore, the study confirms that the influence of turbulence on enhancing the vaporization rate is more significant for fuels with lower vapor mass diffusivity and higher thermal diffusivity. Contrary to the common assumption that turbulence affects more strongly less volatile fuels, the present findings demonstrate that droplet vaporization is more responsive to turbulence when vapor diffusivity is low.

As for combustion, the burning rate of butanol droplets was consistently lower than that of heptane under quiescent conditions across all tested pressures. However, this difference diminished with increasing turbulence intensity, and the burning rates of both fuels became comparable under highly turbulent and pressure conditions. These findings suggest that, under high-pressure and high-turbulence regimes, the burning rate may become largely independent of fuel type. Nonetheless, further investigations involving a broader range of fuels and higher pressures are necessary to validate this hypothesis.

6.1.5 Effect of ambient gas composition

- *Droplet evaporation*

The results demonstrate that ambient gas composition plays a significant role in governing the evaporation rate of butanol droplets. Among the pure gases tested, N_2 consistently yields the highest evaporation rate, followed closely by O_2 , while CO_2 results in a significantly slower evaporation. The suppressive effect of CO_2 is primarily due to its higher specific heat capacity,

which allows it to absorb more thermal energy and delays heat transfer to the droplet surface. Additionally, its lower thermal conductivity and viscosity further hinder heat and mass transfer, leading to prolonged droplet lifetimes. These effects are especially pronounced under stagnant conditions, where natural convection is reduced due to the high density of CO_2 , suppressing buoyancy-driven flow around the droplet and further slowing the evaporation. In contrast, under turbulent flow conditions, enhanced mixing weakens the influence of gas properties, reducing the disparity between gases, although CO_2 still maintains, overall, the lowest evaporation rate.

When examining binary mixtures of ambient gases, the evaporation rate of butanol droplets consistently falls between those observed in the corresponding pure gases. However, the influence of the heavier gas tends to dominate the evaporation behavior. For example, in equal mixtures of N_2 and CO_2 , the evaporation rate is noticeably closer to that in pure CO_2 than in pure N_2 . This trend suggests that the thermophysical characteristics of the heavier component have a stronger impact on the droplet evaporation. Overall, both pure and mixed gas environments show that the thermal and transport properties of the surrounding/ambient gases significantly affect droplet vaporization, and turbulence acts to moderate these differences by enhancing convective transport.

- ***Droplet combustion***

The results showed that the burning rate of butanol droplets is strongly influenced by the concentrations of O_2 and CO_2 . The effects of these gases on the burning rate are investigated separately, with O_2 varied from 18% to 30% and CO_2 from 0% to 41%, while the remainder of the ambient composition was N_2 . Increasing the oxygen concentration in the ambient leads to a consistent enhancement in the burning rate across all test conditions. At low ambient pressures, this improvement follows an almost linear trend, as higher oxygen levels reduce the flame standoff

distance and consequently improve heat transfer toward the droplet surface, thus promoting faster burning. This effect becomes more pronounced under turbulent flow and elevated pressure environments, where oxygen enrichment helps stabilize the flame and prevents flame extinction events. However, beyond a certain oxygen concentration, especially at high pressures, further increases in oxygen yield diminishing returns. This is due to the already high density of oxidizer molecules at elevated pressures and the increased role of heat loss mechanisms such as radiation and conduction, which limit the additional benefit of oxygen enrichment. In low-oxygen environments, turbulence tends to weaken combustion due to the increased frequency of flame extinction events, making the burning process less efficient.

On the other hand, the addition of carbon dioxide to the ambient gas mixture has a clear suppressive effect on the burning rate of butanol droplets. This is primarily due to the reduced thermal conductivity of CO_2 containing mixtures, which weakens heat transfer from the flame to the droplet and thus lowers the burning rate. Even moderate concentrations of carbon dioxide can significantly impair combustion performance. Furthermore, CO_2 increases the flame standoff distance, and thus diminishing flame strength and stability. Overall, CO_2 acts as a combustion suppressant, limiting both flame intensity and droplet burning rate.

6.2 Recommendations for future studies

There are still many areas of research on butanol droplet evaporation and combustion which require further studies. Some research directions are highlighted below.

6.2.1 Binary component droplet evaporation

One possible solution to partially solve the utilization of fossil fuels in CIEs is the use of butanol as a potential alternative to partially substitute traditional diesel. A wealth of literature has explored the use of blends of butanol – diesel in different types of CIEs, and the findings are succinctly

outlined in recent reviews [1-3]. Regarding engine performance, butanol – diesel blends, when compared to only diesel, exhibit lower brake power [4], higher specific fuel consumption [1], and slightly higher brake thermal efficiency [5]. Concerning emissions, the utilization of a butanol-diesel blend can markedly reduce NO_x , PM, and CO emissions, albeit with a slight rise in unburnt hydrocarbon levels [2]. Using a blend of butanol and diesel in advanced CIEs also yields promising results. For instance, it has been found that using butanol - diesel blends in partially premixed compression ignition and homogeneous charged compression ignition engines resulted in higher indicated thermal efficiency [3].

While numerous diesel engine tests with higher alcohol blends have been performed [6], there is significantly less data available on the fundamental processes of droplets evaporation and combustion [7]. Understanding the evaporation and combustion characteristics of binary-component fuel droplets is essential for advancing the application of biofuels in CIEs. Most of the existing studies on butanol-based blends have been conducted under simplified and stagnant conditions that do not represent the high-pressure and turbulent environments present in practical CIEs. Since the ignition delay in CIEs is strongly influenced by the interplay between physical and chemical processes, studying binary droplets under or realistic operating conditions can yield valuable insights into optimizing combustion phasing, improving fuel-air mixing, and reducing pollutant emissions.

Diesel fuel comprises a complex mixture of hydrocarbons with diverse physical properties, varying globally based on crude oil sources, refining processes, and regulations [8]. To streamline research, some studies have employed dodecane as a surrogate fuel to characterize diesel, given its comparable thermo-physical properties [9], while others have opted for hexadecane for the same purpose [10-12]. For future investigations, it is recommended to use n-dodecane as the base fuel

component to pair with butanol. Note that n-dodecane is widely recognized as a reliable diesel single-component surrogate due to its comparable thermophysical properties, such as density, viscosity, and surface tension, as well as its molecular structure and carbon chain length [13].

6.2.2 Ignition delay

As previously mentioned, published studies have identified challenges associated with prolonged ignition delay in CI engines fueled with butanol [14]. This longer ignition delay can contribute to higher unburned hydrocarbon emissions and lower thermal efficiency [15].

Studying spray auto-ignition in a complex turbulent environment, influenced by air inflow, spray injection, and the high-speed motion of a piston, presents significant challenges [16]. To ease this complexity, a developed spray can be conceptualized as an ensemble of droplets. Each droplet, representing a basic heterogeneous system [17], exhibits physical and chemical processes that are analogous to those occurring in a spray [18]. Consequently, investigating the auto-ignition process of a single droplet is not only meaningful but also fundamental to understanding spray auto-ignition.

Numerous studies have presented experimental data on droplet ignition under various conditions. Two widely used methods include the freely moving droplet technique and the suspended droplet technique. The former involves either a droplet freely falling within a furnace or injected into a heated gas stream [19]. For the suspended droplet technique, a droplet held by a fiber is subjected to a hot environment within a preheated furnace [20-22]. All the aforesaid scenarios require a very hot environment, which is not realizable with the current setup in the Energy and Combustion Laboratory (ECL) at the University of Manitoba. However, in some other investigations droplet ignition is caused by an external source, such as a laser beam [23-24], a hot wire [25-26], or a heated coil [18, 27-28]. Based on these studies, it is recommended to investigate the ignition delay

of a butanol droplet using the available ignitor in ECL that has been previously used in butanol droplet combustion experiments ([Chapter 4](#)).

6.2.3 Effect of Fuel Properties

The present study has provided new insights into the influence of fuel type on droplets evaporation and combustion characteristics. Contrary to the common belief that turbulence exerts a greater impact on the less volatile fuels, the present findings indicate that turbulence has a stronger influence on fuels with the lowest vapor diffusivity and highest thermal diffusivity. Additionally, the results suggest that, under high-pressure and intense turbulence conditions, the burning rate of single droplets may become largely independent of fuel type.

To validate this hypothesis, future research should investigate a broader range of fuel types and conduct experiments under more representative engine-like conditions, specifically involving higher ambient pressures and temperatures. Such studies would be instrumental in confirming the observed trends and improving the applicability of these findings in practical combustion systems.

6.2.4 Effects of neighbouring droplets

In engines, liquid fuel is atomized in the combustion chamber as a spray to create a combustible mixture with air [29]. Dense spray forms close to the atomizer and becomes dispersed/diluted farther downstream of the injector. While the distance between droplets surpasses the average droplet diameter in the diluted spray region [30], droplets interaction may still persist and can significantly affect the evaporation process, especially in the spray near-field region. To explore the effects of droplets interaction on the spray overall evaporation process, various configurations have been examined in the literature, including (i) a stream of droplets (e.g., [31-33]), (ii) a cluster of droplets (e.g., [34-36]), (iii) a cloud of droplets (e.g., [30, 37-39]), and (iv) a droplet surrounded by vapor background (e.g., [40-45]). To shed more light on this topic a similar configuration

involving a droplet surrounded by a vapor-rich environment has also been investigated by our group for pentane droplet [46]. In This investigation, we showed the combined effect of background vapor, pressure, and turbulent flow field on the variation of the vaporization rate. For future studies, it is recommended to examine the evaporation and combustion behavior of a droplet group and compare the findings with existing literature to distinguish the influence of background vapor from that of neighboring droplet interactions. This investigation requires modifications to the current droplet suspension technique and the droplet injection method available in ECL. A review of the literature indicates that several configurations have been proposed, although each has its own limitations. For example, Xu et al. [47] employed an approach in which droplets are generated on a frame outside the chamber and the entire frame is then inserted through one of the large windows. However, this technique may restrict studying the effect of elevated pressure conditions. Another possible approach involves creating a free falling droplet stream [31], but this approach is limited by the narrow imaging area. Further investigation is required to determine whether the evaporation rate can be evaluated based on a limited number of images of the droplet's lifetime during free falling.

6.3 References

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Appendix A: Turbulent flow field characterization using PIV

This section provides a brief explanation about the result of turbulent flow characterizations.

A.1. Particle image velocimetry

The two-dimensional, two-component particle image velocimetry (2D2C-PIV) technique was employed to characterize the turbulent flow field inside the chamber. Measurements were limited to the central region of the chamber, where the field of view was approximately $90 \text{ mm} \times 90 \text{ mm}$. This constraint was due to the chamber's large geometry, thick window, the fixed position and size of the optical access ports, and the importance of the chamber center, which serves as the primary location for droplet evaporation and combustion studies.

For this thesis, PIV tests were conducted under different ambient pressures and at various fan speeds. It is important to note that the initial measurements were taken with all eight axial fans and in the absence of any obstructions (i.e., the chamber was empty). A summary of the turbulence characteristics is provided in Table A1, which presents average values calculated over a circular region with a 5 mm radius at the center of the chamber.

Table A1. Summary of turbulence characteristics with empty chamber

conditions	Pair images	$U(m/s)$	$V(m/s)$	$U/U_{rms}(\%)$	$V/V_{rms}(\%)$	$U_{rms}/V_{rms}(\%)$	$V/q^{1/2}(\%)$
1 bar – 200 rpm	8000	-0.0027	0.0068	3.73	9.28	99.24	8.22
1 bar – 400 rpm	8000	-0.0171	-0.0003	11.52	0.61	96.50	9.26
1 bar – 600 rpm	8000	0.0054	-0.0037	2.38	1.55	95.43	2.33
1 bar – 800 rpm	8000	-0.0049	0.0008	1.57	0.86	98.11	1.54
1 bar – 1000 rpm	8000	0.0007	0.0047	0.43	1.16	96.78	1.12
1 bar – 2000 rpm	8000	-0.0052	-0.0013	0.72	0.68	96.11	0.87
11bar – 200 rpm	8000	-0.0091	0.0007	10.9	1.15	97.23	8.83

As shown in Table A1, the average mean velocities are negligible in comparison to the root-mean-square (RMS) velocity fluctuations, indicating that the central region of the empty chamber effectively maintains a zero mean velocity condition.

While a single PIV run is limited to a maximum of 2000 image pairs, combining data from multiple runs can improve the convergence of turbulence statistics, as demonstrated in the results presented in Table A1. However, given the constraints on processing time and data storage, it is deemed sufficient to minimize the number of image pairs as long as statistical reliability is preserved. A comparative analysis showed that the root-mean-square (RMS) velocity fluctuations obtained from 8000 image pairs deviated by less than 5% and 4% from those derived using only 2000 pairs, for fan speeds of 200 and 2000 RPM, respectively, within the central ± 10 mm region. Based on this observation, the rest of PIV datasets in this study were acquired using 2000 image pairs per test condition.

To evaluate the impact of various internal components on the flow field characteristics, several chamber configurations were tested. The experimental conditions are defined as follows:

- 1- Chamber with Heater, Frame, Injector (HFI)
- 2- Chamber with Heater, and Injector (HI)
- 3- Chamber with Frame, and Injector (FI)

All tests were conducted at atmospheric pressure and at varying fan speeds. Table A2 provides a quantitative comparison of the turbulence characteristics for each configuration. The reported values represent spatial averages within a 5 mm diameter circle at the geometric center of the chamber.

Table A2. Summary of turbulence characteristics for different component configurations at 1 bar

Condition	Fan Speed (RPM)	$U(m/s)$	$V(m/s)$	$U / U_{rms} (%)$	$V / V_{rms} (%)$	U_{rms} / V_{rms}	$V / q^{1/2} (%)$
HFI	1000	0.038	-0.022	10.74	5.91	0.98	10.02
	2000	0.074	0.033	9.93	4.24	0.95	8.74
	3000	0.027	-0.016	2.45	2.04	0.94	2.65
	4000	0.102	0.016	10.57	1.18	0.93	8.37
	5000	0.108	-0.030	5.54	1.53	0.95	4.70
HI	1000	0.021	-0.015	5.31	3.66	1.003	5.32
	2000	0.094	-0.022	10.69	2.64	0.94	9.62
	3000	0.111	0.044	9.11	3.44	0.96	7.86
	4000	0.139	0.003	8.46	0.66	0.99	6.93
FI	1000	-0.019	-0.022	5.43	5.72	0.93	6.5
	2000	0.075	-0.029	9.79	3.57	0.95	8.41
	3000	0.048	-0.047	4.23	3.80	0.93	4.76
	4000	0.083	0.027	5.30	1.80	0.96	4.6

The results indicate that the influence of these internal components on the flow field is minimal. Across all tested conditions, the mean velocities remain below 10% of the corresponding velocity fluctuations, confirming that mean flow is negligible relative to the corresponding fluctuating flow field. Additionally, both anisotropy and inhomogeneity are maintained within 10%, indicating that the flow field retains an acceptable degree of homogeneity, isotropy, and low mean velocity, even in the presence of the frame, injector, and heater.

A.2. Effect of ambient composition

So far, the PIV results were obtained with air as the ambient gas. To investigate the effect of ambient composition on turbulent characterization, a series of PIV tests were performed in an N_2 or CO_2 ambience. For these tests, the chamber was first evacuated to ensure it is empty, and then the desired gas was introduced until the target pressure was reached. The spatial average of the statistics are summarized in Table A3. This spatial averages is within a 5 mm diameter circle at the geometric center of the chamber. The results show that changing the ambient composition does

not alter the main characteristics of the turbulent flow field. The table indicates that the mean velocity components are negligible compared to the turbulent velocity fluctuations confirming that the nearly zero mean velocity condition is still maintained at the center of the chamber. Moreover, under both ambient compositions, the chamber exhibits a high degree of isotropy (quantified by $U_{rms}/V_{rms} \sim 1.0$). Finally, the flow demonstrates a high level of homogeneity in this region, where the variation in $q^{0.5}$ relative to its local average remains below 5%.

Table A3. Summary of turbulence characteristics for different ambient compositions

Ambient Composition	Pressure	Fan Speed (RPM)	U / U_{rms} (%)	V / V_{rms} (%)	U_{rms} / V_{rms}	$V / q^{1/2}$ (%)
N_2	1 bar	1000	7.76	2.57	0.9779	6.63
		1000	10.78	5.34	0.977	9.8
		3000	7.68	2.6	0.9656	6.63
		3000	0.82	5.22	0.9701	4.41
		5000	2.61	0.86	0.9836	2.34
		5000	0.96	1.56	0.9324	1.63
		5000	3.5	1.01	0.9902	3.05
	5 bar	1000	2.23	2.26	0.9421	3.02
		2000	2.16	2.35	0.9805	2.72
		2000	0.62	2.74	0.964	2.38
		2000	0.64	1.2	0.9937	1.19
CO_2	1 bar	1000	14.37	1.57	0.9561	11.57
		5000	3.97	1.21	0.9306	3.32
		5000	3.06	3.36	0.97	3.78
	5 bar	1000	2.26	2.41	0.9815	2.93
		2000	5.73	2.2	0.9567	4.97
		2000	3.65	1.94	0.99	3.49

A.3. PIV measurement uncertainty

Quantifying the overall uncertainty in PIV measurements is a challenge, which is due to the intricate interplay between measurement errors and numerous experimental parameters [1]. Some potential error sources can be dismissed due to their minimal impact on measurements. In this study, for example, tracer-particle slip can be considered negligible because the Stokes number—defined as the ratio of the particle relaxation time to the Kolmogorov time scale—remains below 0.01 for all operating conditions, which is well below published threshold [2]. The sources of error in the calculation of instantaneous velocity are as follows:

$$U_i = \left(\frac{\Delta x_i}{\Delta t} \frac{\delta d_r}{\delta M} \right) \quad (\text{A-1})$$

An overall magnification uncertainty, δM , on the order of 0.01 ($\approx 1\%$) is considered realistic when accounting for contributions such as the finite thickness of the laser sheet, minor angular misalignment, and variations in the positioning of the calibration rod. Timing errors, Δt , associated with a properly synchronized commercial Nd:YAG laser are generally insignificant [3], and uncertainties related to pixel pitch, δd_r , can also be disregarded [4]. Consequently, the dominant contribution to the measurement uncertainty arises from the estimation of particle-image displacement, Δx_i , which is expected to exceed the uncertainties of the other influencing factors. Uncertainty in the measured particle-image displacement, Δx_i , is commonly reported to be on the order of 0.1 pixels [5]. The preliminary assessment in [4] suggests that a similar magnitude of displacement uncertainty is appropriate for the present study. This type of error is predominantly random, and its influence can be reduced by increasing the number of samples used in the ensemble averaging process [4].

References

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Appendix B: Image processing analysis

For image processing analysis, the algorithm developed based on strategies proposed in [1], begins by cropping the image to exclude the retracted injector from the initial frames. The cropped image, containing only the droplet and support fibers, undergoes thresholding to generate a binary representation. Thresholding assigns pixel intensities below a specified limit (the threshold) to zero (black/background) and those above the threshold to one (white/foreground). The threshold value is determined using MATLAB's *graythresh* function, which employs Otsu's method to compute a global threshold.

Then, a morphological image processing technique called *opening* is applied to remove the support fibers. In image processing terminology, opening involves sequential erosion and dilation operations. Horizontal and vertical line structuring elements are used in this step to effectively eliminate the fibers while preserving the droplet's integrity. The resulting image is a binary representation of the nearly spherically shaped droplet.

Finally, the droplet diameter, d , is calculated by counting the number of foreground (droplet) pixels, N_{px} , and performing a single calculation as

$$d = \left(\frac{4}{\pi} \frac{N_{px} d_r^2}{M^2} \right) \quad (\text{B-1})$$

where M is the magnification and d_r is the pixel pitch of the camera sensor. More details about this method along with the MATLAB code is available in [2].

B.1. Uncertainty analysis

Uncertainty in droplet image processing affects the measured diameter and, consequently, the evaporation rate. The main sources of error arise from three factors. First, non-spherical droplets introduce geometric deviations, as any departure from a perfect sphere results in slight variations in the measured diameter. Second, camera calibration contributes to uncertainty because inaccuracies in the pixel-to-length conversion directly affect instantaneous diameter measurements. Finally, edge detection introduces error due to sensitivity to image contrast and thresholding, which can affect the precise identification of droplet boundary.

- Droplet sphericity

This research shows that both the cross fiber and single-fiber, with node, techniques, largely preserve droplet sphericity when used with sub -1 mm droplets. However, in highly turbulent environments, aerodynamic forces can cause droplets to deviate from a spherical shape. Additionally, adhesion at the droplet-node interface introduces slight asymmetry. Since the equivalent diameter calculation assumes that droplet image represents the projection of a perfect sphere, deviations such as ellipsoidal distortions can slightly effect accuracy.

To account for this, each processed image can be evaluated for circularity, which serves as a necessary (though not entirely sufficient, due to the two-dimensional nature of the image) indicator of sphericity. The circularity C , is calculated using the following equation:

$$C = \left(\frac{4A_s\pi}{P^2} \right) \quad (B-2)$$

when C is equal to unity, it corresponds to a perfect circle. Droplet images within the curve-fitting range consistently show circularity values above 0.9, indicating that any deviations from perfect sphericity have a minimal impact on the accuracy of the results.

- Camera calibration

As demonstrated in Eq. (B-1) droplet diameter is inversely proportional to the magnification factor.

The magnification is defined as follows:

$$M = \left(\frac{d_r \overline{N_{pixel}}}{d_c} \right) \quad (B-3)$$

where N_{pixel} represents the number of pixels corresponding to the diameter of the calibration object, d_c . The overline notation indicates that the reported value is the average obtained from several independent calibration measurements.

The uncertainty in the calibration object's diameter is taken as the resolution of the micrometer used for its measurement, giving $\delta d_c = 2.54 \mu\text{m}$. For the ball bearing used in this study, which has a diameter of $498 \mu\text{m}$, this corresponds to a fractional uncertainty of $(\frac{\delta d_c}{d_c} = 0.005)$ or approximately 0.5%.

N_{pixel} was determined by averaging the results from multiple independent placements of the calibration object. The corresponding uncertainty, δN_{pixel} was calculated from the standard deviation, σ , of these measurements and expressed using a 95% confidence interval ($Z_c = 1.96$).

By applying this procedure, the fractional uncertainty, $(\frac{\delta N_{pixel}}{N_{pixel}})$ is found to be less than 0.005 (0.5%). Therefore, the overall uncertainty of the magnification calculation is determined using Eq. (B-4) and is expected to be approximately 1%.

$$\frac{\delta M}{M} = \sqrt{\left(\frac{\delta d_c}{d_c} \right)^2 + \left(\frac{\delta N_{pixel}}{N_{pixel}} \right)^2} \quad (B-4)$$

- Edge detection

To quantify Uncertainty associated with edge detection, each droplet image was processed using two independent thresholding approaches. In the first method, the threshold level was selected automatically using Otsu's algorithm, which provides an optimal data-driven estimate and is therefore used to obtain the reported droplet diameter. In the second method, a fixed, intentionally high threshold value (for example, 0.95 in normalized intensity) was applied to preserve nearly all detectable edge pixels. The diameter computed using this high threshold represents an upper bound for the droplet size extracted from the image. The difference between the diameter determined by Otsu's method and that obtained using the elevated threshold provides an estimate of the maximum possible error associated with edge detection. For instance, if Otsu's threshold yields a diameter of 500 μm , whereas applying a threshold of 0.95 results in a diameter of 525 μm , the discrepancy of 25 μm corresponds to an uncertainty of approximately 5% (25/500). This approach offers a practical means of assessing the sensitivity of the measured diameter to the thresholding technique. Table B1 presents representative examples from the worst-case conditions, corresponding to the highest pressure and turbulence intensity examined in this study, in order to evaluate the relative uncertainty. As shown in the table, the relative uncertainty associated with edge detection remains below 2% for the cases listed, and this level of accuracy is consistent across all other experimental conditions.

Table B1. Relative uncertainty of edge detection for different cases

Test conditions	$d_{otsu} (\mu\text{m})$	$d_{0.95} (\mu\text{m})$	$ (d_{otsu} - d_{0.95})/d_{otsu} \%$
$P = 10 \text{ bar}, q^{0.5} = 1.0 \text{ m/s}$	485	490	1.03
$P = 10 \text{ bar}, q^{0.5} = 1.0 \text{ m/s}$	487	492	1.02
$P = 1 \text{ bar}, q^{0.5} = 3.0 \text{ m/s}$	503	507	0.79
$P = 1 \text{ bar}, q^{0.5} = 3.0 \text{ m/s}$	516	520	0.77

References

- [1] C. Solomon and T. Breckon, Fundamentals of Digital Image Processing: A Practical Approach with Examples in MATLAB, *John Wiley & Sons* (2011).
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Appendix C: Considerations regarding the fibers

In this thesis, it is repeatedly asserted that the effect of silicon carbide (SiC) fibers on the evaporation and burning rates is negligible. To support this assertion, this section further examines the influence of fiber size on droplet size determination and its conductive effect on the combustion process.

C.1. Fiber size

To investigate the effect of fiber size on the measurement of droplet size, the volume function $V(d)$ is defined as the ratio of the fiber volume within the droplet (V_f) to the total initial droplet volume (V_d).

$$V(d) = \frac{V_f}{V_d} = \frac{2 \times d_0 \times (\pi d_f^2 / 4)}{(4/3) \pi r_0^3}$$

Here d_f denotes the diameter of SiC fiber ($d_f = 14 \mu\text{m}$), while d_0 and r_0 represent the initial droplet diameter and radius, respectively. In this thesis, d_0 is varied and takes values of 300 μm , 500 μm , 700 μm . Note that this volume function is less than 2% under all the test conditions explored in this thesis. Furthermore, in the most restrictive case, the vaporization rate was evaluated only until the normalized squared droplet diameter reached 0.25, $(d^2/d_0^2) \sim 0.25$, at which point the droplet volume function $V(d)$ corresponds to less than 3% of the initial volume.

Therefore, it can be concluded that the combined volume of the two fibers inside the droplet is less than 3% of the total droplet volume during the evaporation or combustion process, which is deemed too small to affect the measured droplet size.

C.2. Conduction effects of fibers

In droplet combustion experiments, there is no way to avoid flame impingement on the fibers supporting a droplet, but the effect can be mitigated by proper fiber selection. The effect of the selected fiber on the burning rate is believed to be negligible, a conclusion supported by published literature [1]. Previous studies have shown that large fibers can significantly influence the burning rate of droplets by increasing the liquid-gas interfacial area and conducting heat along the fiber [2]. However, the impact of the fiber decreases as its diameter is reduced. Faroukhi et al. [1] conducted a numerical investigation on the effects of fiber type and diameter on the burning rate of a single droplet. Their findings indicate that, under conditions similar to those in the present study, when the ratio of droplet diameter to fiber diameter is approximately 35 ($d_{0-droplet}/d_{fiber} \sim 35$), variations in the average burning rate become negligible for both SiC and quartz fibers, even with a fiber diameter of around 30 μm . In a subsequent study, the same group [3] demonstrated that for a 10 μm SiC fiber, the burning rate was nearly identical to that of a tetherless droplet. Further research has established that in hot ambient environments, the droplet vaporization rate is linearly related to both the square of the fiber diameter, d_f^2 , and the fiber's thermal conductivity, k_f [4, 5]. The optimal conditions occur when the fiber diameter is less than 100 μm , and the thermal conductivity is below $80 \times 10^{-6} (W/(\mu\text{m} \cdot K))$ yielding a product of $k_f d_f^2 = 8 \times 10^{-4} (W \cdot \mu\text{m}/K)$ [7]. In the present study, a 14 μm CG Nicalon fiber was used due to its extremely low thermal conductivity. The calculated thermal conductivity product was $k_f d_f^2 = 4.5 \times 10^{-4} (W \cdot \mu\text{m}/K)$, well below the recommended threshold. These results suggest that the fiber's effect on the burning rate is indeed negligible, in agreement with published findings.

References

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- [3] T. Farouk et al. "Tethered methanol droplet combustion in carbon-dioxide enriched environment under microgravity conditions." *Combustion and Flame* 159.1 (2012).
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Appendix D: Independence and reliability of burning rate

In this section, a brief explanation is first provided to show that the burning rate is independent of coil power and residence time. Subsequently, the consistency of burning rate determination is demonstrated using an example related to the high error bar in Figure 4-3.

D.1. Coil power and residence time

A series of preliminary experiments was conducted to validate the independence of the burning rate from the coil power and the ignition system residence time under both ambient atmospheric and elevated pressure conditions. In these experiments, the minimum power and maximum residence time required for droplet ignition were first determined. Subsequently, both power and residence time were varied until the minimum residence time and maximum power required for complete combustion were achieved. The results are presented in Table D1, and they show that the maximum variation in the burning rate under these extreme conditions is less than 2.0%.

Table D1. Effect of variation of coil power and residence time on droplet burning rate

<i>P</i> (bar)	Power, W	Duration, s	<i>d</i> ₀ , μm	<i>K</i> _b , mm ² /s	wire clear
1.0	15	0.45	1225	0.946	0.9
	15	0.45	1246	0.95	0.9
	15	0.45	1266	0.951	0.91
	Average of above tests:			0.949	0.91
	20	0.45	1258	0.95	0.87
	20	0.45	1271	0.958	0.87
	20	0.45	1249	0.947	0.96
	Average of above tests:			0.952	0.9
	20	0.5	1260	0.957	0.84
	20	0.5	1250	0.948	0.84
	20	0.5	1250	0.95	0.83
	Average of above tests:			0.952	0.84
	20	0.55	1243	0.965	0.8
	20	0.55	1251	0.964	0.81
	20	0.55	1249	0.967	0.81
	Average of above tests:			0.965	0.81
	20	0.6	1254	0.966	0.78
	20	0.6	1258	0.962	0.78
	20	0.6	1257	0.973	0.78
	Average of above tests:			0.967	0.78
3.0	25	0.35	1261	1.218	0.94
	25	0.35	1271	1.22	0.94
	25	0.35	1260	1.226	0.95
	Average of above tests:			1.22	0.94
	25	0.5	1252	1.224	0.83
	25	0.5	1258	1.23	0.88
	25	0.5	1262	1.229	0.83
	Average of above tests:			1.23	0.85
	25	0.65	1263	1.244	0.74
	25	0.65	1254	1.243	0.72
	25	0.65	1253	1.249	0.73
	Average of above tests:			1.25	0.73
	15	0.65	1263	1.247	0.96

D.2. Reliability

In this thesis, to ensure that the results are consistent and reliable, between 4 and 12 tests were conducted for each investigated condition. The consistency of the results was evaluated by calculating the relative standard error (*RSE*) for each condition as follows:

$$RSE = z \cdot \frac{\sigma/\sqrt{N}}{\bar{K}} \times 100 \quad (D1)$$

where σ denotes the standard deviation, N is the total number of the tests, $\bar{K}$ is the average of all tests and z is a constant that depends on the chosen confidence level, which is equal to 1.96 for a 95% confidence interval [1].

This value remains below 5% for all investigated droplet vaporization tests. However, it exceeds 5% in certain cases for the combustion of a single droplet, as shown and discussed in [Chapter 4](#).

To further confirm the reliability of the results and rule out accidental variations, additional tests were conducted on different days whenever the *RSE* exceeded 5%. For example, Table D2 presents results for one condition with a high error bar in Figure 4-3, ($P = 11$ bar, $q^{0.5} = 0.3$ m/s). Under this condition, 11 tests were conducted separately in different days. The *RSE* was 10%, and the average burning rate remained consistent between the two days, yielding an overall value of 1.02 mm²/s. This consistency confirms that the results are reliable, regardless of the number of tests performed, as long as the experimental conditions are kept the same.

Table D2. Test results for two separate days for butanol droplet combustion at $P=11$ bar, $q^{0.5}=0.3$ m/s

Date	Test #	P, bar	T, °C	d_0 , μm	K_b , mm^2/s	Ignition system
240530	1	10.95	25.2	511	1.244	0.91
	2	10.93	25.4	513	0.933	0.75
	3	10.92	25.9	504	1.009	0.88
	4	10.90	25.0	496	0.682	0.94
	5	10.90	25.9	509	0.977	0.89
	6	10.95	25.5	515	1.042	0.93
	7	10.93	25.2	496	1.122	0.8
	8	10.90	25.0	508	1.17	0.88
240531	1	11.05	24.2	514	0.841	0.98
	2	11.01	25.2	505	1.196	0.83
	3	10.97	25.3	496	1.058	0.9

References

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Appendix E: Thesis Details

This thesis was typeset using Microsoft Word 2019 on a Windows operating system. All data presentation figures were generated using MATLAB R2023a and Tecplot 360 2023 R2, and saved as individual PDF and WMF files to preserve image quality. Detailed schematics of the experimental apparatus were developed from accurate CAD models created in Solid Edge ST10. All codes used in this thesis for the calculation of droplet size, evaporation rate, and PIV characterization are reported in [1].

References

- [1] C. Verwey, “An experimental investigation of the effect of fuel droplet size on the vaporization process in a turbulent environment at elevated temperature and pressure”, *M.Sc. thesis, University of Manitoba* (2017).