

**EXPERIMENTAL AND NUMERICAL INVESTIGATION
INTO THE OXY-COMBUSTION CHARACTERISTICS
OF PROPANE IN A SWIRL-STABILIZED,
NON-PREMIXED COMBUSTOR**

BY

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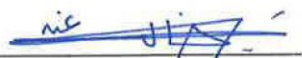
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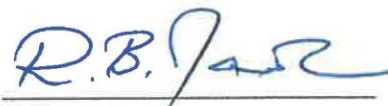
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| To my wife *Daybah* and Children; *Mohammad Bello, Ahmad, and Saadiq* |

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LIST OF ABBREVIATIONS

LED	:	Light Emitting Diode
A	:	Area (m^2)
c_p	:	Specific heat capacity (J/kg-K)
C	:	Speed of sound (m/s)
CH^*	:	Carbyne radical
C_2^*	:	Ethynidyl radical
CO	:	Carbon Monoxide
CO_2	:	Carbon dioxide
CH_4	:	Methane
C_3H_8	:	Propane
C_2H_4	:	Ethylene
Da	:	Damkohler number
D	:	Diameter (m)
E	:	Energy (J)
E_A	:	Activation energy (J/mol)
$\exp$	:	Exponential function

f	:	Mixture fraction
$fuel$	:	Denoting fuel stream
F'_i	:	Fluctuating components of body force per unit mass (N/kg)
FTF	:	Flame transfer function
FFT	:	Fast Fourier Transform
h	:	Convection heat transfer coefficient (W/m ² K)
H ₂	:	Hydrogen
$\bar{H}$	:	Mean enthalpy (J/kg)
i	:	the i^{th} specie
K	:	Coefficient of thermal conductivity (W/m-K)
k	:	Turbulent kinetic energy (m ² /s ²)
k_t	:	Turbulent thermal conductivity (W/m-K)
$k(T)$	:	Rate constant for chemical reaction
L	:	Length (m)
LES	:	Large eddy simulation
m'	:	Rate of mass production per unit volume (kg/m ³)
O ₂	:	Oxygen

OH^*	:	Hydroxyl radical
ox	:	Denoting oxidizer stream
P	:	Pressure (N/m^2)
P'	:	Pressure fluctuations in a disturbance (N/m^2)
$p(f)$	:	Probability density function (PDF)
Q'	:	Heat release fluctuations per unit volume (J/m^3)
RANS	:	Reynolds-averaged Navier-Stoke equations
RNG	:	Renormalization-Group
RI	:	Rayleigh index
S_h	:	Source term for heat transfer (W/m^3)
S_L	:	Laminar flame speed (m/s)
T	:	Temperature (K)
T'	:	Temperature fluctuation in a disturbance (K)
t	:	Time (s)
$u, \vec{v}$	:	Velocity vector (m/s)
u'_i	:	i th direction component of velocity in a disturbance (m/s)
U	:	Uncertainty

V	:	Volume (m ³)
Z	:	Elemental mass fraction
e'_{ij}	:	Strain rate tensor in the disturbance (1/s)
$\mathcal{D}$	:	Molecular diffusivity (m ² /s)
ω	:	Frequency (Hz)
ρ	:	Density (kg/m ³)
τ_{ij}	:	Viscous stress tensor (N/m ²)
τ'_{ij}	:	Viscous stress tensor in a disturbance (N/m ²)
τ_{res}	:	Residence time (s)
τ_{chem}	:	Chemical reaction time (s)
$\dot{w}_i$	:	Reaction Rate (kgmol/m ³ -s)
$\mathcal{V}$	:	Volumetric flow rate (m ³ /s)
μ	:	Molecular viscosity (kg/m-s)
α	:	Thermal diffusivity (m ² /s)
ϕ'	:	Viscous dissipation function in a disturbance
Φ	:	Equivalence ratio
ε	:	Turbulent kinetic energy dissipation rate (m ² /s ³)

ε_r	:	Emissivity
κ	:	Absorption coefficient
σ_t	:	Turbulent Prandtl number
μ_l	:	The laminar viscosity (kg/m-s)
μ_t	:	The turbulent viscosity (kg/m-s)
χ	:	Scalar dissipation rate (1/s)
Γ	:	Vortex strength (m ² /s)
Γ^*	:	Non-dimensional vortex strength
“ ₀ ”	:	Subscript referring to parameters in an undisturbed medium

|

ABSTRACT

Full Name : [Zubairu Abubakar]

Thesis Title : [Experimental and numerical investigation into the oxy-combustion characteristics of propane in a swirl-stabilized, non-premixed combustor]

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[One of the most widely recommended means of tackling CO₂ emission is the carbon capture technique, which includes oxyfuel combustion. Recycled CO₂ from flue gases can be employed as a diluent forming O₂/CO₂ oxidizer mixtures in oxyfuel combustion to mitigate its characteristically excessive temperatures. The CO₂ in the O₂/CO₂ oxyfuel oxidizer affects the combustion characteristics. In this dissertation, the characteristics of C₃H₈-oxyfuel combustion with CO₂ dilution are studied in a non-premixed, swirl-stabilized combustor over a wide range of operating conditions. Air combustion was compared experimentally to two oxyfuel mixtures, namely, oxyfuel I and II, in terms of lean blowout limits. Results show that, for lean mixtures, the C₃H₈-air flame transits from the attached flame to lifted flame before subsequent flame extinction. This is contrary to oxyfuel I and II flames that transit directly from an attached flame to no flame regime at all firing rates studied. Near stoichiometry, however, the oxyfuel flames with CO₂ dilution display distinct flame transitions, including liftup before blowout at high firing rates. These flame transitions before blowout were observed to be flow-induced. Flame blowout under CO₂ dilution is found to be induced by both the chemical effect of CO₂ diluent (decreasing the flame speed and taking away heat), as well as strain imposed by the flow on the flame at high dilution levels. The amount of CO₂ in the oxidizer at

blowout was observed to decrease significantly as the equivalence ratio decreases from 1 to 0.9, signifying enhanced flame stability at stoichiometric conditions under CO₂ diluent influence. Further studies revealed that the oxyfuel flames are more stable at the swirl number of 1.0 when compared to 0.6 and 1.5. The flame transitions with CO₂ dilution were observed based on numerical results to be a consequence of fuel jet-vortex interaction and that this interaction can be employed in the characterization of swirl-stabilized, non-premixed flame macrostructures. Jet-like flames were obtained at zero and low CO₂ dilution while V-shaped flames were obtained at higher CO₂ concentrations. The jet-like flames obtained at low dilution levels were found to have the same non-dimensional vortex strength of 0.2. Also, the flame transition coincides with a sudden increase in the vortex strength value from 0.2 to about 0.3 and continued to increase linearly with increase in CO₂ dilution level. The change in the flame's macrostructure is associated with vortex breakdown and the formation of an inner recirculation zone occurring at high CO₂ dilution as the fuel jet fails to penetrate the created vortex. Vortex-breakdown-induced combustion instability characterized by high amplitude sound was observed to occur at the CO₂ dilution level of 45% which coincides with the flame transition from jet-like to V-shaped resulting from flow separation leading to the formation of IRZ. In the aftermath of this onset, the instability amplified at 50% CO₂ dilution level due to a coupling between heat release and pressure fluctuations. The combustor mode excited is at the frequency of 465 Hz and the limit cycle amplitude was observed at 60 % CO₂ concentration after which the acoustic amplitude decreases due to damping. The CO emission increases with CO₂ dilution due to the combined effect of cooling, low residence time, and CO₂ dissociation, up to the threshold of 50% CO₂

dilution level, beyond which it decreases due partly to a drastic decrease in CO_2 dissociation that is attributed mainly to the cooling effect. Also, flames beyond 50% CO_2 dilution are V-shaped characterized by enhanced mixing. Increasing the H_2 concentration from 0 to 30% extends the blowout limits of the CO_2 diluted oxyfuel flames by 2.5% and lower the acoustic amplitude. Hydrogen enrichment, however, was found to increase CO while lowering CO_2 emission as a consequence of the low residence time and competition for oxygen between the fuel species. Decreasing the equivalence ratio from 1.03 to 0.93 also leads to a significant reduction in CO emission from 8000 ppm to <1 ppm accompanied by an increase in O_2 emission. The flames, however, display better stability at higher equivalence ratios.

ملخص الرسالة

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واحدة من أكثر الوسائل الموصى بها على نطاق واسع لمعالجة انبعاثات ثاني أكسيد الكربون هي تقنية التقاط الكربون ، والتي تشمل الاحتراق الوقود بالأكسجين. يمكن استخدام ثاني أكسيد الكربون المعاد تدويره من غازات المداخل كمخاليط مؤكسدة مكونة من الأكسجين وثاني أكسيد الكربون في احتراق الوقود بالأكسجين لتخفيف درجات الحرارة المرتفعة. يؤثر ثاني أكسيد الكربون الموجود في المؤكسد المكون من الأكسجين وثاني أكسيد الكربون على خصائص الاحتراق. في هذه الرسالة ، تم دراسة خصائص احتراق البروبان والأكسجين مخفف بثاني أكسيد الكربون في احتراق غير ممزوج مسبقا ومستقر باستخدام دوامة على نطاق واسع من ظروف التشغيل. تمت مقارنة احتراق الهواء في المعمل بمزيج من خليط الأكسجين ، وهما المؤكسد الأول والثاني ، من حيث حدود الاحتراق الغير غني بالوقود. تشير النتائج إلى أنه بالنسبة للمخاليط الغير غنية بالوقود ، تنتقل شعلة احتراق البروبان بالهواء من اللهب المتصل إلى شعلة مرفوعة قبل انطفاء اللهب. هذا يتعارض مع لهب المؤكسد الأول والثاني الذي ينتقل مباشرة من اللهب إلى منطقة انعدام اللهب في جميع معدلات الاحتراق التي تمت دراستها. ولكن بالقرب من كمية الهواء والوقود المطلوبة لاحتراق كامل ، تعرض لهب الوقود بالأكسجين المخفف بثاني أكسيد الكربون لتغيرات مميزة ، بما في ذلك الزيادة قبل الاشتعال بمعدلات احتراق عالية. هذا التحول في اللهب قبل الاشتعال لوحظ أنه يكون ناجم عن التدفق. انطلاق اللهب تحت تخفيف ثاني أكسيد الكربون نتيجة كل من التأثير الكيميائي لمخفف ثاني أكسيد الكربون (تقليل سرعة اللهب ورفع الحرارة) ، وكذلك الضغط الذي يفرضه التدفق على الشعلة عند مستويات تخفيف عالية. لوحظ أن كمية ثاني أكسيد الكربون في المؤكسد عند الانفجار تنخفض بشكل كبير حيث تنخفض نسبة التكافؤ من 0.9 إلى 1. مما يدل على ثبات اللهب المعزز في ظروف العناصر المتكافئة تحت تخفيف ثاني أكسيد الكربون. كشفت دراسات أخرى أن لهب احتراق الوقود بالأوكسيجين أكثر استقرارًا عند الدوامة عند 1.0 مقارنةً بـ 0.6 و 1.5. وقد

لوحظت تحولات اللهب مع تخفيف ثاني أكسيد الكربون على أساس النتائج العددية كنتيجة لتفاعل وقود الدوامي النفث وأنه يمكن استخدام هذا التفاعل في توصيف هياكل للهب الكبيرة والمثبتة في دوامة و غير ممزوجة مسبقا . تم الحصول على لهب يشبه النفثاة عند نسبة تخفيف صفر من ثاني أكسيد الكربون بينما تم الحصول على لهب على شكل V بتركيزات أعلى من ثاني أكسيد الكربون. كما تم العثور على السنة اللهب النفثاة التي تم الحصول عليها بمستويات تخفيف منخفضة لها نفس قوة دوامة 0.2. و يتزامن انتقال اللهب مع زيادة مفاجئة في قيمة قوة دوامة من 0.2 إلى حوالي 0.3 واستمرت في الزيادة الخطية مع زيادة مستوى التخفيف من ثاني أكسيد الكربون. يرتبط التغير في البنية الأساسية للهب مع تكسر الدوامة وتشكيل منطقة إعادة الدوران الداخلية التي تحدث عند التخفيف العالي لثاني أكسيد الكربون لأن اندفاع الوقود يفشل في اختراق الدوامة التي تم إنشاؤها. لوحظ عدم استقرار الاحتراق الناجم عن تكسر الدوامة الذي يتميز بصوت عالي السعة يحدث عند مستوى التخفيف من ثاني أكسيد الكربون بنسبة 45% والذي يتزامن مع انتقال اللهب من شكل يشبه النفث إلى شكل V الناتج عن فصل التدفق الذي يؤدي إلى تكوين IRZ. في أعقاب هذه البداية ، زادت حالة عدم الاستقرار عند مستوى التخفيف 50 % من ثاني أكسيد الكربون بسبب الاقتران بين إطلاق الحرارة وتقلبات الضغط. يكون وضع الاحتراق النشط عند تردد 465 هرتز ولوحظ حد السعة للدورة عند تركيز 60% من ثاني أكسيد الكربون ، وبعد ذلك تنخفض السعة الصوتية بسبب التخميد. يزداد انبعاث أول أكسيد الكربون مع تخفيف ثاني أكسيد الكربون نتيجة للتأثير المشترك للتبريد ، ووقت التشغيل المنخفض ، وتفكك ثاني أكسيد الكربون ، حتى بداية مستوى التخفيف من ثاني أكسيد الكربون بنسبة 50% ، والذي يتناقص بعده جزئياً بسبب الانخفاض الحاد في تفكك ثاني أكسيد الكربون الذي يعزى بشكل رئيسي إلى تأثير التبريد. أيضا ، عند مستوي تخفيف لثاني اكسيد الكربون اكبر من 50 % يكون اللهب على شكل حرف V والتي يتميز بالاختلاط النشط. كما تؤدي زيادة تركيز الهيدروجين من 0 إلى 30% إلى تمديد حدود الاشتعال في لهب الوقود بالاكسجين المخفف بنسبة 2.5% بثنائي اكسيد الكربون وتقليل السعة الصوتية. ومع ذلك ، وجد أن زيادة الهيدروجين يزيد أول أكسيد الكربون مع تقليل انبعاثات ثاني أكسيد الكربون نتيجة انخفاض وقت التشغيل والتنافس على الأكسجين بين أنواع الوقود. يؤدي خفض نسبة التكافؤ من 1.03 إلى 0.93 أيضاً إلى انخفاض كبير في انبعاثات أول أكسيد الكربون من 8000 جزء في المليون إلى أقل من جزء في المليون مصحوباً بزيادة في انبعاثات ثاني أكسيد الكربون. ومع ذلك ، فإن الشعلات تظهر ثباتاً أفضل عند نسب تكافؤ أعلى.

CHAPTER 1

INTRODUCTION

1.1 Background and Motivation

Emission of Carbon-dioxide (CO_2) is one of the major environmental considerations emanating from fossil fuels combustion. This is because it takes the largest share of the amount of Global Greenhouse gas (GHG) emissions to our atmosphere with up to 65% of the GHGs being CO_2 [1]. In line with this, the international community sought to unify efforts in reducing CO_2 emission through comprehensive agreements. The most recent of these efforts is the COP21 (Paris Climate Conference of 2015) which after long negotiations proposed a universal and legally binding agreement on climate seeking to keep global warming below 2°C by the year 2100, with CO_2 emissions reduction at the apex of the whole idea [2]. Fossil-fueled power plants are responsible for roughly 40% of total CO_2 emissions with the remaining coming from other sources like the transportation sector, industrial activities, deforestation and desertification [3].

Currently, more than 85% of the world energy demands are met mainly by fossil fuels as can be seen in Figure 1.1 which depicts statistical review of world energy of 2017 conducted by BP Oil Company [4]. With the constant growth in industrialization and urbanization in both developed and emerging economies, energy consumption will rapidly continue to increase. International Energy Agency (IEA) projected 30% increase

in global energy demand by 2040 [5]. Although the use of renewable sources of energy is also projected to increase, Fossil fuel is still projected to account for up to 75% of global energy demand by 2040. Consequently, the expected target over the next two decades, to utilize 40% clean energy technology in the global energy production, includes the use of renewables as well as cleaner combustion of fossil fuels [6]. One of such clean combustion technologies is the carbon capture technology that involves pre-combustion carbon capture, post-combustion carbon capture, or oxy-fuel combustion [7].

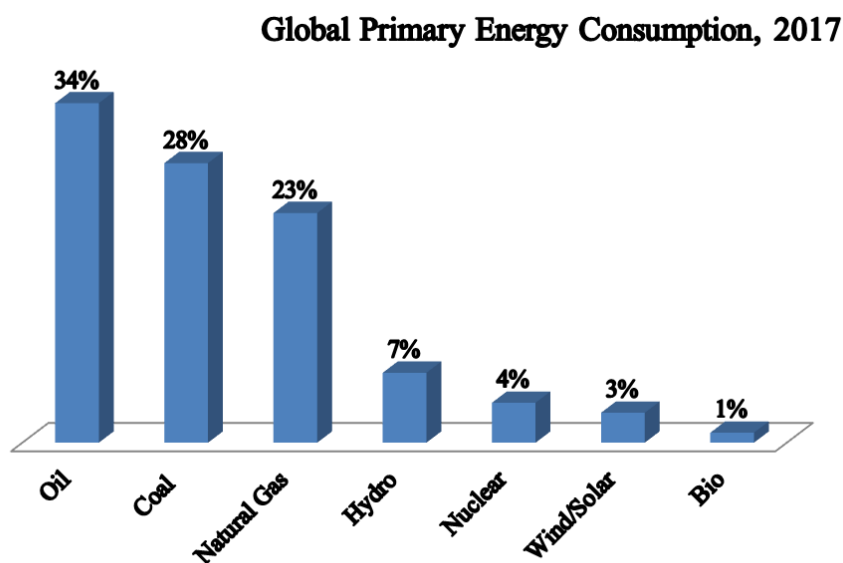


Figure 1.1: Global Primary Energy Consumption Statistics of 2017 Reported by BP [4]

Oxyfuel combustion as one of the means for tackling CO₂ emission is a branch of Carbon Capture and Sequestration (CCS) technology that uses pure oxygen as an oxidizer in combustion systems so that the products will be mainly CO₂ and H₂O. The CO₂ in the

combustion products, therefore, can be captured and sequestered after condensation of the H_2O from the flue gas stream [8, 9]. Subsequently, Oxyfuel combustion with carbon capture has the potential of achieving zero CO_2 emission. This is in addition to the potential elimination of thermal NO_x emissions ensuing from the oxidation of nitrogen in air-oxidized combustion systems, since pure oxygen, instead of air is utilized as an oxidizer in oxyfuel combustion. Pieces of literature are available looking into the optimization of the carbon separation techniques, storage capacities, transportation, cost, and economic potentials [10-12]. Despite many challenges associated with CCS in terms of capture, transportation, and storage of the CO_2 from both technical and economic standpoints, available practices like the utilization of the captured CO_2 in enhanced oil recovery (EOR) is a promising step towards improved CCS [13]. Subsequently, with oxyfuel combustion, cleaner combustion of fossil fuels including economically-under-utilized, highly-carbonaceous fuels like residual oil, coal, and other heavy fuels becomes more viable [14]. Pilot-scale retrofitted plants utilizing oxyfuel combustion, like Doosan Babcock in the United Kingdom, are already in operation and are reporting CO_2 rich flue gas that could be a very good candidate for CCS [15].

Because of high temperatures associated with oxyfuel combustion in a stream of pure oxygen, the use of a diluent is necessary in order to lower these excessive temperatures to limits suitable for components in combustion systems. An obvious choice for such a diluent is recycled CO_2 from the flue gases to form O_2/CO_2 oxidizer employed in oxyfuel combustion [16]. Pure oxygen from an air separation unit (ASU) can, therefore, be injected into the stream of recycled CO_2 to form the oxidizer mixture [17]. Luo et al. [18] explored the use of a control system in flue gas recirculation in order to control the effect

of quality and characteristics of the flue gas using a dynamic exergy evaluation technique. Up to 70% by volume of CO_2 with O_2 was reported in the literature with higher amount said to cause flame instability even near stoichiometric equivalence ratio [19, 20]. This is in sharp contrast to the higher concentration of N_2 in air oxidizer (79%) that air-oxidized flames can propagate stably even at low equivalence ratios. These differences in combustion characteristics between air and O_2/CO_2 oxidizer are due to lower thermal diffusivity of CO_2 , its higher thermal radiation, dissociation, and its cooling effect compared with that of N_2 . Because of this reason, oxygen in the O_2/CO_2 oxidizer should be about 30% of the mixture in contrast to 21% in air, in order to have similar combustion characteristics from the two oxidizers [21, 22]. Effect of O_2 concentration in O_2/CO_2 oxidizer between 20-40% was studied by Kutne et al. [23] and was found to play a greater role in oxyfuel flame stability than the operating equivalence ratio. Also, oxygen concentration affects significantly the production and consumption rates of CO in the combustion products. At high concentrations, depending on the combustion temperature, CO_2 participates in the reaction with evidence from CO concentrations in the product [24]. Therefore, O_2/CO_2 oxidizer ratio or in other words *CO_2 dilution level* affects the oxyfuel flame structure and stability, heat transfer, as well as emissions.

Flame instability is a consequence of the competition between the rate of reaction and the rate of diffusion of species and energy [25-27]. Static instability is a term that refers to flame extinction when the flame cannot be stably anchored in the combustor. Subsequently, the static stability limit of combustors is characterized by their blowout propensity. Flame blowout is sometimes preceded by flame liftup when a flame gets

detached from its anchoring position at the burner rim and stabilizes at a distance downstream. Anchoring or stabilizing non-premixed flames a distance away from burner rim can be advantageous as it helps circumvent thermal contact between the flame, characterized by high temperature, and the burner rim that can get degraded by such temperatures. Also, the dead space in-between the rim and the lifted flame helps in enhancing the mixing of the reactants. Despite these advantages, however, lifted flames are more prone to instabilities and possible blowout. The mechanism driving blowout phenomena is when the time required for the chemical reaction in combustion to occur is longer than the propagation rate of the combustion species [28, 29]. In other words, flame blowout occurs when characteristic chemical time exceeds the characteristic mixing time (or residence time) in the combustor. Critical Damkohler number also known as mixing time scale can be used to predict the range of static stability for a certain range of combustion conditions. It is defined as the ratio of characteristic convective time to chemical time at blowout. Flame blowout, when undetected could allow the accumulation of unburned fuel and oxidizer mixture, intensifying the risk of explosions.

Apart from static instability, dynamic combustion instability is another critical operational concern in real combustion systems. It is also known as thermoacoustic instability as it involves coupling between pressure and heat release fluctuations in the combustor. The fluctuation in heat release and by extension pressure in combustion systems is generally the result of mass flux fluctuation in combustion reactants and/or flame-vortex interaction in swirl or bluff-body stabilized flames [30]. Consequently, any mechanism through which sporadic heat release rates arises due to equivalence ratio perturbation and/or flame-vortex interaction can lead to thermoacoustic instability. Some

of the mechanisms include intermittent flow rates as a result of changes in pressure and velocity, flame extinction and re-ignition (due to heat losses and radicals escape from the reaction zone), and vortex formation in the recirculation zone that can change the flame structure.

Understanding the interaction between acoustic waves and combustion heat release is the key to predicting and controlling thermoacoustic instability. However, it is a very difficult task to comprehensively predict the dynamic response of flames to some finite-amplitude disturbances that renders a linearly stable flame into non-linear dynamics mode [31]. The progress made involves qualitative and quantitative analysis of thermoacoustic instability in combustion systems. Studies generally seek to establish the frequency of the oscillations resulting from combustion instability, circumstances that trigger such oscillations, and the limit-cycle amplitude of the oscillations. Most of the available literature on thermoacoustic instability, however, is focused on air-oxidized premixed combustion systems because of the abundance of these systems in the form of lean premixed combustion technology. Consequently, thermoacoustic instability in non-premixed combustors is not extensively studied even for air-oxidized systems [32]. With most gas turbine combustors for aircraft, power plants, and other industrial applications operating non-premixed combustors, the importance of investigating thermoacoustic instability in such systems is evident. It is even more evident in non-premixed oxyfuel combustion system that will be utilizing oxygen instead of air oxidizer.

It is remarkable that flame static instability, resulting from operating combustors near lean blowout limit, encountered in air combustion to reduce NO_x emissions is not a concern in oxyfuel combustion. This is because, for oxyfuel combustion, there is no

apparent incentive for lean combustion in that regard since the oxidizer utilized is free of nitrogen. Moreover, the cost of oxygen separation is an additional penalty to be paid when operating oxyfuel combustion systems. The use of excess oxidizer, therefore, becomes even more unattractive. Consequently, operating a combustor in oxyfuel mode near stoichiometric equivalence ratio is beneficial with regards stability and cost. Static instability in oxyfuel combustion, therefore, comes down to the dilution level of CO_2 or any other diluent used in the oxyfuel oxidizer mixture. Other combustion characteristics affected by the use of O_2/CO_2 oxidizer mixtures instead of air include the flame length, shape, speed, ignition as well as adiabatic flame temperatures. All of these ultimately affect the ensuing combustion emissions, stability, and energy recovery. From the aforementioned considerations, it is clear that for efficient design and operation of burners and combustion chamber that will be utilizing oxyfuel combustion with its inherent oxidizer mixtures, the combustion characteristics of such mixtures need to be studied under different conditions.

It is worth mentioning that most of the available literature on oxyfuel combustion focus on coal, apparently, because of its comparatively higher carbon content, making its combustion CO_2 -rich, and because of coal's potential in IGCC plants. This includes a comprehensive review of the state of the art oxy-fuel combustion fundamentals, their modeling, and models implementation [33] and other studies dealing with oxyfuel combustion of coal [34-39]. Some pieces of literature are also available on oxyfuel combustion of methane, with other higher carbon fuels like propane receiving little attention. Oxyfuel combustion, which is one of the CCS technologies is generally recommended for fuels with high carbon content (such as coal). This is because, the

higher carbon content in the fuel increases the amount of CO_2 to be captured from oxyfuel combustion exhausts, which can help justify the extra cost of utilizing the technology. Furthermore, a high amount of CO_2 produced is complementary to the cost of oxyfuel combustion that targets the utilization of the captured CO_2 in processes like enhanced oil recovery. It is, however, important to point out that oxyfuel combustion of gaseous fuels like Methane and Propane can also be economically viable for CO_2 production. An example of that is in cases where the fuel's on-site availability is of the essence to curb cost associated with transportation.

This study is conducted using both experimental and numerical techniques in a swirl-stabilized, non-premixed combustor. Different O_2/CO_2 oxidizer mixtures were employed to study propane-oxyfuel flame and combustion stability under different combustor firing rates and different swirl numbers. It is stated above that lean combustion is not encouraged in oxyfuel combustion systems. However, for the purpose of comparison, the lean stability limits, combustor temperature distribution, as well as emissions from propane-oxyfuel and propane-air combustion, are studied. Furthermore, the effect of CO_2 dilution level on propane-oxyfuel flames in terms of flame's macrostructure, temperature, thermoacoustic instability as well as emissions are studied near stoichiometric condition. Finally, the effect of adding hydrogen on the blowout limit and thermoacoustic instability of propane oxyfuel flames with CO_2 dilution is studied.

1.2 Objectives

The main objective of this study is to conduct a parametric study under different fuel and oxidizer conditions in order to investigate the effect of such conditions on static and dynamic instability, emission, flame structure, and temperature profiles of propane-oxyfuel flames in a non-premixed, swirl-stabilized combustor.

The following are the outline of the specific objectives of this study;

- I. To carry out detailed experimental studies using propane with air and O_2/CO_2 oxidizer mixtures, establishing the effects of fuel firing rates, equivalence ratio, and CO_2 dilution level on the flame structure and instability in a swirl-stabilized, non-premixed combustor. Including;
 - a) Study of the emission characteristics for the conditions in (I) above.
 - b) Measurements of the temperature profiles for the various conditions in the combustor.
- II. To carry out experimental studies using propane enriched with hydrogen in both air and O_2/CO_2 oxidizer mixtures, in order to study its effect on the flames instability, structure, and emissions.
- III. To use the data from the experimental study to develop and validate a numerical model for the combustor.

CHAPTER 2

LITERATURE REVIEW

This chapter is devoted to a review of existing literature related to combustion emissions formation, flame macro-structure, and flame and combustion instability as regards both premixed and non-premixed flames. Considerable attention is given to reviewing the conditions and fundamental mechanisms driving static and dynamic instabilities. Furthermore, the effects of combustion technology, fuel compositions, operating equivalence ratios, and geometric considerations among other things on these combustion characteristics are reviewed.

2.1 Combustion Emissions

One of the most common environmental considerations emanating from combustion systems is the oxidation of nitrogen at high temperatures when air is used as an oxidizer to produce thermal NO_x . Some fuels like syngas are also prone to the formation of fuel-bound NO_x depending on the feedstock used in their production or sources. The Zeldovich mechanism as a pathway for the formation of thermal NO_x is particularly prominent for diffusion flames where the combustion proceeds at near-stoichiometric conditions [40]. Higher combustion temperatures are associated with higher NO_x formation, but with lower CO and HC emissions, and higher combustion efficiency. Some of the approaches employed to reduce the adiabatic flame temperature, thereby

lowering the amount of NO_x formation involves the use of diluents like steam, EGR (exhaust gas recirculation) or nitrogen [41, 42]. While this has shown to lower NO_x emissions, it does it at the detriment of the overall cycle efficiency due to the additional overhead of supplying the diluent to the combustion region. Additional alternatives include the removal of the NO_x from the combustion products by the utilization of selective catalyst reduction system (SCR) which is prohibitively expensive, the utilization of preheated reactants in MILD combustion and/or staged combustion [43-45].

Lean Premixed Combustion (LPM) also known as excess air combustion is another promising approach for NO_x reduction that is widely accepted because of lesser constraints like the cost in SCR or cycle efficiency in steam injection. It involves using a lean premixed oxidizer-fuel mixture characterized by lower combustion temperatures compared to non-premixed flames. Fuel-lean conditions are also reported to lower the residence time due to the increase in the overall combustor volume flow rate thereby lowering NO_x formation [46, 47]. The disadvantage however in LPM is combustion instabilities arising from the premixed condition and low equivalence ratios (near blowout) that have to be employed in order to achieve the lower NO_x emissions [48]. In cases like syngas combustion, in order to maintain the power from turbines, comparatively excessive flow rates may be required to supplement the loss of energy due to a possible lower calorific value. These excessive flow rates, together with high oxidizer flow rates of LPM amplify the tendency of the system to exhibit combustion instabilities. Oxyfuel combustion that utilizes pure oxygen instead of the nitrogen-containing air as an oxidizer is another means of tackling thermal NO_x emissions.

Another important pollutant (carbon dioxide; CO_2), is known to cause global warming and ultimately a potential for climate change. CO_2 is produced in the combustion of every hydrocarbon fuel. Several techniques are proposed over the years to reduce CO_2 emission. These include reducing the fuel's carbon content by increasing its H_2 -to-C ratio like in syngas combustion in an integrated gasification combined cycle (IGCC). IGCC power plants take in fossil fuel, reacts it in a gasifier with steam and oxygen to produce the syngas fuel (primarily mixture of CO , H_2 , CO_2 , and traces of other gases depending on conversion efficiency) that can be utilized in the gas turbine combined cycle [49]. The fossil fuels that can be exploited in this process include coal and the economically underutilized residual oil [14, 50]. IGCC plants provide an opportunity by which carbon can be captured prior to combustion. The syngas can undergo additional processing before combustion like subjecting it to water-gas shift reaction in order to convert CO and H_2O to H_2 and CO_2 so that CO_2 can be separated ensuring almost pure H_2 combustion that is carbon-free. Physical or chemical adsorption processes are generally employed in separating the CO_2 in the H_2/CO_2 mixture through the use of solvents, sorbents, or membranes [51]. A major drawback to this pre-combustion carbon capture is its high cost including the capital investment required for the gasification process.

Post-combustion carbon capture involves capturing carbon after combustion of fossil fuels. If air is used as an oxidizer in the combustion process, the main challenge in post-combustion carbon capture is separating CO_2 from N_2 and its compounds in the flue gas. Just like in the case of pre-combustion separation, post-combustion carbon separation also utilizes solvents, sorbents, or membranes. In the solvent-based CO_2 separation, the CO_2 gas is absorbed into a liquid carrier. Typical solvent being utilized for post-

combustion carbon separation is an amine solution which can bind with CO_2 easily. The CO_2 is recovered from the solvent solution by heating the solvent- CO_2 mixture, where the CO_2 will be liberated and, subsequently, cooled for reuse. High energy requirement for the solvent regeneration is among the challenges for this carbon capture technique. Studies are available in the literature focused on advanced solvents characterized by lower regeneration energy requirement compared to the typical amine solution [52]. Away from the aqueous solvents, use of sorbents, characterized by comparatively lower regeneration energy requirement (due to the lower heat capacity of solids compared to aqueous solution) is considered advantageous. Cost, adsorption capacity, CO_2 selectivity, and the sorbent's endurance to multiple regeneration cycles are some of the most important factors driving the development of sorbents for carbon capture [53]. Finally, in the membrane-based carbon capture, permeable or semi-permeable membrane that is CO_2 -selective and resistant to flue gas contaminants is utilized. The membrane's stability and permeability, its durability, as well as cost, are some of the key challenges with the use of membranes in post-combustion carbon capture [54].

Oxyfuel combustion with carbon capture makes use of pure oxygen as an oxidizer in the combustion system so that the main combustion products will be CO_2 and H_2O . Once the H_2O is condensed in the flue gas, the leftover will be mainly CO_2 , ready for sequestration. This CCS technology presents a unique opportunity in utilizing our fossil reserves cleaner with a zero or an ultra-low NO_x and CO_2 emissions. The main challenges in oxyfuel combustion are the cost for oxygen separation and achieving sequesterable exhaust having the maximum acceptable limits for other gas components apart from CO_2 and H_2O . Consequently, the combustion system should utilize the minimum possible

amount of costly oxygen by targeting stoichiometric conditions while ensuring acceptable flue gas composition. The issue of the flue gas composition is a vital one in CCS using oxyfuel combustion since the captured CO_2 needs to be transported and sequestered. Depending on pipeline specifications, the so-called sequesterable exhaust restricts CO emission to about 0.1% to prevent reactions and formation of pentacarbonyls in CO_2 transport pipelines. Oxygen in the combustion products, on the other hand, should be limited to less than 50 ppm to avoid corrosion in pipelines and reactions in geologic reservoirs containing the sequestered CO_2 [55].

2.2 Swirl-stabilized, non-premixed flames macrostructure

The flame structure is a direct manifestation of the active combustion reaction zone and, hence, it changes with combustion variables like burning velocity, swirl intensity, and the characteristics of the fuel and oxidizer streams. High burning velocities produce a short flame that requires small flame surface area and shorter combustor lengths which is desirable in gas turbine applications because of space optimization. Fuel-oxidizer mixing rates affect burning velocity, with high mixing rates associated with higher burning velocities, and hence, shorter flames having extended stability limits. The mixing rate is generally enhanced by the use of bluff bodies or swirlers in combustors to produce large scale recirculation vortex, which acts as a flame anchoring position. The created toroidal vortex reduces the centerline axial velocity of the combustion mixture, allowing for longer residence times and recycling of combustion products including radicals for

reignition. In a swirl-stabilized combustor, the flame is typically anchored in the shear layer, in-between inner and outer recirculation zones generated by the swirling flow [56].

In non-premixed swirl-stabilized combustion systems, it is customary to supply fuel as an axial jet via a central nozzle, while having a swirling oxidizer surround the jet. Consequently, the analysis for such flow arrangement is drawn from the interaction between the fuel jet and the toroidal vortex generated by the swirling oxidizer flow also known as an oxidizer-driven vortex. As a result of this interaction, and depending on the properties (strength) of fuel jet and the oxidizer driven vortex, there could be a fuel-driven vortex and, therefore, inner and outer recirculation zones that form the basis for flame anchoring in swirl-stabilized, non-premixed combustors [57]. The outer recirculation zones (ORZ) are generally a consequence of the sudden expansion of flow, from each side of a central annular fuel jet, as combustion mixtures enter into a larger volume. Inner recirculation zone (IRZ), on the other hand, is a vortex-breakdown-induced recirculation zone.

A non-dimensional vortex strength proposed by Dahm [58] can be used to characterize flames in a classical jet-vortex interaction of swirl-stabilized flames. The non-dimensional vortex strength is a ratio of momentum fluxes defined as the ratio of the square root of vortex-induced momentum to the square root of fuel jet momentum. Vortex strength momentum is quantified by the product of oxidizer density (ρ_{ox}) and the square of vortex strength (I^2), while the fuel jet momentum is quantified by the product of fuel density (ρ_f), square of the jet velocity (U_f^2), and the square of fuel jet diameter (d_f^2). Subsequently, the non-dimensional vortex strength (I^*) is scaled by the equation:

$$\Gamma^* = \rho_{ox}^{1/2} \Gamma / (\rho_f U_f^2 d_f^2)^{1/2} \quad (2.1)$$

Non-dimensional vortex strength can be employed to characterize flames and predict or target specific flame macrostructure by controlling the jet momentum and the vortex strength momentum. The flames macrostructures, which are time-averaged flame shapes, can exhibit a jet-like appearance of a simple jet flame if fuel jet dominated the flame, because of large jet momentum relative to vortex-induced momentum. If the vortex-induced momentum dominates the flame, on the other hand, the flame will become wider but shorter due to high vortex strength. The vortex strength can be directly increased by increasing the velocity of the flow into the swirler as it is linearly related to the velocity of the recirculating flow, or by increasing the geometric swirl number.

2.3 Instability in combustion systems

Instability in combustion systems can be static or dynamic and it is among the most critical operational challenges encountered in real combustion systems like gas turbine combustors, industrial boilers, and furnaces. Static stability happens when the flame cannot be physically anchored in the combustor and this phenomenon is also called flame blowout. Dynamic instability, on the other hand, involves pressure fluctuations driven by heat release fluctuations in the combustor. In subsequent sections, dynamic and static instabilities in combustion systems will be reviewed.

2.3.1 Thermoacoustic instability

Thermoacoustic instability encapsulates flames dynamic response as energy is added or removed to/from the acoustic field of a combustor due to heat release oscillation. The process involves a feedback mechanism, where sporadic heat release rate acts as a source of energy to the combustor natural acoustic mode in a classical combustion-acoustic interaction. Also, the process can be intrinsic (self-excited) or can arise due to the interaction of flames with their surroundings (excited by a source external to the system). Instability in gas turbine combustors can be of low frequency (< 100 Hz), intermediate frequency (100-1000 Hz) and high frequency (> 1000 Hz) related to acoustic disturbance [59]. The low-frequency mode is generally associated with Helmholtz mode (breathing mode). Intermediate frequency instability is said to be associated with the natural acoustic modes of combustors and is the most commonly reported in the literature. Very limited amount of information is available as to what triggers high-frequency dynamics (> 1000 Hz) in combustors since, at high frequency, most of the coupling mechanisms for combustion instability are damped [60]. While the mechanisms that trigger the three modes are different, all involves coupling between pressure and heat release fluctuations. Less than 5% in the amplitude of pressure fluctuations relative to the mean combustion chamber pressure can be considered stable, while higher amplitudes are considered to be instability in the system.

Combustion systems are categorized as premixed or non-premixed depending on whether the reactants (fuel and oxidizer) are initially mixed or are supplied as distinct streams into the combustor, respectively. For both premixed and non-premixed flames, any inherent

mechanism through which fluctuation in pressure and heat release rate arises can lead to thermoacoustic instability. Flames could be short relative to the combustor longitudinal acoustic wavelength and it could be located at the pressure anti-node point so that oscillation in heat release could trigger the instability. Subsequently, an otherwise stable flame can go into spontaneous oscillations as a response to perturbations in heat release triggered by some disturbance.

The fluctuation in heat release and by extension pressure in combustion systems is generally the result of mass flux fluctuation in combustion reactants, and/or flame-vortex interaction in a swirl or bluff-body stabilized flames [30]. The mass flux fluctuation in fuel or oxidizer upstream of the mixing nozzle in the premixed system, or where the two reactants meet in a non-premixed system, will result in equivalence ratio perturbations [61]. This equivalence ratio fluctuation will be convected at the rate of the mean flow downstream into the combustion zone, where the mixture will burn with fluctuating heat release rates. The mass flux combustion instability is more prominent with premixed combustion systems, particularly in lean premixed combustion (LPM) systems. In such systems, the convective time delay results in equivalence ratio fluctuations, leading to large acoustic fluctuations due to low flame temperature characterized by LPM. For bluff-body or swirl stabilized flames, the vortices created as a means of flame stabilization in these systems, interact with the flame since typically combustion process has faster reaction rates than vortex shedding frequency [62]. Hence, the flame will ride on these unstable structures as they convect together downstream causing fluctuations in heat release [62, 63]. Also, during their formation, vortices (which contain combustible mixture) entrain hot products leading to ignition and subsequent combustion within the

vortex. This can lead to the sudden breakdown of the vortex into smaller scales turbulence causing heat release oscillations. Consequently, any mechanism through which sporadic heat release rates arises due to equivalence ratio perturbation and/or flame-vortex interaction can lead to combustion thermoacoustic combustion instability. Some of the mechanisms include intermittent flow rates as a result of changes in pressure and velocity, flame extinction and re-ignition (due to heat losses and radicals escape from the reaction zone), and vortex formation in the recirculation zone that can change the flame structure [25-27].

Figure 2.1 shows the feedback mechanism for thermoacoustic instability in which perturbation in the flow or equivalence ratio excites heat release fluctuation, which consecutively, excites pressure fluctuation due to heat addition or removal to the combustor acoustic field. The pressure fluctuation, in turn, generates the next perturbation in the flow and/or equivalence ratio, completing the loop, and the cycle is repeated. Consequently, the feedback loop is created when the oscillatory heat release excites one or more natural acoustic modes in a combustor. A sustained feedback mechanism in which the subsequent disturbance (heat release fluctuation) is in phase with the previous one (pressure fluctuation) can lead to amplification of the combustion instability accompanied by large amplitudes of pressure fluctuations. In other words, the coupling between unsteady heat release and pressure fluctuations can lead to self-amplifying thermoacoustic instability. In a coupled mode, the amplification is exponential with time until the oscillation reaches its *limit-cycle* amplitude. The fluctuations are of common occurrence in almost all combustion systems because of the

large amount of energy release in the process due to chemical reaction and the characteristic closed acoustic environment of combustors [63].

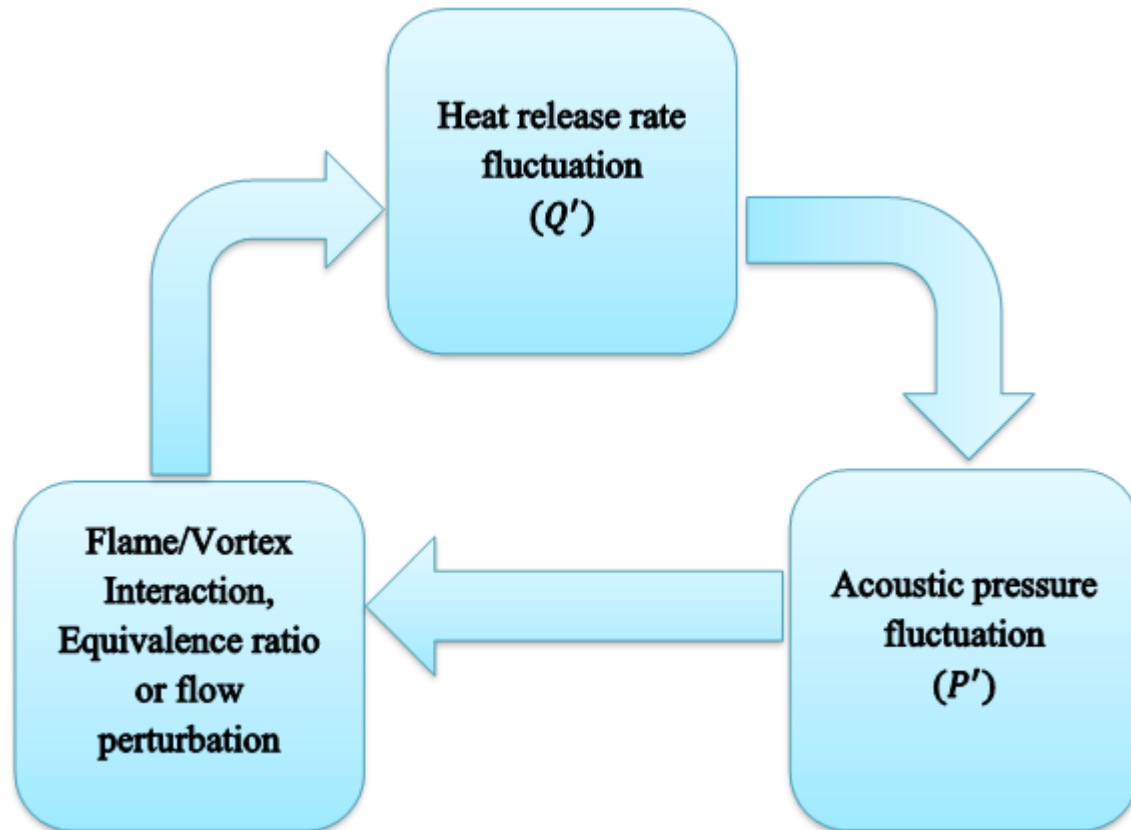


Figure 2.1: Thermoacoustic instability feedback loop

Instability in combustion systems is potentially dangerous phenomena. It can lead to structural damage in the system due to excessive vibrations and heat transfer to the combustion chamber and can translate into a serious safety issue. The catastrophic damage to combustors by combustion instability can be seen in Figure 2.2 which shows a new burner assembly and one damaged by combustion instability. It is noteworthy that not all oscillatory combustion is undesirable as these oscillations can serve to enhance

mixing and hence increase burning rates; a favorable scenario in *continuous combustion* systems, and are employed in pulsed combustors [64].



Figure 2.2: A new Burner assembly (left) and a burner assembly damaged by combustion instability (right) [65]

Intrinsic combustion instability occurs as a result of the combustion process itself with no influencing factors from the surroundings. In premixed flames, intrinsic instability is generally hydrodynamic in nature resulting from thermal expansion. However, in non-premixed flames, the instability is, largely, the result of diffusive-thermal effects [66]. Combustion instability resulting from thermal expansion occurs as a fluid element becomes heated during combustion causing it to expand and exerts a compressive force to the adjacent fluid layers. Consequently, a pressure wave that propagates in the region surrounding the fluid element is created. Upon reaching the boundary of the combustor, this pressure wave could get reflected and, as a consequence, affects the flame structure (which can cause fluctuation in heat release rate) on its return path, thereby, triggering

another wave from fluid element affected by the reflected wave [67]. Thus, the periodic change in volume of a fluid element in combustion zone due to thermal expansion serves as a source for the instability as it supports inherent fluctuations in heat release as well as pressure. The diffusive-thermal effects attributable to intrinsic instability in non-premixed flames are related to preferential diffusion effects (underscored by Lewis number; Le) and heat losses [68]. Instability can manifest as expansion and contraction of the flame at a certain frequency or in a back and forth movement along the surface of stoichiometry [66]. Ripples can also form on a surface of a flame that is stretched as a result of expansion giving the flame a wrinkled appearance.

2.3.2 Theoretical background on thermoacoustic instability

The onset of thermoacoustic instability was first postulated by Lord Rayleigh [69] in 1878 as follows: “If heat be periodically communicated to, and abstracted from, a mass of air vibrating in a cylinder bounded by a piston, the effect produced will depend upon the phase of the vibration at which the transfer of heat takes place. If heat be given to the air at the moment of greatest condensation or to be taken from it at the moment of greatest rarefaction, the vibration is encouraged. On the other hand, if heat be given at the moment of greatest rarefaction, or abstracted at the moment of greatest condensation, the vibration is discouraged”.

It goes from the Rayleigh criterion that thermoacoustic instability is derived by heat addition or removal to an acoustic field, and therefore, a coupling between heat release

(Q') and pressure (P') fluctuations in combustors. The first mathematical representation of the Rayleigh criterion was put forward by Putnam and Dennis in 1953 [70, 71]. This is the commonly known Rayleigh index (RI) denoted by Equation 2.2.

$$RI = \oint dt \int p' Q' dV \quad (2.2)$$

For a chosen integral volume, a positive RI (the fluctuations are in phase) entails amplification of the thermoacoustic instability while a negative quantity (the fluctuations are out of phase) entails decay of instability in the system. While Rayleigh criterion is necessary for thermoacoustic instability, it does not *guarantee* its occurrence as that will depend on heat losses and energy dissipation being lower than the energy in the fluctuation that is driving the process [72]. The choice for the volume (dV) to evaluate RI integral is also very important. Selecting the entire computational domain as the volume could mask regions of amplification or damping of the instability through averaging (global RI). Computing local RI by using volume less than the entire domain, on the other hand, could identify these regions.

A more general criterion than the RI that is representative of the net energy of a disturbance can be derived from the conservation laws. The quantity of this net energy represents the level of fluctuations present in an oscillatory system. This energy exhibits similarities with acoustic energy encountered in the sound's theory but with added parameters to capture the flow and thermal properties in systems involving heat release like combustion. Therefore, the amplification or attenuation of the disturbance energy has a direct bearing on the acoustic instability. The expression for the disturbance energy was derived by Chu [73] using the basic conservation laws. The mass, momentum,

energy, and species fundamental equations, each having source term, were added and the resulting equation is integrated after some mathematical manipulations to come up with the integral expression for the fluctuation energy.

The resulting fluctuation's energy equation obtained is written as:

$$\frac{dE}{dt} = \frac{1}{\rho_0} \int p' m' dV + \frac{1}{T_0} \int T' Q' dV + \rho_0 \int F'_i u'_i dV - \frac{1}{T_0} \int T' \mu_{0i} \dot{M}'_i dV - \frac{K_0}{T_0} \int \frac{dT'}{dx_j} \frac{dT'}{dx_j} dV - \int \Phi' dV \quad (2.3)$$

Where T' and p' are pressure and temperature in the disturbance, m' is the rate of mass production per unit volume, u'_i is the i th direction component of velocity in the disturbance, and Q' is heat release rate per unit volume. The viscous dissipation function in the disturbance Φ' is denoted by $\Phi' = 1/2 \tau'_{ij} e'_{ij} \geq 0$ where τ'_{ij} and e'_{ij} are viscous stress and strain rate in the disturbance respectively.

Thus the first four terms of Equation (2.3) represent sources for perturbations in mass, energy, momentum, and species, respectively. These terms are responsible for any increase or decrease in the energy of the system and, therefore, the fluctuation level within the disturbance. The last two terms represent thermal and viscous dissipation respectively. It is, therefore, apparent from the equation that if the sum of the first four terms is a positive quantity greater than the sum of the dissipation terms, finite amount of energy in the disturbance will endure. Subsequently, this fact is useful in the control of instability in a thermoacoustic environment [67]. This is because; it is evident from Equation (2.3) that amplification or attenuation of energy in the disturbance depends on whether the fluctuations are in phase (a distinct part of a sequence occurring over time) or

out of phase, respectively, in each of the first four integrals. For example, energy will be added to the disturbance if fluctuation in mass is in phase with pressure fluctuations, fluctuation in heat release rate is in phase with temperature fluctuations, fluctuation in body force is in phase with velocity fluctuations, and species generation in phase with chemical potential. Hence, periodic addition of mass, body force, heat or species anti-phase with pressure, velocity, temperature, or chemical potential, respectively, will result in an attenuation of the fluctuation energy, and form the basis for the *active* control of dynamic instability [74]. The heat energy addition could be accomplished by utilizing a heat source like a heater at one of the combustor ends, while a magnetic field can be used as a source for body force addition to affects the velocity field. Creating a periodic pressure gradient (by periodic geometric changes or periodic evaporation of liquid droplets), on the other hand, could be utilized for mass addition. Since the active scheme of combustion instability control requires extraction or addition of energy from/to the fluctuation through secondary sources, such systems will require a feedback control system [75]. A passive control, on the other hand, involves among other things, introducing geometrical changes such as baffles aimed at suppressing the acoustic standing wave or operating within the established stability limit of the combustor [76]. Part of passive control of combustion instability also involves the introduction of damping and dissipation through acoustic liners and Helmholtz resonators [77]. The resonant frequency of Helmholtz resonator, $\omega_o = c/2\pi\sqrt{A_{neck}/L_{neck} \times V}$ can be determined in order to establish its instability behavior. Parameters to vary includes the resonator's volume (V) and the area and length of its neck (A_{neck} and L_{neck}).

It is worth mentioning here that in acoustic mode, temperature fluctuations are in-phase with pressure fluctuations and hence the second term in Equation (2.3) is proportional to the Rayleigh index (Equation 2.2) [67, 73]. Rayleigh criterion entails that the integral of the Rayleigh index (*RI*) represented by Equation 2.2 has to yield a positive quantity for thermoacoustic instability. A modified Rayleigh criterion, on the other hand, takes into account, also, the energy dissipation from the system. Equation 2.4 represents the so-called modified Rayleigh criterion, in which, for the instability to be sustained, the Rayleigh index has to be a positive quantity greater than the sum of viscous and thermal dissipation.

$$\int P' Q' dV > T_0 \int \Phi' dV + K_0 \int \frac{dT'}{dx_j} \frac{dT'}{dx_j} dV \quad (2.4)$$

Other damping mechanisms for combustion instability include sound convection and transfer of energy between different acoustic modes (higher to sub-harmonics or vice-versa; $2\omega_o$, $3\omega_o$ or $\omega_o/2$, $\omega_o/3$ etc. with ω_o is natural frequency) in the combustor. The sound convection in an open-ended tubular combustor can be scaled by; $(\omega D/c)^2$, where ω is the frequency, D is the diameter of the tube, and c is the speed of sound [60]. From the fluctuation energy equation (Equation 2.3), if we assume an instability that is prompted purely by thermal oscillations (heat release fluctuations), the fluctuation in mass, body force, and species will be zero. Also, by incorporating the effect of heat losses through the boundaries of the system by conduction and radiation and considering thermal and viscous dissipation, we can write Equation 2.3 in the following form;

$$\frac{dE}{dt} = \frac{1}{T_0} \int T' Q' dV - \frac{hK_0}{T_0} \int T'^2 dA - \frac{K_0}{T_0} \int \frac{dT'}{dx_j} \frac{dT'}{dx_j} dV - \int \Phi' dV \quad (2.5)$$

Where h is the convection heat transfer coefficient and K_o is the thermal conductivity at temperature T_o . The energy in the fluctuation will be sustained if a finite amount of energy is obtained by integrating Equation 2.5 over a volume of interest and the period considered.

In the foregoing discussions, the effect of adding energy to an acoustic field via heat release fluctuation resulting into the amplification of energy in the disturbance (if the energy addition is coupled with the acoustic disturbance) was examined theoretically. However, understanding the physical phenomena that characterize this coupling mechanism in flames requires analyzing the flame transfer function (FTF). The FTF quantitatively assess flames susceptibility to thermoacoustic instability. Furthermore, FTF (ω) embodies the dynamic response of a flame heat release rate to a flow perturbation upstream of the flame as a function of frequency [78]. For a heat release fluctuation $Q'(\omega)$, fluctuation in reference velocity $u'_{ref}(\omega)$, and their respective mean values $\bar{Q}$ and $\bar{u}_{ref}$, FTF (ω) can be defined [79] as:

$$FTF(\omega) = \frac{Q'(\omega)/\bar{Q}}{u'_{ref}(\omega)/\bar{u}_{ref}} \quad (2.6)$$

The reference velocity perturbation arises from the perturbation in fuel or oxidizer velocity (in non-premixed combustion systems) or the mixture velocity (in premixed systems) upstream of the flame. Formulation of FTF requires the identification of the driving mechanism of heat release fluctuation, which changes depending on combustion conditions. The conditions include whether the system is premixed or non-premixed, confined or un-confined flame and whether the fuel is gas or liquid fuel that requires

atomization [80]. For example, the driving mechanism for non-premixed flames was reported to be dominated by mass burning rate fluctuations. This is more sensitive to flow perturbations than premixed flames in which the driving mechanism is dominated by flame surface area fluctuations [81]. Other important driving mechanisms include equivalence ratio oscillations and oscillations arising from liquid fuel atomization and evaporation [79]. A combination of two or more driving mechanisms on flame dynamics is also a real possibility. Consequently, the development of FTF generally focuses on the dominant mechanism (s) that is (are) driving the flame heat release fluctuations.

An involved FTF analysis is a computationally expensive endeavor that requires an unsteady CFD study to be conducted on the domain of interest to obtain the time-dependent solution of velocity and heat release rate. From the solution of the CFD model, the fluctuation in velocity and heat release can be obtained by subtracting their respective averages from instantaneous values. This subtraction process was reported to be straightforward when unsteady Reynolds-averaged Navier–Stokes equations (URANS) are used compared with Large eddy simulation (LES), which requires a characteristics-based filter to extract the acoustic signals [80, 82]. Han et al. [83] studied a bluff-body-stabilized, partially-premixed turbulent flames non-linear response to acoustic perturbation using LES. The authors successfully predicted, numerically, using LES, the limit cycle behavior of the flame. A similar analysis was conducted by Li et al. [84] in turbulent premixed flames. One of the proposed means of reducing the computational cost involves developing multiple flame transfer functions (FTFs), each based on a driving mechanism, and subsequently apply them simultaneously depending on the given operating conditions [79, 85].

2.3.3 An experimental approach to the study of thermoacoustic instability

Experimentally, thermoacoustic instability studies focus on the determination of amplitude and frequency of oscillations, as well as establishing the phase relationship between heat release and pressure fluctuations in a wide range of combustion conditions. Subsequently, the key to these studies is the ability to carry out real-time measurements of these fluctuations. Dynamic pressure transducers are generally used for the measurements of pressure fluctuations, while flame chemiluminescence or the light emission intensity of flames is commonly utilized for the quantification of heat release fluctuations. The flame transfer function (FTF) can also be deduced from the measurement of velocity perturbation using a hot wire anemometer and heat release from chemiluminescence intensity. Flame chemiluminescence provides a decent means for the quantification of energy release from combustion [86].

The unstable intermediate radical molecules produced during combustion like OH^* , CH^* and C_2^* emit light in a narrow spectral band of 308 nm, 431 nm, and 513 nm, respectively, with CO_2^* emitting in a broader spectral range [87]. Band-pass filters are usually used to detect a spectral band for those or other radicals, thereby, establishing the presence of the target radical and measuring its intensity. It is stated that the chemiluminescence intensity of a combustion process is proportional to its heat release rate. A photomultiplier tube (PMT) or a charged coupled device (CCD) camera can be used to acquire the chemiluminescence emission signal. The former is used for time acquisition of the spectral data while the latter is used for spectrum and image analysis

[88]. Intensified CCD cameras are used together with filters to map-out the radical distribution in the combustion zone using an imaging technique.

The major limitation to the utilization of flame chemiluminescence obtained using the optical technique discussed above for the quantification of heat release is that it basically gives only an integral heat release. Because of turbulence-chemistry interactions, the information about the local heat release rate cannot be determined by chemiluminescence without some corrections that involve statistical modeling [89]. This limitation, however, does not extend to the use of flames chemiluminescence in quantifying equivalence ratio in both premixed and non-premixed flames [90, 91]. The ratio; $\text{OH}^* / \text{CH}^*$ was reported to be a monotonic function of the equivalence ratio and hence can be employed in the determination of local equivalence ratio in non-premixed flames [92]. This $\text{OH}^* / \text{CH}^*$ ratio is said to be considerably lower in non-premixed flames when compared to stoichiometric premixed flame forming a basis for differentiation between the two.

High strain rate is understood to affect the intensities of radicals employed in flame chemiluminescence. Intensities of OH^* and CH^* radicals were shown by, Ponoutsos et al. [92], to strongly depend on the strain rate of turbulent diffusion flames. The use of their ratio for equivalence ratio determination, however, was reported to be accurate even for highly strained swirl-stabilized premixed flames [93]. Lauer et al. [87] had extensively studied the effect of turbulence on the determination of spatially resolved heat release rate using chemiluminescence. They found, in their study, that high turbulence intensities (characterized by local variations in flames reaction zones) have an effect of suppressing chemiluminescence, which renders its use in the determination of

spatially resolved heat release rate inaccurate. In the study, a correction, developed statistically, is further proposed. The correction accounts for turbulence-chemistry interaction in heat release rate determination using chemiluminescence for turbulent flames.

Another important observation pertaining to the use of band-pass filters in the measurement of chemiluminescence by targeting specific radicals is the superimposition of CO_2^* spectral band with the target radicals. Figure 2.3 shows this superimposition between the narrowband radicals emissions and the broadband CO_2^* spectrum. It can be observed from the figure that any measurement in a carbonaceous mixture targeting, for instance, OH^* emission will contain some amount of CO_2^* chemiluminescence at that wavelength. Consequently, such measurement will not be quantifiable of the number of electronically excited OH^* radicals [89]. A subtraction procedure for the CO_2^* from the band-pass filtered OH^* emission measurement was proposed by Lauer and Sattelmayer [91]. Multiple band-pass filters centered at different wavelengths were used in the proposed representative measurement technique with the final correction process carried out using the data substituted into equations developed by the authors. Band-pass filtered measurement, therefore, can only be used without correction to measure the relative integral intensity of the intermediate radicals, and that is proportional to an integral heat release rate. This type of measurement has been carried out for thermoacoustic stability analysis in different studies [94-96].

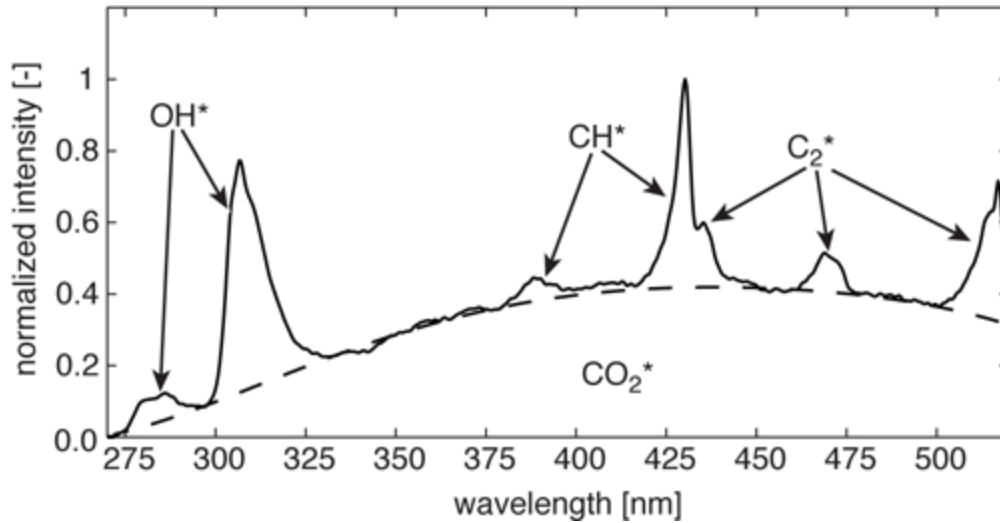


Figure 2.3: Typical chemiluminescence spectrum of a turbulent, premixed flame [89]

2.3.4 Effect of combustion conditions on thermoacoustic instability

While there is no such thing as a stable fuel, combustion of hydrocarbon fuels is reported to lead to different instability characteristics compared to other fuels like syngas because of their respective differences in heat release characteristics [97]. In other words, irrespective of the fuel, it is the interaction between the flame and the acoustic field of the combustor that leads to dynamic instabilities. Consequently, for the same burner and combustor assembly, combustion of different fuel mixtures will exhibit varying amplitudes and frequencies of instability. This is because as the fuel nature changes, important combustion characteristics like flame speed equally changes altering both the flame's shape and position. These factors are of paramount importance to the nature and magnitude of thermoacoustic instability. A flat-shaped flame, for instance, is thermally compact and, therefore, releases energy to a comparatively smaller area leading to

acoustic intensifications. High concentrations of hydrogen in fuel mixture is shown to drastically affect, in a positive manner, the flame anchoring as well as shaping the flame into an elongated V-shape that dampens acoustics strength. Allison et al. [97] reported lower acoustic amplitude from a V-shaped, anchored, non-resonating flame for hydrogen-rich syngas fuel in contrast to a flat-shaped flame produced by some hydrocarbon fuels. Narrower region for amplification or damping of combustion instability, accompanied by high heat-release density, is however reported for hydrogen-rich flames [98].

Swirling flows are characterized by vortex breakdown. Flow separation from flame holders causes the formation of vortical structures known as recirculation zones. The size, shape, and location of these coherent structures changes with combustor geometry and combustion parameters like the fuel and oxidizer composition. Coupling between the flame's heat release fluctuations and flow vortex can lead to amplification of thermoacoustic instability. Flame oscillations in swirl-stabilized combustors can be a direct consequence of flow-vortex interactions occurring primarily in the region around the outer shear layer, downstream of the injector nozzle [99]. For fuel having comparatively higher reactivity like hydrogen, due to high flame speed, the vortex may be very small or even not visibly present rendering the flame-vortex coupling unlikely. Therefore, a comparatively lower acoustic amplitude is reported for hydrogen-rich syngas combustion when compared with methane combustion [100, 101]. Similarly, wider flammability limit of hydrogen in hydrogen-containing fuels hinders heat release oscillation that results from recurrence of extinction and re-ignition. It is in line with this, that hydrogen injection onto a premixed mixture of hydrocarbon fuel and oxidizer was proposed as a technique for the control of combustion instability [102].

Flames have their highest speed at stoichiometric or slightly rich mixtures. Hence, an equivalence ratio perturbation affects the flame speed. As flame speed increases, the flame correspondingly shortens reducing the distance to the center of heat release. This reduction in distance shortens the convecting time for equivalence ratio perturbations, rendering an unstable flame stable. The reversed case can also be true for a stable flame [103]. It is reported by Speth et al. [103] that higher equivalence ratios are associated with a higher frequency of oscillations in contrast to a lower frequency, weakly oscillating, quasi-stable flames observed at intermediate equivalence ratios. The effects of hydrogen concentration and equivalence ratio on flame stability for methane blended with hydrogen and a syngas fuel mixtures were also studied by Zhang et al. [104]. High equivalence ratios and hydrogen concentration in the methane-hydrogen mixture was found to increase the frequency of pressure oscillations for the premixed, air-oxidized flames as opposed to the vortex-driven instability discussed above. As can be seen in Figure 2.4, beyond the equivalence ratio of 0.65, an increase in the frequency of pressure oscillation is apparent. Also from the figure, in contrast to methane-hydrogen flames, the thermoacoustically unstable zones for syngas flames are confined in a narrow range of lean equivalence ratios (about a mean of 0.24). That range slightly enlarges with an increase in hydrogen concentration. High hydrogen content in fuel mixtures and high equivalence ratio of operation are sources of high heat release densities in combustion systems. Increasing hydrogen content is shown to enhance the flame's extinction resistance (Blowout limit) while making the flame more prone to flashback. A hydrogen volume of about 60% will trigger the occurrence of flashback.

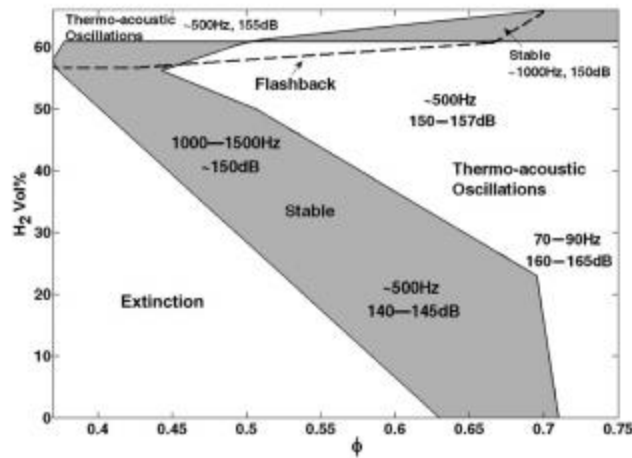


Figure 2.4: Effect of hydrogen concentration and equivalence ratio on stability of hydrogen-enriched methane flames blended with N₂ [104]

Thermoacoustic instability has been extensively studied in air oxidized premixed combustion systems as reviewed by Lieuwen [105]. Flames dynamic response relative to operating conditions in propane/hydrogen premixed flames was studied by Hong et al. [106]. The authors reported that the operating conditions (parameters like H₂ concentration and equivalence ratio) studied collapses into a family of curves that defined the state of the combustor within a mode. Other studies involving air-oxidized premixed flames include [30, 67, 75]. Some of the work on non-premixed flames focuses on utilizing acoustic excitation to enhance mixing and to reduce NO_x in air-oxidized combustion systems. Flame-vortex interaction of turbulent hydrogen non-premixed flames under acoustic forcing was studied by Kim et al. [107] and a decrease in flame length up to 15% accompanied by a reduction in NO_x emissions was reported. A similar study also reported the use of acoustic excitation in NO_x reduction for non-premixed flames [108].

Thermoacoustic instability literature focusing on non-premixed combustion are mostly based on air-oxidized combustion systems. These include Tyagi et al. [109]; a qualitative study of thermo-acoustics, which reported that Damkohler number (Da ; the ratio of residence to chemical time) plays an important role in determining the phase and amplitude of heat release fluctuations relative to flow fluctuations. Balasubramanian et al. [32] studied the combined effect of non-normality and nonlinearity in combustion systems in triggering thermo-acoustic instability mode. Idahosa et al. [96] studied the response of non-premixed swirl-stabilized flames to forced acoustic perturbations and formulated a flame response index analogous to Rayleigh index in non-forced systems. Thermoacoustic instability in colorless distributed combustion (CDC) of methane accomplished by maintaining oxygen concentration below 15% in oxidizer mixture through N_2/CO_2 dilution was studied by Khalil et al. [95]. The authors reported a decrease in heat release fluctuations and hence decrease in sound pressure level (SPL) with a decrease in equivalence ratio. Furthermore, they reported an increase in heat release fluctuation with an increase in CO_2 dilution at low concentrations. These fluctuations, however, were reported to get dampened at high CO_2 concentrations resulting in low acoustic amplitude in CDC mode (Figure 2.5).

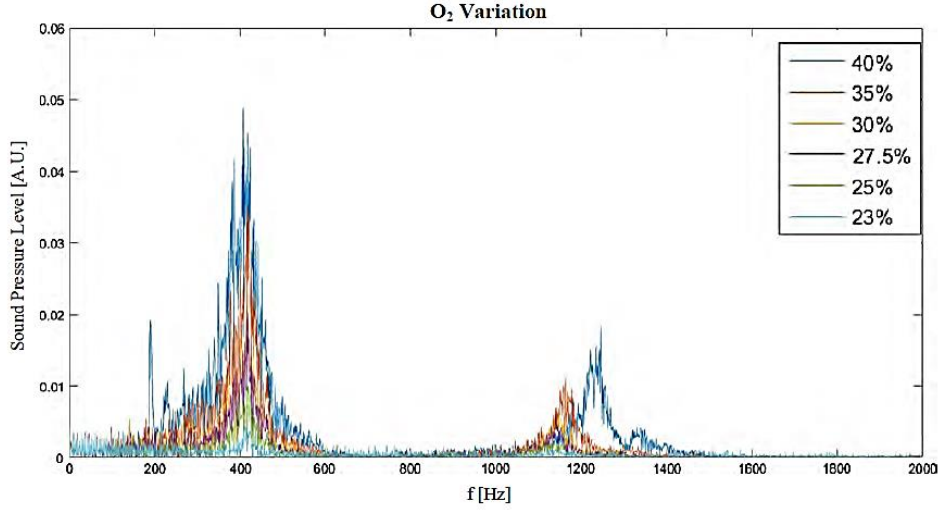


Figure 2.5: Acoustic frequency response for CDC combustion in O₂-CO₂ mixture[95]

Oxyfuel flame's dynamic instability in a premixed burner with sudden expansion was studied by Ditaranto et al. [19] where low frequency and low amplitude oscillations controlled by the flame length were reported. Furthermore, they reported that variation in mass flow rate is attributable to the heat release and pressure fluctuations observed. Instability in a partially premixed gas turbine combustor utilizing O₂/CO₂ oxyfuel oxidizer mixture was studied by Kutne et al. [23]. They reported that depending on O₂ concentration, there exists a window, where thermoacoustic pulsations were observed in the combustor. At the O₂ concentrations resulting in these oscillations (34% and 38% O₂), the oxyfuel flames were observed to be flat-shaped in contrast to conically shaped non-pulsating flames. Li et al. [110] studied dynamic instability of CH₄/O₂/CO₂ oxyfuel flames in comparison to CH₄/O₂/N₂ flames in a swirl-stabilized combustor and reported strong acoustic oscillations in relation to the oxyfuel cases. They also reported temporal pressure oscillations of large magnitudes. Table 2.1 summarizes the effect of combustion conditions on thermoacoustic instability obtained from the literature.

Table 2.1: Effect of combustion conditions on thermoacoustic instability in air and oxyfuel combustion

References	Combustor Geometry	Mixture Studied	Parameters Varied	Measurements carried out	Comments
Allison et al. [97]	Non-premixed, dual-swirl burner of square cross-section	Air-oxidized, H ₂ /CO compared with C ₂ H ₄ , C ₃ H ₈ , and CH ₄	Equivalence ratio, Fuel Compositions, air flow rate, and burner geometry	Pressure was measured. Frequency and amplitude of pressure oscillation was obtained from the measurement	Burner geometry, air flow velocity, flame speed, and the amount of H ₂ in fuel affect thermoacoustic instability. Also, syngas fuels exhibit different instability behavior from hydrocarbons.
Lee et al. [100]	Non-premixed, swirl-Stabilized annular combustor	Air-oxidized, Syngas (H ₂ /CO) compared with Natural gas	Fuel composition and flow rate varied	Pressure, temperature, and emissions	Amount of H ₂ strongly affects the formation of recirculation zone and, therefore, vortex-breakdown-induced instability. As a result, no instability was observed with hydrogen-rich fuel as was observed in natural gas combustion
Lee et al. [98]	Partially premixed, Swirl-stabilized annular combustor	Air-oxidized, Syngas (H ₂ /CO/C H ₄)	Syngas Fuel composition varied	Pressure, flame images, and Temperature	High H ₂ reactivity in the syngas mixture affects the flame structure and consequently combustion instability
Davis et al. [101]	Premixed, Low-Swirl Injection (LSI) cylindrical combustor	Air-oxidized, CH ₄ and H ₂ /CH ₄ mixtures	H ₂ /CH ₄ and CH ₄ Flames were compared	Pressure, Heat release using OH* chemiluminescence, and PIV used for flow	Different flame structures observed. The vortices formed in CH ₄ flames results in fluctuating heat

				characterization	release rates compared to a consistent burning of H ₂ -enriched CH ₄ .
Therkelsen et al. [99]	Premixed, Low-Swirl Injection (LSI) Cylindrical chamber	Air-oxidized, CH ₄ And H ₂ /CH ₄	Equivalence ratio and fuel composition	Pressure, flame motion using laser detection, and PIV used for flow characterization	Based on the laser detected flame motion, location and frequency of the flame oscillations were determined. More self-excited oscillations at rich conditions.
Speth et al. [103]	Premixed, Swirl-Stabilized Cylindrical tube	Air-oxidized, Syngas (H ₂ /CO)	Fuel composition and equivalence ratio varied	Pressure and high-speed video	Strained flame speed can be used instead of the multi-functional parameterization (fuel composition and equivalence ratio) to characterize the instability modes in the combustor.
Lee et al. [111]	Non-premixed, Swirl-stabilized annular combustor	Air-oxidized, Syngas (H ₂ /CO) with H ₂ O, CO ₂ , and N ₂ diluents	Syngas Fuel composition and flow rate varied	Pressure, temperature, and emissions	The diluents affected emissions but little effect on combustion instability was observed
Garcia et al. [29]	Premixed, Swirl-stabilized cylindrical quartz combustor	Air-oxidized, H ₂ /CO/C H ₄	Fuel composition	Pressure, Temperature, Flame images and Heat release using OH* chemiluminescence	At high H ₂ concentration in the fuel mixture, blowout limits are extended while flashback-induced thermoacoustic instability was observed
Khalil et al. [94]	Partially premixed, swirl-	Oxyfuel combustion, CH ₄	CO ₂ dilution level in O ₂	Pressure, CH* chemiluminescence using PMT,	Heat release fluctuations increase with the

	stabilized colorless distributed combustion (CDL) burner	with varying CO ₂ concentrations in O ₂		flame images and temperature	increase in CO ₂ dilution at low concentrations. At high CO ₂ concentrations, the fluctuations get dampened
Khalil et al. [95]	Partially premixed, swirl-stabilized colorless distributed combustion (CDL) burner	Oxyfuel combustion, CH ₄ with varying CO ₂ and N ₂ /CO ₂ concentrations in O ₂	Equivalence ratio, CO ₂ and N ₂ /CO ₂ dilution level in O ₂	Pressure, CH* chemiluminescence using PMT, flame images and temperature	Heat release fluctuations decrease with the decrease in equivalence ratio. Although, at around frequency of 200 Hz, some level of coupling between pressure and heat release fluctuations exists for equivalence ratios
Ditaranto et al. [19]	Premixed, sudden expansion burner with a square cross-section	Oxyfuel combustion, CH ₄ with varying CO ₂ concentrations in O ₂	CO ₂ dilution level in O ₂ , Equivalence ratio, and Reynolds number	Pressure, CH* chemiluminescence, and velocity	The flame oscillations are controlled by its length. Subsequently, variation in mass flow rate is attributable to the heat release and pressure fluctuations
Kutne et al. [23]	Partially premixed, swirl-stabilized gas turbine model combustor	Oxyfuel combustion, CH ₄ with varying CO ₂ concentrations in O ₂	CO ₂ dilution level in O ₂ , Equivalence ratio, and combustor power	Pressure, OH* chemiluminescence. Also, species concentrations, mixture fraction and temperature using Raman scattering technique	Depending on O ₂ concentration, there exists a window where thermoacoustic pulsations were observed in the combustor. The oxyfuel flames were observed to be flat-shaped in the pulsating mode

Li et al. [110]	Non-premixed, swirl-stabilized combustor	Oxyfuel combustion, CH ₄ /O ₂ /C O ₂ oxyfuel flames in comparison to CH ₄ /O ₂ /N ₂ flames	CO ₂ dilution level in O ₂ , Equivalence ratio, and combustor power	Pressure, temperature, and species concentration	A distinctive feature of combustion instability was observed when the two different oxidizers were employed even at the same O ₂ concentrations. Also, a strong acoustic oscillation was reported in relation to the oxyfuel cases.
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2.3.5 Static instability in combustion systems

Static stability limit of combustors is characterized by their blowout propensity. This aspect of instability results from a flame getting lifted from its anchoring position followed by its subsequent extinction or even directly going extinct without apparent transitions [112]. The driving mechanism for such instability requires that the essential time for the combustion chemical reaction to occur be longer than the residence time (or mixing time) of the combustion species such that the reaction cannot be sustained [28]. Consequently, static instability is a result of the competition between the rate of reaction and the rate of diffusion of species and energy [25-27]. Blowout phenomena in premixed flames, therefore, occurs when the characteristic chemical reaction time is longer than the propagation rate of the combustion species [28]. Or in case of non-premixed flames, it occurs when characteristic chemical time exceeds the characteristic mixing time (local

fluid mechanical mixing time) in the combustor. The mixing time is the time available for “back-mixing” of hot combustion products with fresh reactants by large-scale flow structures [113].

Critical Damkohler number also known as mixing time scale defined as the ratio of residence time to chemical time at blowout can be used to predict the range of static stability for certain combustion conditions [29]. If the residence time is quantified by the ratio of a length scale (L) to velocity scale (reference velocity; U_{ref}) and chemical time by the ratio of thermal diffusivity (α) to the square of laminar flame speed (S_L^2), Damkohler number (Da) can be expressed as follows:

$$\text{Damkohler number, } Da = \frac{\text{Residence time } (\tau_{res})}{\text{Chemical time } (\tau_{chem})} = \frac{LS_L^2}{U_{ref}\alpha} \quad (2.7)$$

The expression can also be written using the Arrhenius kinetic rate formula by replacing the characteristic chemical time as seen in Equation (2.8).

$$Da \sim \frac{\tau_{res}}{\alpha} \exp\left(\frac{-E_A}{RT_f}\right) \quad (2.8)$$

Where T_f is the flame temperature in Kelvin, E_A is the activation energy (the minimum energy needed for the reaction to occur expressed in joules per mole), and R is the gas constant. A high magnitude of Damkohler number ($Da \gg 1$) entails reaction rate that is much greater than the diffusion rate leading to fast chemistry and chemical equilibrium. Low magnitude Damkohler number ($Da \ll 1$) on the other hand entails that diffusion of species occurs much faster than the chemical reaction leading to slow chemistry or even flame extinction at some critical value [114].

To use Damkohler number in predicting static stability limits, each of the defining parameters needs to be measured or determined. For turbulent flames, the residence time is proportional to the turbulent integral time scale [115]. The laminar flame speed and thermal diffusivity can be obtained from any chemical kinetics modeling codes like CHEMKIN. To quantify the residence time using length scale and reference velocity, these two quantities need to be obtained. The characteristic length scale could be the length of the recirculation zone in a swirling flow while the reference velocity could be the flow velocity of incoming reactants. Use of reactants flow velocity (U_0), however, would leave out the effect of burned gas velocity which is a strong function of temperature. Subsequently, the reference velocity is the function of both the flow velocity and that of the ratio of the burned gas temperature to reference temperature ($\frac{T_b}{T_0} U_0$) [116]. Broadwell et al. [117] propose quantifying the mixing time by the ratio of length scale d_s to centerline axial velocity U_s (proportional to d_f and U_f , respectively) evaluated at an axial distance proportional to the flame length (L) in non-premixed turbulent flames. The chemical time was quantified by the authors as the ratio of thermal diffusivity of stoichiometric, hot gas in flame, α_s (proportional to α_f) to the square of laminar flame speed (S_L^2).

Another approach to predicting blowout limits is to look at the flame propagation concept. This is achieved by relating the turbulent flame propagation velocity with the velocity of the incoming mixture to the combustion zone. Turbulent flame velocity is quite challenging to measure as it is a function of all the three-dimensional velocity fluctuations as well as the combustor geometry [118]. In recent practical combustion

applications, issues related to static instability has been partly attributable to the following:

- The drive for lean combustion to reduce NO_x emissions in air oxidized systems[119]; a lean flame is more susceptible to blowout.
- Changing the working fuel and/or oxidizer like in syngas combustion or oxyfuel combustion. Excessive flow rates may be required to maintain the power generated by a gas turbine optimized for a different fuel. This increase in flow rates further strengthens the blowout propensity as it reduces the flow residence time [120]. Also, differences in oxidizer properties need to be accounted for in case of oxyfuel combustion [21].
- Optimum design of flow passages in combustors. The use of swirlers, for instance, affects the blowout propensity since variation in swirl number affects the tendency of external air entrainment, the mixing, and consequently the quenching effect [56].

Apart from blowout, a flame can also *flashback* by physically propagating upstream of its anchoring position primarily as a consequence of higher flame speed relative to the flow velocity in premixed flames [121, 122]. For flashback mechanism emanating from turbulent flame propagation, the local turbulent flame speed is higher than the local flow velocity. In a boundary-layer-driven flashback mechanism, the burning velocity has to be higher than the unburned gas velocity. This happens at the so-called critical velocity gradient, which is proportional to the ratio of the squared laminar burning velocity to thermal diffusivity [123, 124]. The constant of proportionality, in this case, depends on

the geometry of the burner. Flame flashback could also arise from vortex breakdown induced by combustion, particularly in swirl-stabilized combustors. In this mechanism, the flame itself or its anchoring position shifts continuously upstream as a result of vortex breakdown caused by the flame. This is because as the flame causes vortex breakdown, it will trigger a negative flow area downstream that will cause a change in the location of the subsequent vortex breakdown and therefore the flame moves upstream [125, 126].

Flashback is particularly prominent with premixed flames as the fuel and air are already mixed, and could easily be ignited by the backward moving flame, to be propagated upstream. A flame that flashes back eventually finds its way into the premixing chambers intensifying concern for high temperatures in regions not designed primarily to withstand that. Example of such regions includes combustor hardware like fuel nozzle as well as the piping work upstream of the combustor. Flashback is particularly an issue in fuels with a varying composition like syngas due to different concentration of the fuel constituents like hydrogen that is known to alter the kinetics of the mixture [127]. When in a mixture, hydrogen can alter the local equivalence ratio as a result of its high molecular diffusivity and accordingly increase local flame speed. Consequently, fuel-rich mixtures containing hydrogen display intense flashback propensity [128]. Flame blowout and flashback could trigger thermoacoustic instability in combustors leading to high amplitude pressure oscillations that can cause severe damage.

2.3.6 Effect of combustion conditions on static instability

Experimental investigations into the blowout limits generally employ the use of visual techniques from imaging, whereas, for flashback, temperature sensors upstream of the flame are used to detect a possible rise in temperature. In hydrogen enriched fuels and syngas the major role as regards static stability is played by hydrogen concentration. Hydrogen-containing fuels depending on its concentration are characterized by relatively higher flame speeds. As a result, the blowout limit is enhanced as their hydrogen concentration increases. Consequently, fuel mixtures containing a higher amount of hydrogen will stably burn at relatively leaner equivalence ratios [27, 129-132]. Flashback propensity, however, increases with an increase in hydrogen concentration.

Table 2.2 shows blowout and flashback limits, for methane and syngas mixtures in a premixed burner using air as oxidizer [118]. The limits are given for different insert (a restriction in the injection duct) geometries and locations. It can be observed from the table that higher hydrogen concentration in the fuel mixture enhances the blowout limit while aggravating flashback tendencies. At high hydrogen concentrations, flashback occurs even at lean equivalence ratio. The strong dependence of boundary layer driven flashback on combustor pressure and mixture inlet temperature has been also reported [133]. High inlet temperatures are associated with an increase in flashback propensity. Due to the enhanced resistance to extinction exhibited by flames containing hydrogen, it is widely recommended for extending blowout limits of lean premixed combustion [26, 121]. Consequently, hydrogen-enriched flames blowout at comparatively lower equivalence ratios [131]. Many authors have reached similar outcomes on sustaining

flames at low equivalence ratios around 0.5 at gas turbine conditions because of hydrogen enrichment [134-136]. Also, flames with relatively lower hydrogen concentration were reported to “blowout” abruptly. This is in contrast to a clear and distinct liftoff and subsequent blowout that was reported at higher percentages of H₂ in fuels [121].

Table 2.2: Stability limits for methane and syngases for different insert geometries and locations. () denotes cases in which flashback was accompanied by strong flame oscillations. Reproduced from Cheng et al. [118]**

Fuel	30° @ 0mm	30° @ 28mm	45° @ 0mm	45° @ 28mm
Fuel 1: 100CH ₄	0.6/>1.1	0.57-1.05	0.64/>1.15	0.57-1.1
Fuel 2: 90CH ₄ :10H ₂	0.62-1.05	0.56-0.86	0.62-1.1	0.65-0.91
Fuel 3: 75CH ₄ :25H ₂	0.57-0.97	0.54-0.79	0.57-1.05	0.56-0.7
Fuel 4: 50CH ₄ :50H ₂	0.46-1.02	0.46-0.57**	0.46-1.1	0.47-0.56**
Fuel 5: 40CH ₄ :50H ₂ :10CO	0.45-0.77	0.43-0.53**	0.45-0.77	0.49-0.56**
Fuel 6: 30CH ₄ :50H ₂ :20CO	0.43-0.66	0.39-0.5**	0.43-0.72	0.45-0.54**
Fuel 7: 20CH ₄ :50H ₂ :30CO	0.38-0.61	0.38-0.47**	0.38-0.61	0.36-0.48**
Fuel 8: 50H ₂ :50CO	0.31-0.44	0.31-0.38**	0.31-0.44	0.32-0.37**

The effect of swirl number on flame blowout was studied by Abdulsada et al. [137] for five different fuel blends with hydrogen and reported relatively extended static stability limit at high swirl numbers. Also, a positive influence of exhaust confinement on flame blowout was reported by the same authors. Open combustors were reported to display higher vulnerability to blowout compared to combustors having exhaust confinement.

Similarly, gravity effect was reported to affect the prediction of flames extinction rates. This is due to buoyancy imposed on the species convection by gravity [138].

Flame flashback that is driven by combustion induced vortex breakdown for syngas mixtures was studied by Bidhan et al. [139]. Using a PIV system, the vortices formation in the swirling flow field was studied by the authors exposing intricate vortex-combustion interactions. Subsequently, a decreasing flashback propensity with an increase in swirl number was reported. The examination of the flow field in both stable and flashback situations gives some insight into the mechanism triggering the transition from a stable flame to flashback regimes. A more detailed explanation of the effect of the swirling flow on flashback propensity can be found in reference [140]. It is suggested that during eccentric conditions, a transitory escalation in swirl eccentricity could result in a reduction in flow angular velocity causing a decrease in swirl number. Accordingly, this could hold up or reverse the flashback incidence. Flashback could also be triggered by periodic pressure fluctuations accompanying thermoacoustic instabilities and vice versa. This is because of the coupling of periodic flashback with the combustor acoustics modes through a sustained positive feedback mechanism [141].

For oxyfuel combustion, additional concern as regards static stability arises from the use of diluent to lower high temperatures associated with the use of pure oxygen. This is because the substitution of air with pure oxygen in combustion systems will warrant exhaust/flue gas recirculation (EGR) in order to maintain similar combustion conditions. The common suggestion is to inject recycled CO_2 into pure oxygen to form O_2/CO_2 oxidizer with the CO_2 concentration in the mixture utilized to achieve the desired lower combustion temperatures oxidizer mixture [16, 17]. Consequently, for oxyfuel

combustion, the O_2 /diluent oxidizer ratio plays an important role in terms of static stability [19]. Up to 70-79% by volume of CO_2 concentration in the O_2/CO_2 oxidizer mixture was reported in the literature for gas turbine applications [94, 142]. The experimental conditions varied by Habib et al. [142] includes O_2/CO_2 oxidizer mixture from 100/0 to 25/72 and equivalence ratio from 1.0 to 0.5 for the methane fuel used. Below 30% oxygen in the oxidizer mixture, however, the flame was reported to be unstable even near stoichiometric conditions while the combustion temperature becomes lower in comparison to air-oxidized systems [20, 143]. This is in clear difference to the higher concentration of N_2 in air oxidizer (79%) where flames can propagate stably even at lean equivalence ratios higher than the lean blowout limit. The dissimilarities between air and O_2/CO_2 oxidizer arise as a result of lower thermal diffusivity of CO_2 , its greater thermal radiation, and its cooling effect in comparison to N_2 [21, 22].

There are some studies focusing on the effect of CO_2 dilution on the static stability of oxyfuel flames [144]. Effect of O_2 concentration in O_2/CO_2 oxidizer mixture in the range of 20-40% was studied by Kutne et al. [23]. They reported that the CO_2 concentration in the O_2 oxidizer plays a more important role regarding flame stability than the operating equivalence ratio. The stability of non-premixed, swirl-stabilized, Methane-oxyfuel flames was studied by Saanum et al. [145]. It was reported that the flames transit from V-shaped to an M-shaped structure before liftup and subsequent blowout. It is remarkable that one of the major drivers of static instability in air combustion systems; operating combustors near lean blowout limits is not a concern in oxyfuel combustion. This is because the need for lean combustion to minimize thermal NO_x emissions is eliminated by the use of pure oxygen instead of air. Moreover, the cost of oxygen separation for

oxyfuel combustion makes lean combustion very costly and unattractive. Therefore, operating a combustor near stoichiometric equivalence ratio is favorable with respect to static stability as well as cost.

In an air oxidized combustion systems utilizing lean mixtures, the use of hydrogen enrichment to enhance the static stability limit of the flames is a common practice. A similar approach can be employed to enhance the oxyfuel flame stability limit under the influence of a diluent like CO₂. Sanusi et al. [146] and Said et al. [147] studied experimentally the effect of hydrogen addition to Methane-oxyfuel flames in non-premixed gas turbine model combustors. Hydrogen enrichment was reported to increase the CO₂ concentration at which the onset of static instability was observed. When hydrogen concentration was increased from 0 to 50 % in the methane/hydrogen fuel mixture, up to 15 % increase in CO₂ concentration at blowout was reported by Said et al. [147]. Table 2.3 summarizes the effect of combustion conditions on static instability obtained from the literature.

Table 2.3: Effect of combustion conditions on static instability in air and oxyfuel combustion

References	Combustor Geometry	Mixture Studied	Parameters Varied	Measurements carried out	Comments
Daniele et al. [129]	Premixed, Swirl-stabilized coaxial cylindrical quartz combustor	Air-oxidized, H ₂ /CO/CH ₄	Composition, velocity, and pressure	OH* chemiluminescence using photomultiplier tube and turbulent burning velocity using OH-LIF	Near lean blowout limit (LBO), local extinction ensures leading to high CO emissions. Also, low-frequency oscillations were observed near LBO that can feed thermoacoustic instability leading

					to blowout
Strakey et al. [148]	Premixed, Swirl-stabilized cylindrical quartz combustor	Air-oxidized, CH ₄ and H ₂ /CH ₄	Hydrogen concentration, equivalence ratio, inlet velocity, and pressure	Optical access for blowout visualization	For H ₂ concentration in CH ₄ varied from 0 – 80%, the equivalence ratio at blowout decreased from 0.46-0.3. Also, little effect of pressure in the combustor (varied from 1-8 atmospheres) on blowout was observed.
Hwang et al. [26]	Nom-premixed, Rectangular-shaped combustor with Coaxial air supplied	Air-oxidized, Syngas (H ₂ /CO)	Fuel and air velocities, Compositions, and nozzle diameter	OH* chemiluminescence and Imaging	Flow velocities and fuel compositions affect the stability limits; flashback, flame attachment, and blowout
Noble et al. [121]	Premixed, Swirl-stabilized square combustor and cylindrical quartz tube	Air-oxidized, H ₂ /CO/CH ₄	Fuel Composition and Equivalence ratio	Temperature upstream of the combustor for flashback and an optical system for blowout	Fuel composition, as well as the equivalence ratio, affects both the Blowout and Flashback characteristics
Abdulsada et al. [137]	Premixed, swirl-stabilized combustor with confinement and unconfined	Air-oxidized, H ₂ /CH ₄	Fuel composition, Swirl number, burner geometry	Velocity and visual observations	Both the fuel composition and swirl number affects the mechanism of Blowout. Also, confinement affects the blowout characteristics
Zhang et al. [138]	Premixed, Counter-flow micro-gravity combustor	Air-oxidized, H ₂ /CO/CH ₄ CO ₂ , and N ₂	Equivalence ratio and composition at both Micro and Normal Gravity	Flame imaging captured using a high-resolution CCD camera	Gravity affects flame stabilization and extinction characteristics due to buoyancy
Sanusi et al. [146]	Non-premixed,	Oxyfuel combustion	CO ₂ dilution level in O ₂ ,	Temperature and flame	The high CO ₂ concentration in

	swirl-stabilized cylindrical combustor	of H ₂ -enriched CH ₄ with varying CO ₂ concentrations in O ₂ oxidizer	H ₂ concentration, and combustor firing rates	images	(O ₂ /CO ₂) oxidizer reduces the flame burning rate leading to static instability. Static stability of the oxyfuel flames under CO ₂ dilution can be enhanced by hydrogen enrichment.
Saanum et al. [145]	Non-premixed, swirl-stabilized, pressurized combustor	Oxyfuel combustion of CH ₄ with varying CO ₂ concentrations in O ₂ oxidizer	CO ₂ dilution level in O ₂ oxidizer, fuel power loads and combustor pressure	Flame images, emissions, and pressure	A trade-off between static instability and excessive temperature in the combustor is reported. The combustor pressure and power loads affect the O ₂ concentration at blowout.
Habib et al. [142]	Non-premixed, swirl-stabilized cylindrical combustor	Oxyfuel combustion of CH ₄ with varying CO ₂ concentrations in O ₂ oxidizer	CO ₂ dilution level in O ₂ , and Equivalence ratio	Temperature, emissions and flame images	The flames irrespective of the range of operating conditions (like equivalence ratio) blowout at O ₂ concentration below 21%
Syred et al. [128]	Premixed, Swirl-stabilized tubular burner	Air-oxidized, CH ₄ , H ₂ /CH ₄ and H ₂ /CO/CH ₄ with diluents CO ₂ and N ₂	Fuel composition, and Swirl number	Flame imaging captured using high-resolution CCD	Boundary layer flashback mechanism dominates at low swirl numbers and combustion-induced vortex breakdown at higher swirl numbers
Dam et al. [124]	Premixed, Honeycomb-induced, laminar flow, cylindrical burner, and swirl-	Air-oxidized, H ₂ /CO, and H ₂ /CH ₄	H ₂ concentration, swirl number, and external excitation	Establish flashback via visual technique by recording video and images	H ₂ % affects both the boundary layer and combustion-induced vortex breakdown flashback mechanisms.

	stabilized cylindrical burner				Boundary layer flashback tendencies vary non-linearly with H ₂ %
Tuncer et al. [141]	Premixed, Swirl-stabilized cylindrical quartz tube with exhaust confinement	Air-oxidized, CH ₄ , and H ₂ /CH ₄	Fuel composition	Pressure, emissions and heat release using OH-PLIF	The amount of H ₂ in CH ₄ flames intensifies the flashback propensity. Also, the study distinguishes the nature of flashback induced by thermo-acoustic instability and regular flashback
Dam et al. [139]	Premixed, Swirl-stabilized quartz combustor	Air-oxidized, CH ₄ , H ₂ /CO and H ₂ /CO/CH ₄ with diluents CO ₂ and N ₂	Fuel constituents & compositions, and Swirl number	Imaging system and PIV for flow characterization	The combustion-induced vortex breakdown (CIVB) flashback is dominantly affected by H ₂ % in fuel mixtures, also its propensity decreases with swirl number increase

CHAPTER 3

RESEARCH METHODOLOGY

3.1 Overview

The research methodology employed in this study to achieve the set objectives involves both experimental and numerical techniques. In the experimental technique, the reactants are combusted in a swirl-stabilized, non-premixed burner, having a quartz glass cylindrical confinement. Over the wide range of operating conditions studied, the reactants are supplied accordingly into the combustor, while measurements of the parameters of interest are conducted under steady state conditions. The parameters of interest measured in the experiments are temperature, emissions, sound pressure, heat release intensity, flame images, and blowout point. Schematic of the experimental rig used in this study is shown in Figure 3.1. The rig consists of Propane and Hydrogen fuel cylinders, oxidizer cylinders, stainless steel flow lines and fittings, and computer controlled mass flow meters. The CO₂ diluent used in the oxidizer was mixed with the pure oxygen stream in a mixing chamber upstream of the combustion chamber. Propane fuel and hydrogen are similarly mixed in cases dealing with hydrogen enrichment. The propane, hydrogen, and oxygen gases used throughout the experiments are acquired from Specialty Gases Company Ltd (SGC) and have a purity of 99.9%. Air oxidizer is supplied by an air compressor that can supply pressurized air at pressure up to 150 bar. All the

reactants are supplied to the combustor from their respective sources via mass flow controllers manufactured by Bronkhorst High-Tech.

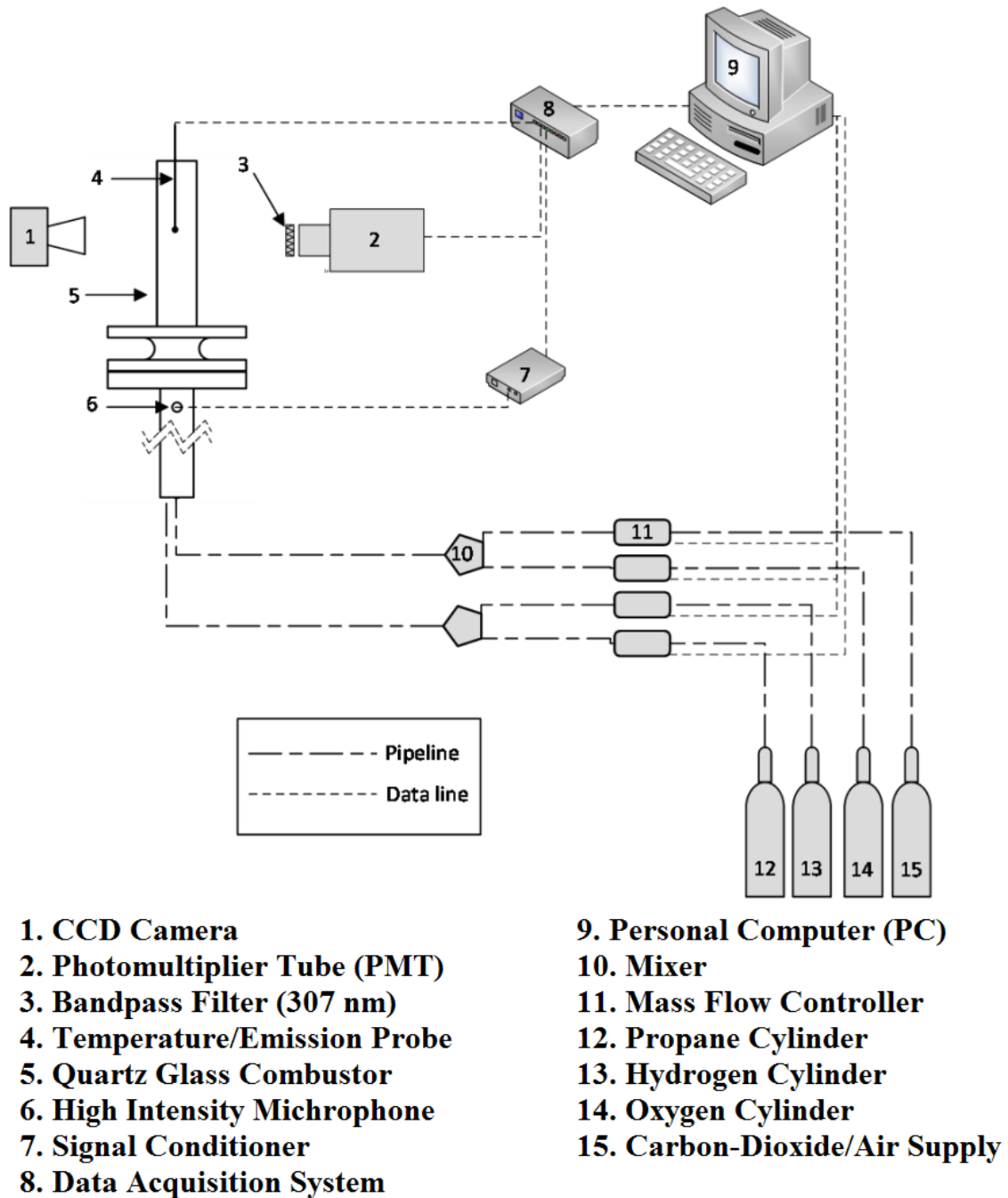


Figure 3.1: Schematic of the experimental setup

In addition to the experimental study, a numerical study was conducted using computational fluid dynamics (CFD) codes to gain more insight into the combustion characteristics. The CFD code used in this study is ANSYS Fluent; a commercial code based on the finite volume scheme. The conservation equations for mass, momentum, energy, and species are solved using the CFD codes in a meshed, 2-dimensional domain under steady state conditions. In addition to these conservation equations, radiative transport equation (RTE) is solved to account for the radiation contribution to the overall heat transfer. Furthermore, the turbulence in the flow is accounted for through an averaging technique.

3.2 The Burner Details

The combustor used in this study, together with the flange containing the swirler, fuel supply pipe, and an oxidizer supply channel is shown in Figure 3.2. The combustion chamber is a cylindrical quartz glass tube of 70 mm diameter and 300 mm length that is open to the atmosphere at the exhaust side.

Figure 3.3 shows the details of fuel and oxidizer supply lines. The combustor fuel nozzle is a 6.35 mm diameter pipe having 16 fuel channels ($0.13 \text{ mm} \times 0.45 \text{ mm}$) arranged around its circumference. These channels are created by the use of a bluff body centered on top of the fuel pipe. The swirler is located beneath a cone-like oxidizer orifice designed to increase the velocity of the swirling oxidizer.

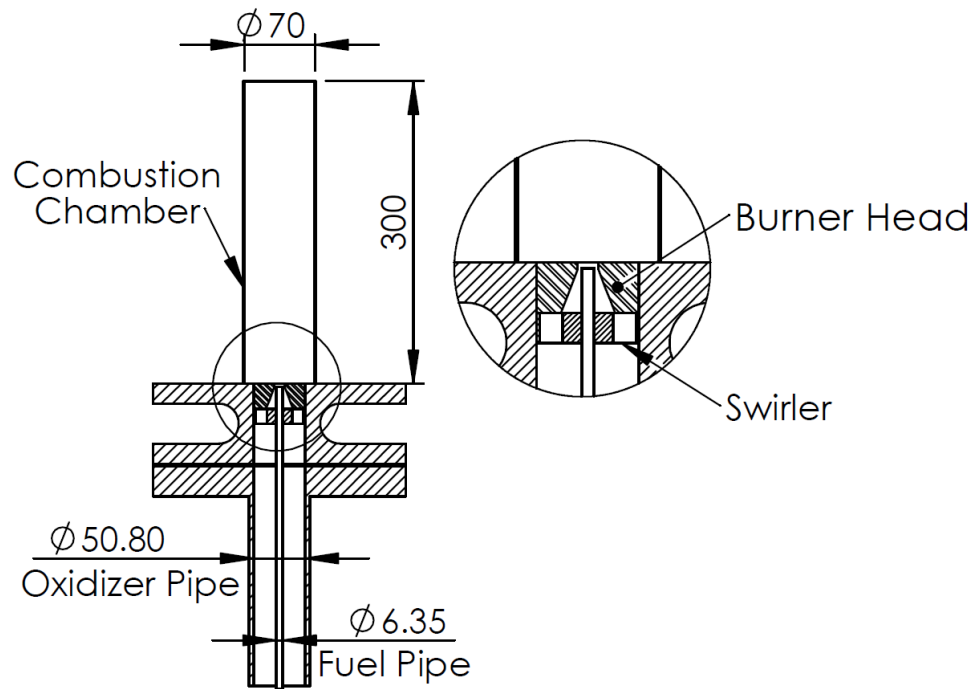


Figure 3.2: Details of the combustion chamber, fuel, and oxidizer pipes (all dimensions are in mm)

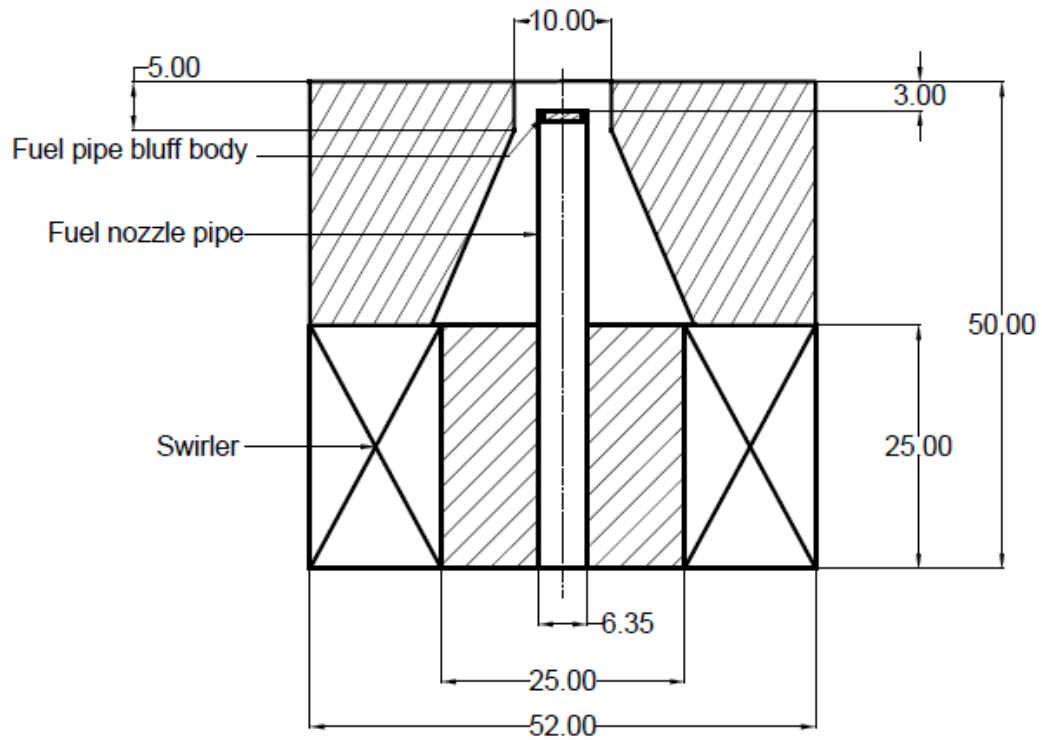


Figure 3.3: Details of the burner head (all dimensions are in mm)

The swirler used for flame stabilization is an axial type having 8 vanes, and it is situated upstream of the combustor dump plane. Three different swirlers having swirl numbers corresponding to 0.6, 1.0, and 1.5 based on their vane angles (30, 45, and 55 degrees, respectively) are used in this study. The swirl number defined as the ratio of the axial flux of angular momentum to that of the axial flux of axial momentum is calculated using the simplified equation based on the geometry of the swirler as:

$$SW = \frac{2}{3} \left[\frac{1 - (R_h/R_n)^3}{1 - (R_h/R_n)^2} \right] \tan \theta \quad (3.1)$$

Where R_h and R_n are the radii of the swirler's inlet duct and center body, respectively, and θ is the vane angle. Table 3.1 shows the respective R_h and R_n as well as the approximate calculated swirl number for the different swirlers used.

Table 3.1: Dimensions of the swirlers used and calculated swirl number

Swirl angle (θ°)	R_h (mm)	R_n (mm)	Swirl number (SW)
30	12.5	11.5	0.6
45	13.5	12.5	1.0
55	13.5	12.5	1.5

3.3 Experimental Measurements Techniques

The Bronkhorst High-Tech. flow meters used in supplying the appropriate flow of reactants to the combustor have an accuracy of $\pm 0.5\%$ Reading plus $\pm 0.1\%$ Full Scale, repeatability of $< \pm 0.2\%$ Reading, and the control stability of $\leq \pm 0.1\%$ Full Scale. The temperature within the combustor at several locations is measured using an R-type thermocouple. For the temperature measurements, the uncertainty is $\pm 2.7\%$ of the measured value. Flame images are taken with a D5200 NIKON digital camera having 24.1 Megapixel DX-format CMOS image sensor. High-intensity microphone (MIC-093) manufactured by Kulite semiconductor products INC is used for the measurement of sound pressure level fluctuations. A photomultiplier tube module (PMT: H10722-110) manufactured by Hamamatsu Photonics UK LTD is used together with an OH filter for the measurement of heat release fluctuations in the flame. The OH filter is a bandpass interference filter centered at 307 nm wavelength (to target OH radicals) acquired from OPTOSIGMA, USA. Data from these sensors is acquired using National Instruments (NI) data acquisition card (DAQ) with LABVIEW software. The emissions (including NO_x) are measured with “TESTO 350 combustion and emission analyzer” having a dilution factor of $\times 5$ for CO measurements. In experiments involving H₂-enrichment, CO emission is measured using KANE 250 combustion meter having a resolution of 1 ppm and an accuracy of $\pm 5\%$ as reported by the manufacturer.

The uncertainty in the independent variables; equivalence ratio (Φ) and CO₂ dilution level (dil) is calculated using Equations 3.2 and 3.3 respectively under the assumption that the inaccuracy arises only from the flow meters supplying the reactants and the

diluent. Details of the equations for the uncertainty analysis can be found in the work of Coleman et al. [149].

$$U_{\Phi}^2 = \left[\frac{\partial \Phi}{\partial \forall_{O_2}} \right]^2 (U_{O_2})^2 + \left[\frac{\partial \Phi}{\partial \forall_{C_3H_8}} \right]^2 (U_{C_3H_8})^2 + \left[\frac{\partial \Phi}{\partial \forall_{H_2}} \right]^2 (U_{H_2})^2 \quad (3.2)$$

$$U_{dil}^2 = \left[\frac{\partial dil}{\partial \forall_{CO_2}} \right]^2 (U_{CO_2})^2 \quad (3.3)$$

Where $\forall$ is the volume flow rate and U_i (U_{O_2} , $U_{C_3H_8}$, U_{H_2} , U_{CO_2}) is the uncertainty from the respective flow meters which is equal to the sum of precisions (P_1 and P_2) and bias (B) given as;

$$U_i^2 = P_{1,i}^2 + P_{2,i}^2 + B \quad (3.4)$$

Where $P_{1,i}$ and $P_{2,i}$ for the Bronkhorst flow meters used are given as;

$$P_{1,i} = 0.002\forall_i \quad (3.5)$$

$$P_{2,i} = 0.001\forall_{FS} \quad (3.6)$$

Where $\forall_{FS}$ is the full scale (FS) volume flow rate of the flow meter used (see Table 3.2).

The bias, on the other hand, is calculated using;

$$B_i = 0.005\forall_i + 0.001\forall_{FS} \quad (3.7)$$

The equivalence ratio (Φ) is the ratio of oxygen-to-fuel ratio at stoichiometry to the actual oxygen-to-fuel ratio calculated as;

$$\Phi = \left(\frac{O}{F} \right)_{stoic} / \left(\frac{O}{F} \right)_{act} \quad (3.8)$$

For propane oxy-combustion with no hydrogen enrichment, the oxygen-to-fuel ratio at stoichiometry is 5 which means at the same temperature, for each one liter per minute of propane, five liters per minute of oxygen volume flow rate is required at stoichiometry. Therefore, for propane enriched with 20% hydrogen (the oxygen-to-fuel ratio is 4.1), the data reduction equation of Φ can be written as;

$$\Phi = 4.1 * \frac{1}{O/F} = 4.1 * \left[\frac{\forall_{H_2} + \forall_{C_3H_8}}{\forall_{O_2}} \right] \quad (3.9)$$

Equations 3.9 can be differentiated accordingly and the results can be substituted in Equation 3.2 together with other results to obtain the uncertainty in Φ . The calculated uncertainty in Φ ranges from 3% to 1% depending on the operating conditions. Values for the uncertainty are reported throughout this dissertation accordingly.

The dilution level in cases to do with CO₂ diluent is defined as the percentage of CO₂ in O₂/CO₂ oxidizer mixture. Subsequently, the dilution level can be calculated as:

$$dil_{CO_2} = \left[\frac{\forall_{CO_2}}{\forall_{CO_2} + \forall_{O_2}} \right] * 100\% \quad (3.10)$$

Table 3.2: The type of Bronkhorst flow meters used with their respective full scale

Flow Meter Model #	Gas Type	Full-Scale Flow Rate
F-201-CI	Hydrogen (H ₂)	10 L/Min
F-122-AI	Propane (C ₃ H ₈)	70 L/Min
F-202-AI	Oxygen (O ₂)	247 L/Min
F-202-AI	Air	250 L/Min
F-202-AI	Carbon-Dioxide (CO ₂)	250 L/Min

3.4 Experimental Procedures and Conditions

Table 3.3 shows the experimental conditions adopted in the study. The experimental procedures employed include:

- I. For static stability studies with CO₂ dilution, initially, the fuel is burnt at a certain firing rate (power density; MW/m³.bar at atmospheric conditions) and global equivalence ratio in a stream of pure oxygen. CO₂ is then added while monitoring its concentration in O₂/CO₂ oxidizer until flame blowout. Note that for the combustor in this dissertation with a volume of 0.0011545353 m³, the combustor firing rate of **4 MW/m³.bar** corresponds to the combustor power of **4.68 kW**.
- II. A 5% by volume increment of CO₂ concentration in the O₂/CO₂ mixture is used at initial stages of dilution. Beyond 60% CO₂ dilution in the mixture, this increment

was reduced to 0.5% in order to achieve gradual sweep and establish the blowout point.

- III. The combustor firing rate is varied at a fixed global equivalence ratio and procedures I and II are repeated at the different combustor firing rates studied.
- IV. The global equivalence ratio is varied near stoichiometry and procedures I through III is repeated to establish the effect of equivalence ratio on the static stability of oxyfuel flames under CO₂ dilution.
- V. The previous procedures are conducted using swirlers with different swirl number (1.5, 1.0, and 0.6) to study the effect of swirl number.
- VI. The propane fuel is enriched with H₂ in different concentrations while repeating procedures I through IV to study the effect of H₂ addition on the static stability of the flames under CO₂ dilution.
- VII. For dynamic stability studies, an approach similar to static stability studies (procedures I-VI) is adopted while recording data on heat release and sound pressure level fluctuations.
- VIII. For static stability studies that compare Air oxidizer with oxyfuel oxidizer mixture, the fuel is burnt at a certain firing rate and stoichiometric global equivalence ratio in a stream of Air and fixed O₂/CO₂ mixture respectively. The O₂/CO₂ ratios used in this study are 31/69% and 21/79% named Oxyfuel I and Oxyfuel II respectively. The Oxyfuel I mixture is estimated to produce the same adiabatic flame temperature as that of air-propane combustion.
- IX. Equivalence ratio sweep is carried out by gradually decreasing (by 0.01) the global equivalence ratio (Φ) until flame blowout.

- X. All measured parameters in the experimental study – flame images, species concentration, temperature, sound pressure level, and heat release - are measured as the flame reach steady state under the specified conditions of interest (equivalence ratio, firing rate, CO₂ dilution level, H₂ concentration, etc)
- XI. Recorded data are analyzed and reported

Table 3.3: Conditions for the experimental study

Conditions for experimental study into blowout characteristics of oxyfuel flames with different oxidizer mixtures				
Study	Swirl number	Combustor firing rate [MW/m³]	Global equivalence ratio; Φ	Oxidizer mixture
Effect of oxidizer mixture (fixed composition)	0.6	3.0-4.5 in steps of 0.5	From stoichiometry to Φ at blowout	• Oxyfuel I (O₂/CO₂: 31/69) • Oxyfuel II (O₂/CO₂: 21/99) • Air oxidizer
Effect of CO ₂ dilution (varying O ₂ /CO ₂ oxidizer composition)	0.6	3.0- 6.0 in steps of 0.5	1.0 and 0.9	From 0 % CO ₂ dilution level to the % at flame blowout
Effect of swirl number	1.5, 1.0, and 0.6	3.0-6.0 in steps of 0.5	Stoichiometry ($\Phi = 1.0$)	From 0 % CO ₂ dilution level to the % at flame blowout
Conditions for experimental study into blowout characteristics of oxyfuel flames with H₂ enrichment				

Study	H₂ %	Combustor firing rate [MW/m³]	Global equivalence ratio; Φ	Oxidizer CO₂ dilution level
Effect of H ₂ enrichment	0-30	2.0 - 3.5 in steps of 0.5	1.00	From 0 % CO ₂ dilution level to the % at flame blowout
Effect of global equivalence ratio (Φ)	20	2.0-3.5 in steps of 0.5	1.0, 0.95, and 0.90	From 0 % CO ₂ dilution level to the % at flame blowout
Conditions for experimental study into Dynamic Instability of oxyfuel flames				
Study	Swirl number	Combustor firing rate [MW/m³]	Global equivalence ratio; Φ	Oxidizer mixture
Effect of CO ₂ dilution (varying O ₂ /CO ₂ oxidizer composition)	1.0	4.0	1.0	From 0 % CO ₂ dilution level to the % at flame blowout
Effect of H ₂ enrichment	1.0	4.0	1.0	From 0 % CO ₂ dilution level to the % at flame blowout
Effect Of firing rate	1.0	4.5-3.0 in steps of 0.5	1.0	From 0 % CO ₂ dilution level to the % at flame blowout

3.5 Mathematical Modeling

Generally, combustors are not perfectly stirred, which entails a non-uniform distribution of chemical species. Therefore, it is necessary to model the flow and mixing of these chemical species in order to accurately predict their state throughout the combustor. This is in addition to modeling chemical kinetics, which predicts the composition of the combustion species. Consequently, combustion process couples one of the most complex flow and heat transfer processes with chemical reaction. Modeling such a phenomenon requires a deep analysis of the conservation laws that adequately describes the process. The principle requires that the mass, momentum, energy, and species of the system are conserved [150].

In this section, the mathematical modeling employed in this study is presented. The section covers only general aspects of mathematical modeling. These include flow (turbulence) modeling and radiation modeling which are common to all the numerical studies undertaken. Detailed chemical reaction modeling and numerical procedures used will be presented together with the results obtained from such models in their respective chapters.

3.5.1 Conservation Equations

The continuity equation for *mass conservation* in steady flow having velocity component u_j j th direction is given as:

$$\frac{\partial}{\partial x_j}(\rho u_j) = 0 \quad (3.11)$$

Similarly, the equation for the conservation of momentum known as the momentum equation is given as:

$$\frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial P}{\partial x_i} + \frac{\partial(t_{ij} + \tau_{ij})}{\partial x_j} \quad (3.12)$$

Where t_{ij} is the viscous stress tensor [151] given by:

$$t_{ij} = \mu \left\{ \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right\} \quad \delta_{ij} = 1 \text{ if } i = j, \delta_{ij} = 0 \text{ if } i \neq j \quad (3.13)$$

And P is the pressure while τ_{ij} is the Reynolds stress tensor related to the velocity gradients through Boussinesq hypothesis (which assumed isotropic turbulent viscosity) as:

$$\tau_{ij} = -\rho u'_i u'_j = \mu_t \left\{ \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right\} - \frac{2}{3} (\rho k \delta_{ij}) \quad (3.14)$$

The energy equation (equation for the conservation of energy) which accounts for energy transfer resulting from convection, conduction, species diffusion, viscous dissipation, and any other source of energy production [152] is given as:

$$\frac{\partial}{\partial x_j}(\rho E + P)u_j = \frac{\partial}{\partial x_j} \left(K_{eff} \left(\frac{\partial T}{\partial x_j} \right) - \sum_j h_j J_j + \tau_{eff} u_j \right) + S_h \quad (3.15)$$

Where $E = h - \frac{P}{\rho} + \frac{v^2}{2}$, k_{eff} is the effective conductivity, $K_{eff} = k + k_t$, and S_h is the energy source term that encompasses the heat of chemical reaction and radiation heat exchange.

The species conservation transport equation takes into account for each species, the convection, diffusion, and reaction source components. The concentration of each species

Y_l is determined through the solution of a convection-diffusion equation for the l^{th} species, given by:

$$\frac{\partial}{\partial x_i}(\rho u_i Y_l) = -\frac{\partial}{\partial x_i} Y_{l,i} + R_l \quad (3.16)$$

Where $Y_{l,i} = -\left(\rho D_{l,i} + \frac{\mu_t}{Sc_t}\right) \frac{\partial Y_l}{\partial x_i}$, R_l is the mass rate of creation or depletion by chemical reaction of the species l , and $D_{l,i}$ is the diffusion flux of species l due to concentration gradients.

3.5.2 Turbulence Modeling

Fluctuations in the velocity field are one of the common characteristics of turbulent flows. These fluctuations in the flow field can translate into subsequent fluctuations in energy and species concentrations because of their coupling. Turbulence modeling involves incorporation of these fluctuations in the transport equations. Direct modeling of the fluctuations, however, is not an easy task since they are generally of high frequency and small scale. Rather, attempts were made to modify the governing equations through time averaging or ensemble averaging, among other means. The modified set of equations resolved the issue of the turbulence scales and provides a less expensive computational tool for turbulence modeling. Several turbulence models are available for the solution of different turbulence problems. Some of the considerations guiding the selection of a particular model include the physical nature of the flow, level of accuracy required, available computational resources, and the available time at hand. A k- ϵ model with renormalization group (RNG) is employed in this study.

The $k - \epsilon$ model is one of the most effective models used to solve turbulent-swirling flows. The k in the model represents turbulent kinetic energy and the ϵ stands for dissipation rate of that energy. The model was derived from the exact Navier-Stokes equations, using a statistical technique called renormalization group (RNG) method [153]. A more detailed description of the RNG model and its application to turbulence can be found in [154].

The transport equations for the RNG k - ϵ model are:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\overline{\rho k u_i})}{\partial x_i} = \frac{\partial}{\partial x_j} \left(\alpha_k \mu_{eff} \frac{\partial k}{\partial x_j} \right) + G_k + G_b - \overline{\rho \epsilon} - Y_M + S_k \quad (3.17)$$

and

$$\frac{\partial(\overline{\rho \epsilon})}{\partial t} + \frac{\partial(\overline{\rho \epsilon u_i})}{\partial x_i} = \frac{\partial}{\partial x_j} \left(\alpha_\epsilon \mu_{eff} \frac{\partial \epsilon}{\partial x_j} \right) + C_{1\epsilon} \frac{\bar{\epsilon}}{k} (G_k + G_b C_{3\epsilon}) - C_{2\epsilon} \bar{\rho} \frac{\bar{\epsilon}^2}{k} - R_\epsilon + S_\epsilon \quad (3.18)$$

Where G_k is given in equation (3.19) and denotes the generation of turbulence kinetic energy due to the mean velocity gradients, G_b represents the generation of turbulence kinetic energy due to buoyancy (Equation 3.20), and Y_M is the contribution of the fluctuating dilatation, in compressible turbulence, to the overall dissipation rate. The parameters α_k and α_ϵ represents the inverse effective Prandtl numbers of k and ϵ respectively, S_k and S_ϵ are user-defined source terms. The model constants (default in FLUENT) is given as;

$$C_{1\epsilon} = 1.42, C_{2\epsilon} = 1.68, C_{3\epsilon} = \tanh \left| \frac{v}{u} \right|, \text{ and } \alpha_\epsilon = \alpha_k \approx 1.393$$

Where v and u are the flow components parallel and perpendicular to gravitational vector respectively.

The generation of kinetic energy due to the velocity gradient G_k is given as;

$$G_k = \mu_t \left[\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \frac{\partial \bar{u}_i}{\partial x_j} - \frac{2}{3} \frac{\partial \bar{u}_i}{\partial x_j} \delta_{ij} \left[\mu_t \frac{\partial \bar{u}_k}{\partial x_k} + \overline{\rho k} \right] \right] \quad (3.19)$$

The rate of generation of turbulent kinetic due to buoyancy G_b is given as;

$$G_b = \beta g_i \frac{\mu_t}{Pr_t} \frac{\partial T}{\partial x_i} \quad (3.20)$$

Where; $\beta = \frac{-1}{\rho} \left(\frac{\partial \rho}{\partial T} \right)_P$ and g_i is the gravitational vector in the i^{th} direction.

The RNG swirl adjustment that can take care of highly swirling flow has a modified turbulent viscosity that takes the following functional form;

$$\mu_t = \mu_{t0} f \left(\alpha_s, \Omega, \frac{k}{\varepsilon} \right) \quad (3.21)$$

Where μ_{t0} represents turbulent viscosity for non-swirling flow, Ω is a characteristic swirl number and the constant α_s have a default value of 0.07 in FLUENT. An increase in α_s increases the level of swirl in the flow [155].

3.5.3 Radiation Modeling

Heat transfer by radiation can be categorized into surface-to-surface effect (wall radiations) and the volumetric (participating media) effect in which both the walls and the fluid medium it confines participate in the radiation. The second case of participating gas is more prominent in combustion applications [156].

For an absorbing, emitting, and scattering medium, the radiative transfer equation (RTE) must be solved to establish radiation contribution to the overall heat transfer. The RTE is then coupled to the energy equation for total heat transfer analysis of the system. Due to the complexity of the RTE, and complications involved in radiation (coupled with the other modes of heat transfer) in turbulent reacting flows, the exact solution of RTE is nearly impossible. Subsequently, several models were proposed aiming at some simplification. The choice of any model will depend on the problem at hand, as well as the application, among other things. In this study, the discrete ordinate (DO) radiation model is used. In the DO model, the full solid angle (4π) in the scattering term of the RTE is divided into a number of discrete angular intervals, whereas the continuous direction (of radiative intensity) is replaced by a discrete set of direction vectors. Consequently, the integral scattering term of the RTE equation (Equation 3.22) is replaced by a summation in the DO model. Weighted-sum-of-gray-gases model (WSGGM) is employed for the determination of the absorption coefficient. The WGSSM is more accurate than the oversimplified gray gas model as it takes into account particular absorption bands. Ultimately, the models (DO and WGSSM) can adequately predict the thermal radiation exchange between the combustion gases and the combustion chamber walls.

The RTE depicted as a field equation in the direction $\vec{s}$ represents the contribution of emission, absorption, and scattering in the medium to the overall radiation intensity I [155]. The equation is given as;

$$\nabla \cdot (I(\vec{r}, \vec{s}) \vec{s}) + (a + \sigma_s)I(\vec{r}, \vec{s}) = an^2 \frac{\sigma T^4}{\pi} + \frac{\sigma_s}{4\pi} \int_0^{4\pi} I(\vec{r}, \vec{s}) \Phi(\vec{s}, \vec{s}') d\Omega' \quad (3.22)$$

Based on the WSGGM, the total emissivity over the distance s can be computed using;

$$\varepsilon = \sum_{i=0}^I a_{\varepsilon,i}(T)(1 - e^{-\kappa_i p s}) \quad (3.23)$$

Where T is the temperature, $a_{\varepsilon,i}$ is the emissivity weighting factor for the i^{th} fictitious gray gas, κ_i is the absorption coefficient of the i^{th} gray gas, p is the sum of the partial pressures of all the absorbing gases and the quantity $(1 - e^{-\kappa_i p s})$ is i^{th} emissivity [157].

3.5.4 Chemical Reaction Modeling

Modeling chemical reaction entails the evaluation of the reaction source term in species conservation equation. Over the years, many techniques are proposed to model chemical reaction. In this study, the Eddy Dissipation Concept (EDC) is used with a reduced chemical reaction mechanism to model the oxyfuel reactions of propane that does not involve hydrogen addition. For cases involving hydrogen-enriched oxyfuel mixtures, the reaction is modeled using the non-premixed combustion model (NPC) with mixture fraction (f) transport equation. The transport equation for f is obtained from the species conservation equations under the assumption of equal diffusivities of the species, which help cancels the reaction source terms in the equations. Details of EDC, NPC, and the numerical schemes used will be given together with the results obtained from the respective models in Chapters 5 and 6, respectively.

CHAPTER 4

EXPERIMENTAL ANALYSIS OF THE STATIC STABILITY AND COMBUSTION CHARACTERISTICS OF OXYFUEL AND AIR FLAMES

In this chapter, results from the static stability analysis of propane-air and propane-oxyfuel flames studied in the non-premixed, swirl-stabilized combustor are presented. Different O_2/CO_2 oxidizer mixtures were employed to study propane-oxyfuel flame stability under different combustor firing rates and different swirl numbers. The lean stability limits, combustor temperature distribution, as well as emissions from propane-oxyfuel (oxyfuel I and oxyfuel II) and propane-air combustion, are also compared and discussed. Oxyfuel I was fixed to have 21% oxygen concentration by volume like air with the remaining 79% being CO_2 . Oxyfuel II, on the other hand, contains 31% oxygen concentration by volume in the O_2/CO_2 oxidizer mixture chosen because, at that ratio, the adiabatic temperature is similar to that of air-propane combustion.

4.1 Air versus Oxyfuel Combustion

4.1.1 Flame static stability

Flame transitions images depicting flames macrostructure for air, as well as Oxyfuel II combustion, are shown in Figure 4.1 and Figure 4.2, respectively. The images were obtained for swirl number of 0.6 at a fixed firing rate of 5 MW/m^3 by gradually decreasing (by 0.01) the global equivalence ratio (Φ) until flame extinction while monitoring the flame transitions. This equivalence ratio sweep test was conducted from stoichiometric conditions to equivalence ratio at flame blowout for the two oxidizers. For propane-air, at stoichiometry, the primary reaction zone of the flame manifested as a deep blue flame anchored on the fuel nozzle, around which a reddish swirling plume was observed, as seen in Figure 4.1. The reddish plume has been previously reported to be resulting from the presence of carbon as a consequence of incomplete combustion [46]. As more oxidizer was supplied by decreasing the equivalence ratio, more oxygen is made available for combustion, and consequently, the plume was observed to vanish completely around $\Phi = 0.8$, forming a V-shaped flame at $\Phi = 0.7$, as shown. A further decrease in Φ weakens the flame base, leading to its liftup at $\Phi = 0.62$, forming an M-shaped flame, suggestively stabilized in the outer recirculation zone formed by the swirling flow. Subsequent flame transitions occur at lower equivalence ratios, forming an oscillating, cone-shaped flame at $\Phi = 0.5$ that further elongates and continues to thin out in the base at $\Phi = 0.48$ until its eventual blowout recorded at $\Phi = 0.47$. The macrostructure of the oxyfuel II flame does not change with the equivalence ratio, because it remains compact and V-shaped irrespective of the equivalence ratio, as shown

in Figure 4.2. Also, unlike propane-air flames, oxyfuel II flames do not undergo any transition in the macrostructure until blowout.

It is worth noting here that, despite having the same adiabatic flame temperatures, air and oxyfuel II combustion display different flame characteristics. This could be attributable to differences in heat loss characteristics from the two flames. Moreover, the reddish luminescence observed for air-propane combustion was also observed for the oxyfuel case having pure oxygen without dilution. However, with CO₂ dilution, e.g., oxyfuel II case, no reddish luminescence was observed, even at stoichiometric conditions. This is attributed to the fact that added CO₂ has the effect of enhancing the mixing by helping create vortical structures, increasing the turbulence, and, consequently, helping to achieve complete combustion in the combustor.

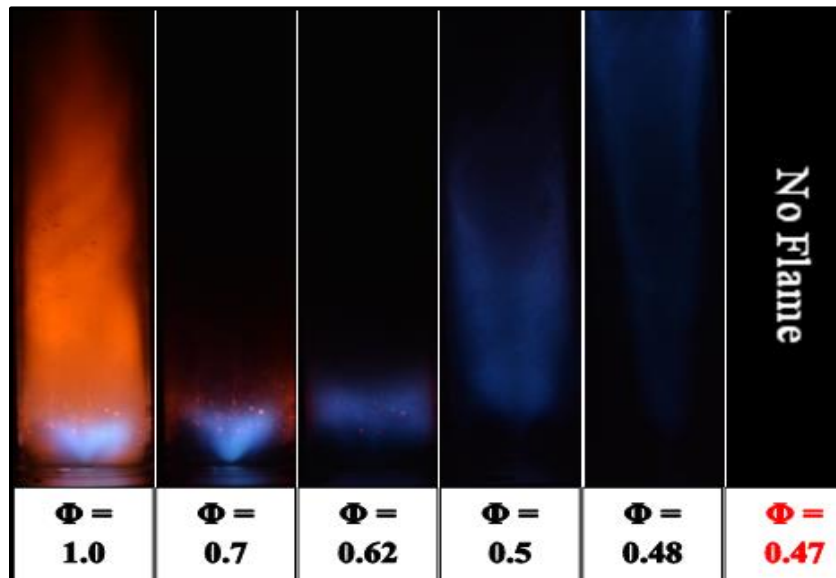


Figure 4.1: Flame transitions of propane-air at a firing rate of 5MW/m³ and 0.6 swirl number

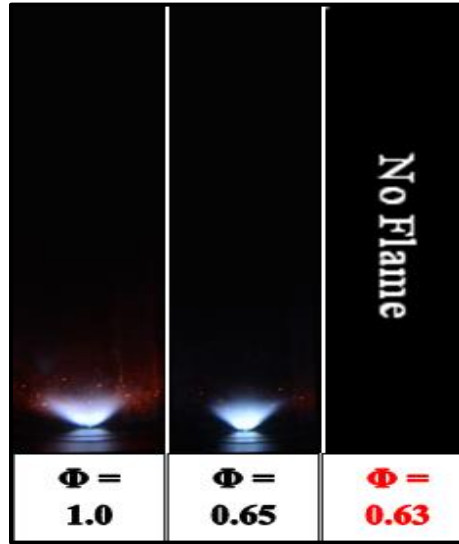


Figure 4.2: Flame transitions of propane-oxyfuel II at a firing rate of 5MW/m³ and 0.6 swirl number

The stability map depicting the blowout limits for the three different oxidizers (air, oxyfuel I, and oxyfuel II) is shown in Figure 4.3 with an inset showing the flame-no flame regions of the profiles. The uncertainty in equivalence ratio (ϕ) in the figure is 1.2%. For a swirl number of 0.6, and for each firing rate studied, the blowout points were obtained by continuously increasing the oxidizer flow rate until flame blowout occurs. The blowout points for propane-air and propane-oxyfuel II flames were observed to be very close to each other compared with oxyfuel I, particularly at a low firing rate. This is expected because the oxyfuel II mixture has an adiabatic flame temperature similar to propane-air combustion. As seen in the figure, for propane-air, the blowout points are nearly constant, irrespective of the firing rate. This suggests its strong dependence upon heat loss from the reaction zone, such that the flame goes extinct at nearly the same adiabatic flame temperature. For oxyfuel II flames, however, the equivalence ratio at

blowout increases marginally as the firing rate increases, indicating a departure from the propane-air cases. This suggests that heat loss from the flames is different, suggestively due to a higher amount of CO_2 in the oxyfuel II cases. In other words, while the two flames might have the same rate of liberation of heat by chemical reactions, their respective rate of heat loss is not the same. The same trend is observed for oxyfuel I flames, with the blowout equivalence ratio, however, being far higher than those of oxyfuel II flames. This is consistent with the results reported by Kutne et al. [23] and is a consequence of a higher amount of CO_2 diluent in oxyfuel I flames. In Figure 4.4 the stability map for propane-air combustion is shown, depicting the blowout as well as liftup points at different firing rates. The liftup phenomenon was observed to occur at a constant velocity ratio of 0.50 (ratio of fuel velocity/oxidizer velocity), irrespective of the combustor firing rate, suggesting that it is flow-induced. Figure 4.5 depicts the blowout points for oxyfuel I and II cases as a function of the oxidizer Reynolds number for a swirl number of 0.6. An increase in the fuel Reynolds number is accompanied by a corresponding increase in the oxidizer Reynolds number at blowout.

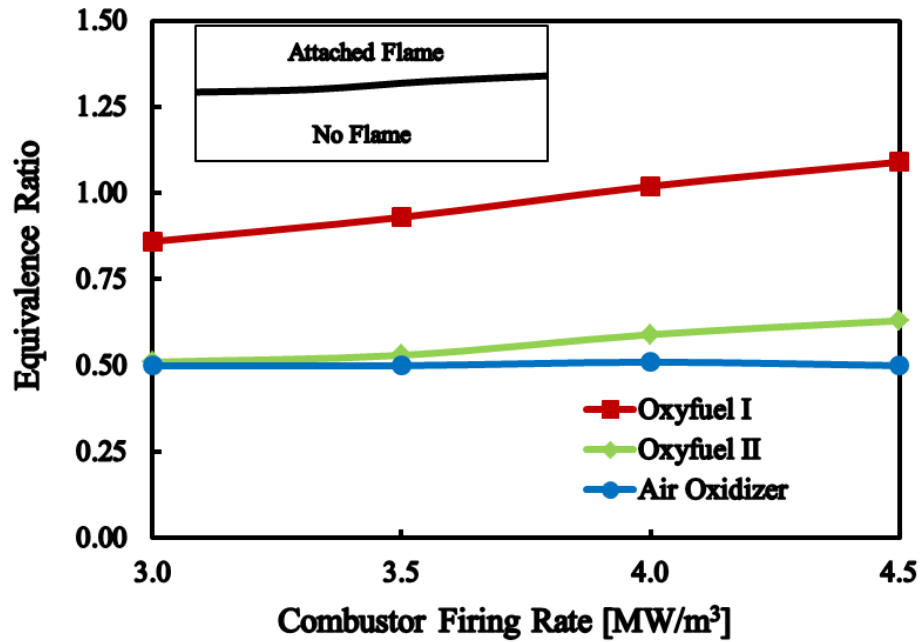


Figure 4.3: Blowout points for air and oxyfuel flames at 0.6 swirl number

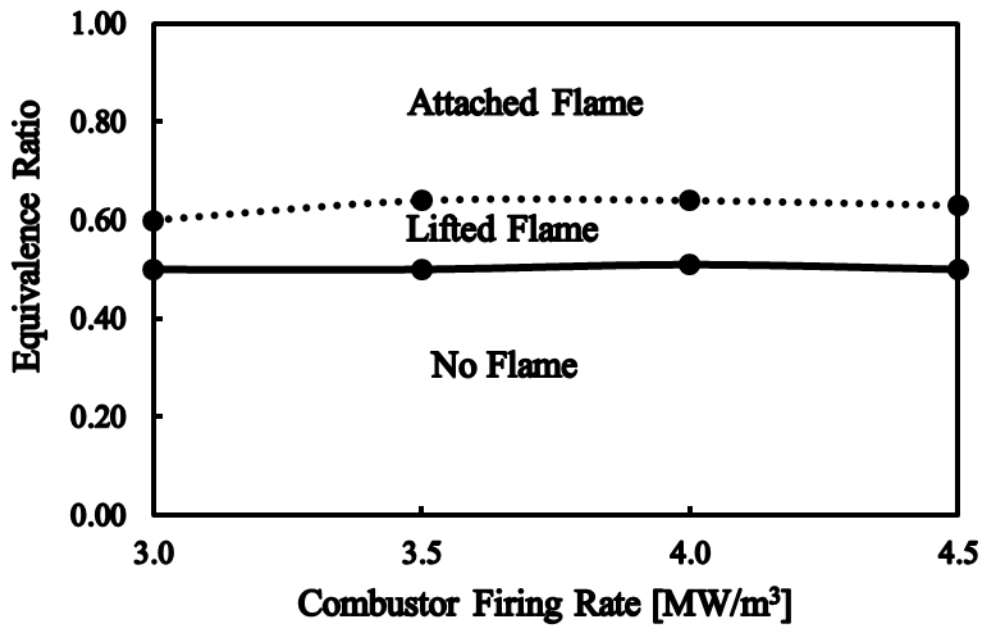


Figure 4.4: Blowout and Liftup point for propane-air combustion at swirl number 0.6

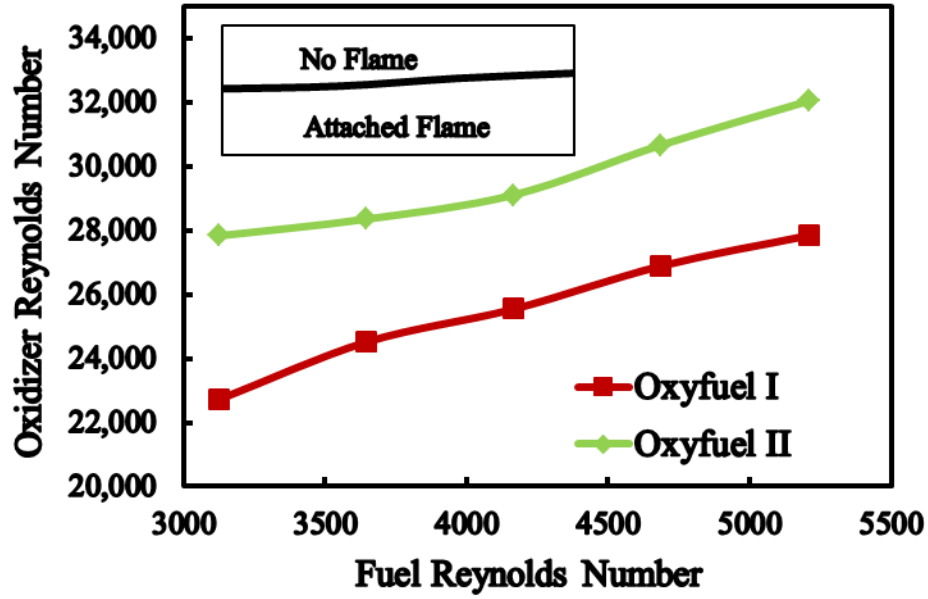


Figure 4.5: Fuel and oxidizer Reynolds number at blowout for oxyfuel flames at 0.6 swirl number

The superior stability window exhibited by air combustion over the oxyfuel cases results from differences in properties of N_2 and CO_2 in the oxidizers. This is because the flame speed of O_2/CO_2 mixture combustion is lower than that of air combustion at the same level of the oxygen concentration and within a certain range (as we will see in the next chapter). The lower flame speed is due to lower values of thermal diffusivity (α) and flame temperature (T_f) in the O_2/CO_2 mixtures compared to those in the air (O_2/N_2) mixture, all of which affect the Damkohler number, as evident in Equations 2.7 and 2.8 [21]. Also at high concentrations, CO_2 was reported by Heil et al. [24] to participate in the reaction with the effect of lowering burning rates. This effect, however, dampens at high O_2 concentrations in the mixture. This direct link between the stability limits and flame speed explains the extended stability limits exhibited by both air and oxyfuel flames with the addition of hydrogen, as shown in Figure 4.6, Figure 4.7, and Figure 4.8,

respectively. Figure 4.6 and Figure 4.7 were obtained for air at a fixed firing rate of 3.5 MW/m^3 with the hydrogen content in the fuel varied from zero (100% propane) to 40% H_2 by volume. From the figures, it can be observed that higher hydrogen concentration in the fuel enhances the blowout limit as evident from the high Reynolds number of oxidizer at blowout which corresponds to lower equivalence ratios. Similar behavior was observed in oxyfuel combustion stability map (Figure 4.8) obtained at a fixed firing rate of 2.5 MW/m^3 and stoichiometric equivalence ratio (at fixed equivalence ratio, only CO_2 was added until flame blowout). The higher flame speed of hydrogen helps enhance the flame stability when hydrogen was added in the fuel, as evident from both the air and oxyfuel cases.

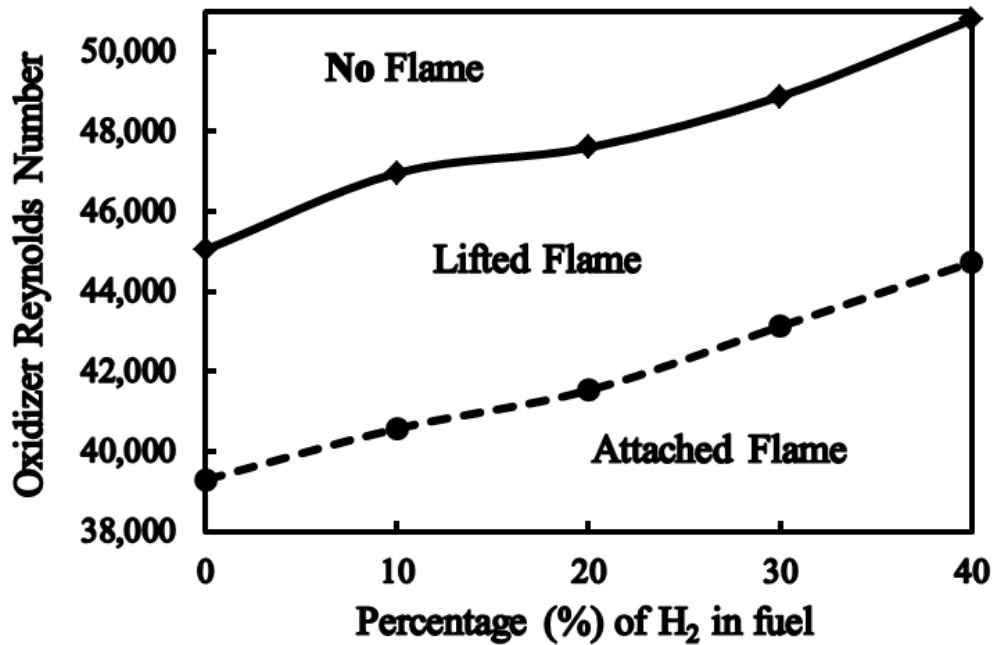


Figure 4.6: Stability map in terms of Reynolds no. for air combustion with H_2 addition at a firing rate of 3.5 MW/m^3 and 1.0 swirl number

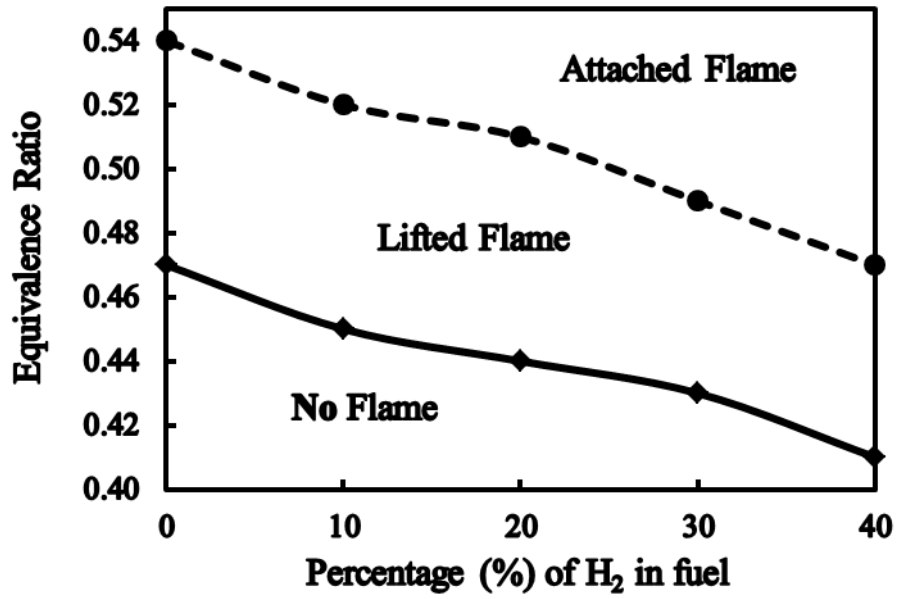


Figure 4.7: Stability map in terms of Φ for air combustion with H_2 addition at a firing rate of 3.5MW/m³ and 1.0 swirl number

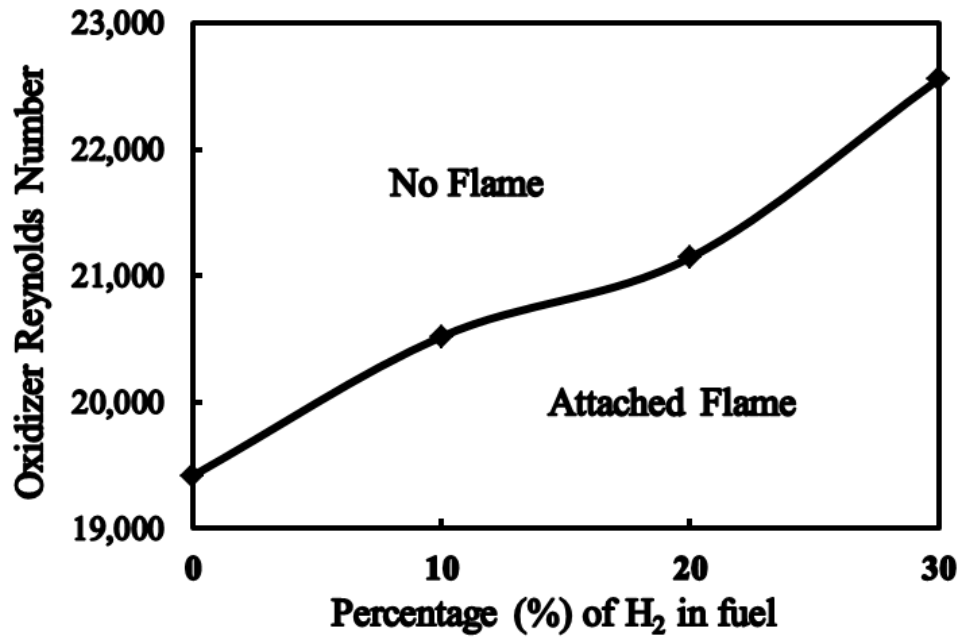


Figure 4.8: Stability map for oxyfuel combustion with H_2 addition at a firing rate of 2.5MW/m³, 1.0 swirl number, and $\Phi = 1.0$

4.1.2 Temperature Profiles and Emissions

Figure 4.9 and Figure 4.10 depict the axial temperature distributions for air and Oxyfuel II combustion, respectively, measured along the centerline of the combustor at the distance of 150-250 mm from its dump plane. The profiles were obtained at a fixed firing rate of 5 MW/m^3 , swirl number of 0.6, and different equivalence ratios as shown. For all of the profiles, decreasing the equivalence ratio decreases the temperature as expected, owing to the cooling effect resulting from supplying more oxidizer at a lower equivalence ratio. Also, the temperature in both cases decreases downstream of the combustor, signifying heat loss by convection, conduction, and radiation from the combustion gases as they move toward the exhaust. Figure 4.11 gives a comparison between air and oxyfuel II axial temperature profiles at a fixed firing rate of 5 MW/m^3 , 0.6 swirl number, and 0.8 global equivalence ratio. The temperatures were measured along the centerline of the combustor at the distance of 150-250 mm from the dump plane of the combustor. Although the oxygen concentration in the oxyfuel II oxidizer mixture was chosen specifically to establish the same adiabatic flame temperature with propane-air combustion, the air combustion resulted in higher temperatures downstream in the combustor, as shown. This is attributable mainly to the high thermal radiation of CO_2 , keeping in mind the characteristically higher CO_2 concentrations in the oxyfuel gases. Subsequently, more heat loss by radiation and, hence, lower temperatures are recorded for the oxyfuel II case compared to the propane-air case.

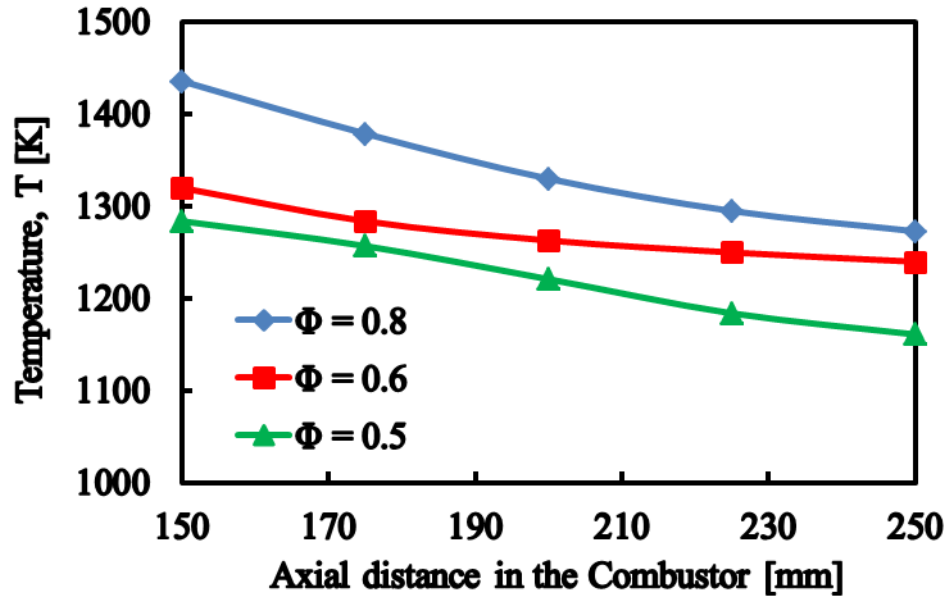


Figure 4.9: Axial temperature distribution for air combustion at a firing rate of 5MW/m³ and 0.6 swirl number

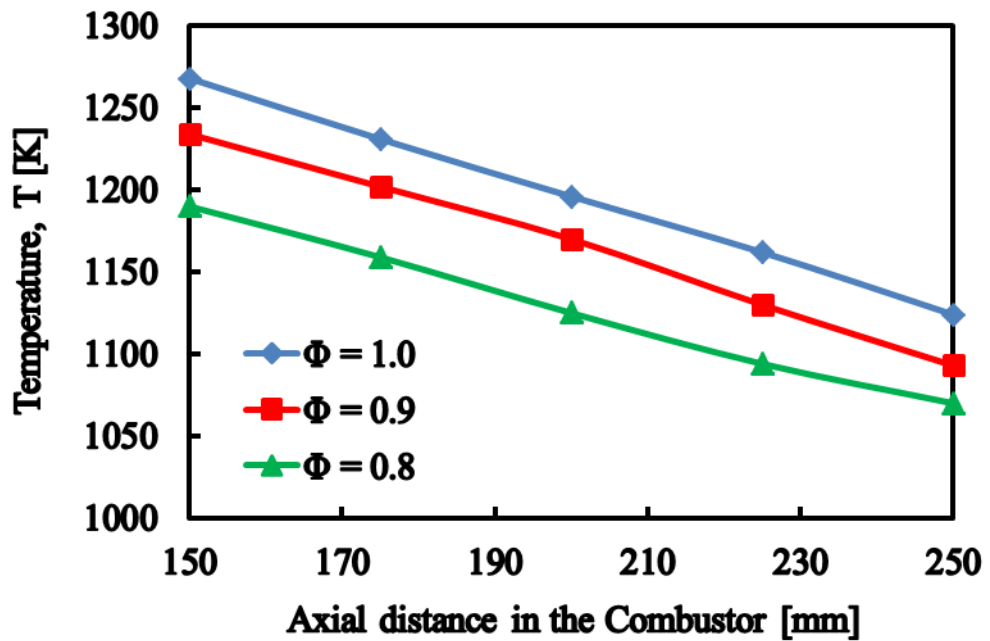


Figure 4.10: Axial temperature distribution for oxyfuel II combustion at a firing rate of 5MW/m³ and 0.6 swirl number

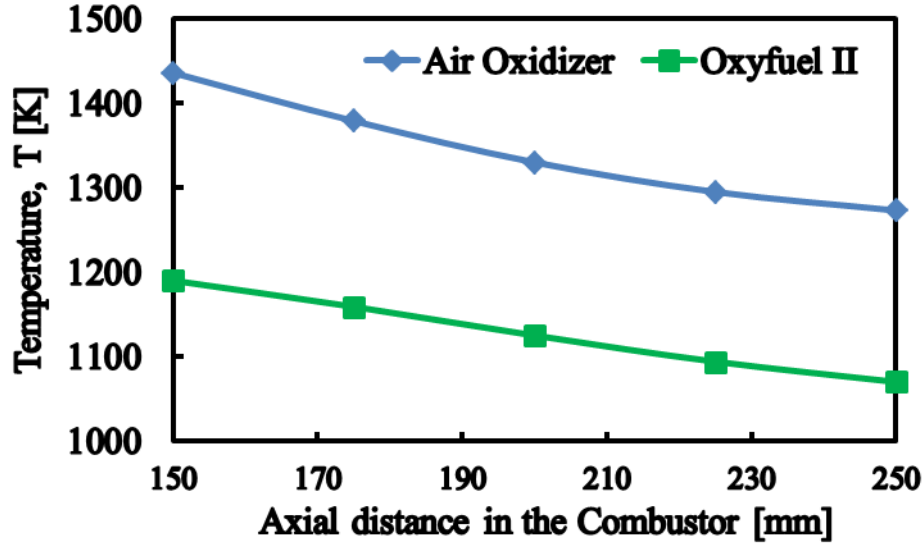


Figure 4.11: Axial temperature distribution comparison air and for oxyfuel II combustion at a firing rate of 5 MW/m^3 , 0.6 swirl number, and $\Phi = 0.8$

In Figure 4.12 and Figure 4.13, NO_x and CO emissions are shown as a function of equivalence ratio for air and oxyfuel combustion, respectively. For the air combustion case, the NO_x emission was obtained close to the combustor exit at a fixed firing rate of 4 MW/m^3 and swirl number of 1.0. As seen in Figure 4.12, NO_x emission increases with an increase in the equivalence ratio. This is because increasing the equivalence ratio increases the temperature as we have seen earlier in this section. Consequently, higher air combustion temperatures resulted in the production of more thermal NO_x via the Zeldovich mechanism. Figure 4.13 shows CO emission from oxyfuel II at a fixed firing rate of 2 MW/m^3 and a swirl number of 1.0 recorded near the combustor exit. As expected, lower temperatures corresponding to lower equivalence ratios are associated with high CO emission. This is because, at lower temperatures, the conversion of CO to CO₂ becomes dampened as a result of cooling. It is, however, important to note that in this case, the temperature is not high enough to encourage CO₂ dissociation as the oxy-

flame is diluted with CO_2 . At very low dilution level, dissociation resulting from excessive oxyfuel temperatures can encourage the formation of more CO at stoichiometry as we will see in the next chapter.

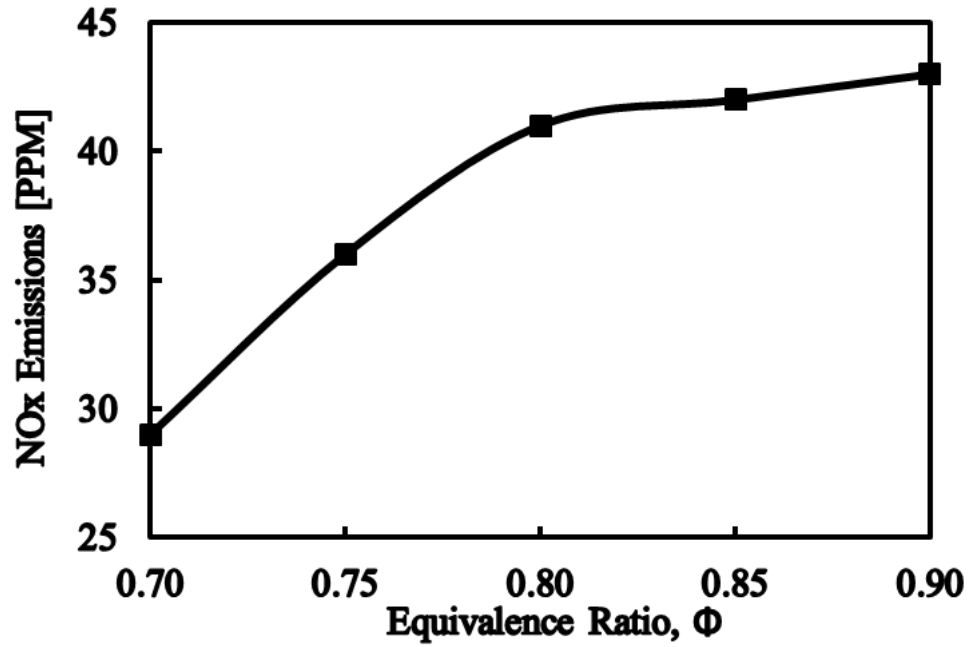


Figure 4.12: Thermal NOx emission from propane-air combustion at a firing rate of 4MW/m^3 and swirl number of 1.0

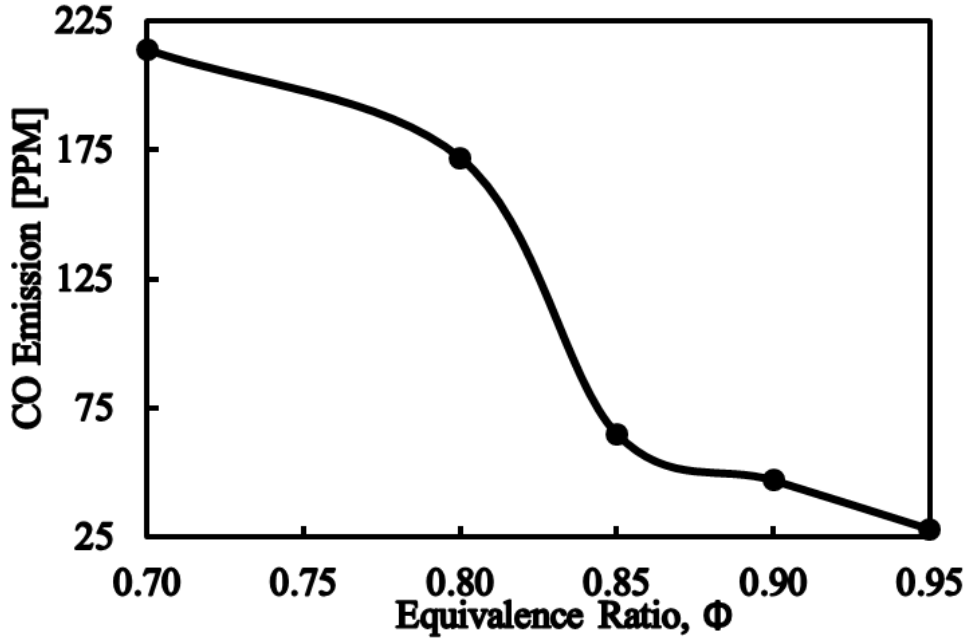


Figure 4.13: CO emission from oxyfuel II combustion at a firing rate of 2MW/m^3 and swirl number of 1.0

4.2 Effect of CO_2 dilution on oxyfuel combustion stability

In the previous section, the stability of propane-air and propane-oxyfuel flames at lean global equivalence ratios (lean blowout limits) was discussed. There is a strong motivation in lean combustion involving an air oxidizer for NO_x reduction. This motivation, however, does not extend to oxyfuel combustion using high-purity oxygen because there is almost no nitrogen present in the oxidizer. More importantly, a penalty will be incurred for excessive usage of oxygen as a result of the cost of its production. Consequently, for oxyfuel combustion, operating at a stoichiometric equivalence ratio is beneficial in reducing oxygen usage, as well as, eliminating lean combustion-related instabilities. Oxyfuel combustion, however, is associated with excessive temperatures, which poses material, and structural safety concerns in combustion systems. This concern

for excessive combustion temperatures can be mitigated by employing CO₂ as a diluent so that O₂/CO₂ oxidizer mixture is utilized for oxyfuel combustion. Therefore, in this section, we investigate the effect of the CO₂ concentration in the O₂/CO₂ oxidizer mixture on oxyfuel flame stability near stoichiometric equivalence ratio.

In the experiments carried out, starting with 100% oxygen at a certain equivalence ratio and firing rate, CO₂ was added continuously while monitoring the flame transitions until flame blowout. Figure 4.14 shows transitions in flame macrostructures represented by images obtained at different CO₂ dilution levels, fixed firing rate of 5 MW/m³, swirl number of 0.6, and stoichiometric equivalence ratio. Unlike the abrupt flame extinction observed earlier for oxyfuel I and II at low equivalence ratios, at high firing rates and around stoichiometric equivalence ratios, CO₂ dilution resulted in a distinct flame transition, leading to blowout at high CO₂ concentrations, as seen in the figure. At zero CO₂ dilution level (100% oxygen), an elongated, annular, jet-like flame having reddish luminescence was observed. As the CO₂ dilution level increases, the flame becomes shorter and more compact with a V shape. This is because the addition of CO₂ increases the oxidizer flow rate, resulting in enhanced turbulent mixing in the combustor, thereby enhancing the combustion process. But the resistance to extinction of the flames at high CO₂ dilution is lowered due to high strain and slower chemistry. This is because CO₂ dilution is known to have the effect of decreasing the flame temperature and burning velocity [158]. Reduced temperature and burning velocities in flames and high strain rates imposed by the flow on the flame can lead to a reduction in the resistance of the flame to extinction. Consequently, at a higher CO₂ dilution level, the flame resistance becomes weakened, causing it to lift up and stabilize at a distance away from the fuel

nozzle at the recorded 76% CO₂ dilution level. A further increase in CO₂ level causes the elongation of the lifted flame, forming an oscillating, swirling, cone-like flame that blows out at 79% CO₂ in the (O₂/CO₂) oxidizer mixture.

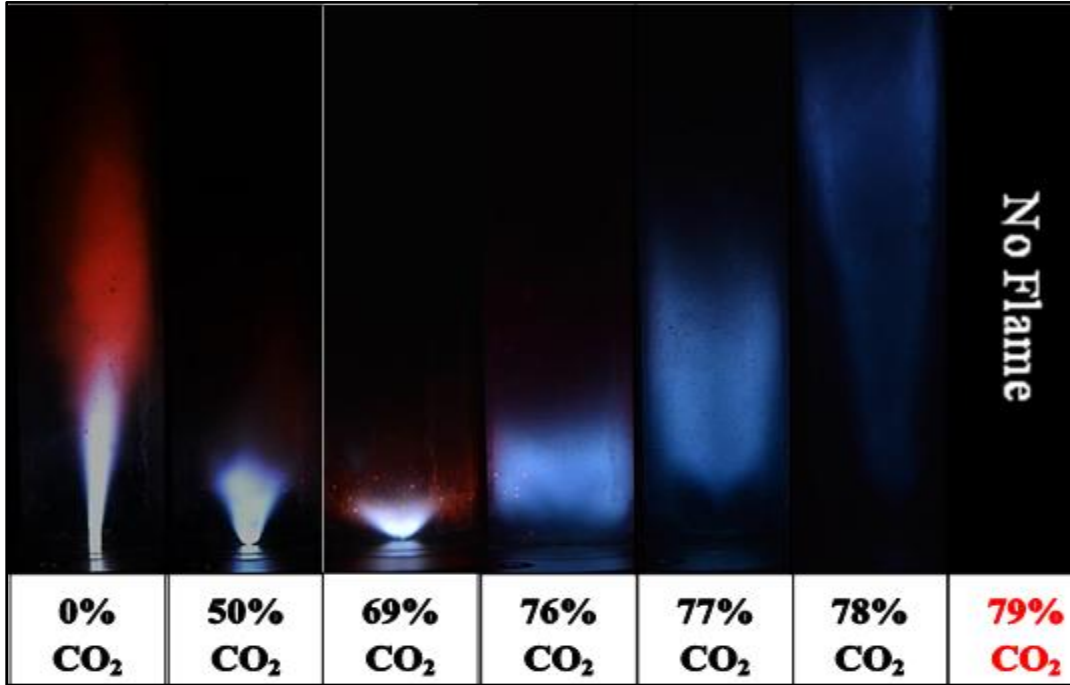


Figure 4.14: Propane-oxyfuel flame transitions at different CO₂ dilution levels, the firing rate of 5MW/m³, swirl number of 0.6, and $\Phi = 1.0$

Figure 4.15 shows the stability map in terms of Reynolds number obtained at the stoichiometric equivalence ratio and swirl number of 0.6 for the propane-oxyfuel flame. From Figure 4.15, it can be observed that the stability window widens (high oxidizer Reynolds numbers at flame blowout) at a high fuel Reynolds number. This can be attributed to greater heat release rates at higher firing rates. Also, it was observed that the flame transits directly from the attached flame to no flame regime at a combustor firing

rate of ≤ 4.5 . Beyond this firing rate, the flame transits from the attached flame to lifted flame before a subsequent transition to the no flame regime. This is a consequence of higher fuel flow rates with an increased firing rate, which further reinforces the previous suggestion that the liftup phenomenon is flow-induced. An average value of 3.0 for the ratio of fuel to oxidizer velocity at blowout was observed in all the lifted flames irrespective of the firing rate. In Figure 4.16, the stability map is presented in terms of the amount of CO_2 diluent in the oxidizer mixture at two different equivalence ratios (1.0 and 0.9). It can be seen from Figure 4.16 that the oxyfuel flames at stoichiometric conditions withstand more CO_2 at flame blowout compared to a leaner equivalence ratio of 0.9, irrespective of the firing rate. The availability of excess oxygen at a lean equivalence ratio leads to the reduction of the flame temperature, aiding the early flame transition. The blowout limit, in terms of the CO_2 concentration in the oxidizer, decreases with the increase in the firing rate up to 4.5 MW/m^3 and then begins to increase, signifying a higher flame resistance to extinction for the lifted flame (characterized by local premixing of reactants). Increasing the combustor firing rate is expected to increase the local flame temperature, thereby extending the flame blowout limit to withstand a higher CO_2 concentration in the oxidizer. However, increasing the firing rate increases the flow field strength due to high Reynolds number, and hence, the flames are subjected to flow-induced strain. That could explain the decrease in CO_2 concentration at blowout with an increase in firing rate before the lifted flame region. Subsequently, the enhanced blowout limit under CO_2 dilution shown by the flames beyond the firing rate of 4.5 MW/m^3 can be attributable to the fact that beyond this firing rate, the flames are lifted before the blowout, which helps enhance mixing at the flame base.

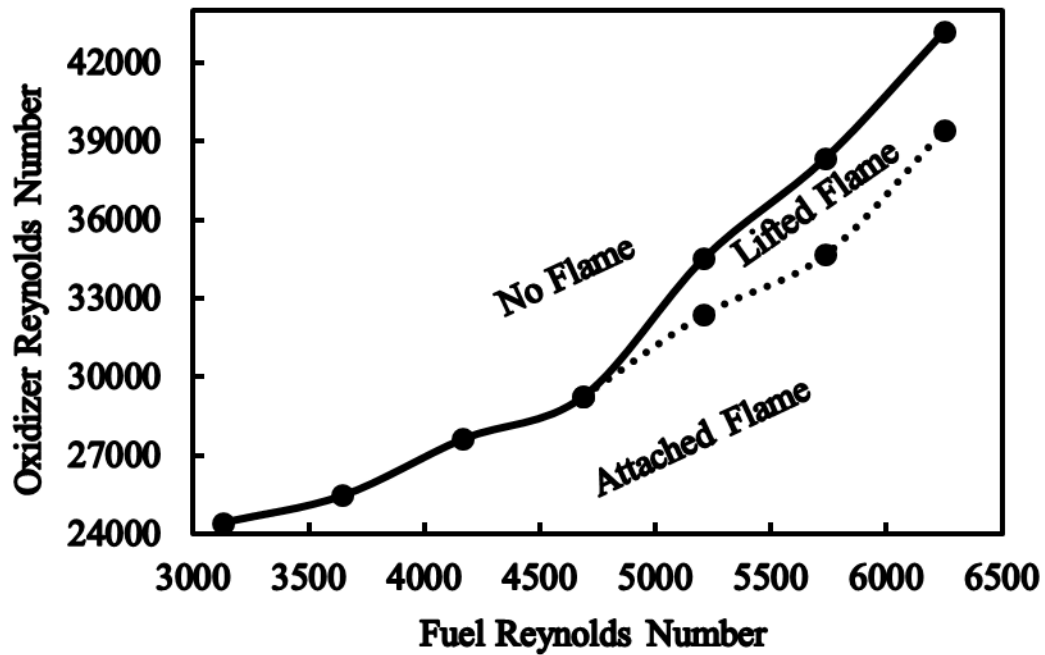


Figure 4.15: Stability map depicting blowout Reynolds number for fuel and oxidizer at $\Phi = 1.0$ and swirl number of 0.6

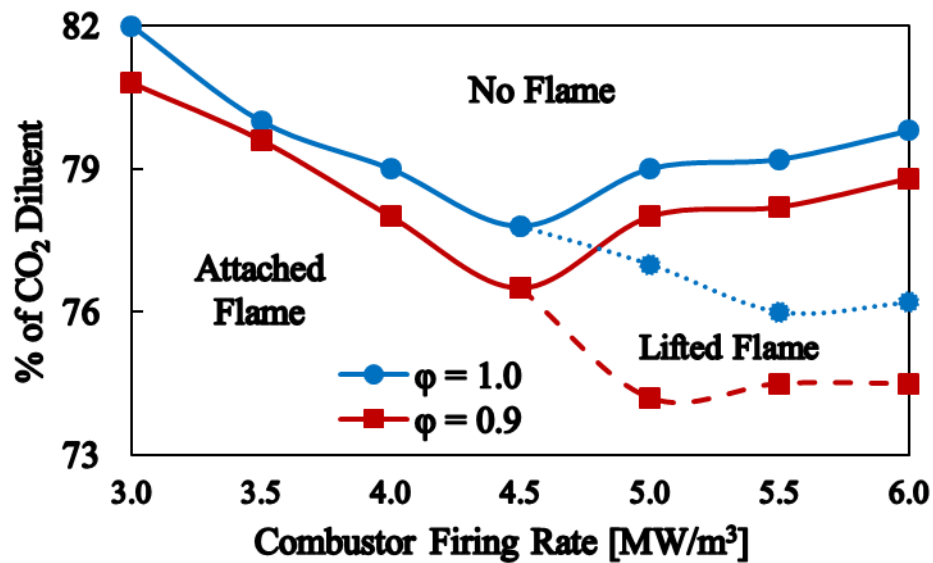


Figure 4.16: Stability map for oxyfuel flames at different CO_2 dilution level and Φ for swirl number of 0.6

4.3 Effect of Swirl Number

Swirlers and bluff bodies are used in flame stabilization because of recirculation zones that they induce in flows as a result of flow separation. Flames are, therefore, anchored in these zones characterized by low flow velocity and even stagnation points. In the case of swirling flows, their use in enhancement of flame stability manifests through the flow recirculation, allowing for longer residence times and recycling of combustion products for flame re-ignition. Swirling flow is also reported to enhanced flame stability as a result of the increase in local velocity fluctuation, causing an increase in the turbulent flame speed [56]. Flames, in swirl-stabilized combustors, are normally anchored in the shear layer in-between inner and outer recirculation zones generated by the swirling flow.

Figure 4.17 and Figure 4.18 depict the blowout points obtained at stoichiometric equivalence ratio in terms of CO₂ dilution level and Reynolds number, respectively. Three swirlers having swirl numbers of 0.6, 1.0, and 1.5 were compared, as shown in the figures. From Figure 4.17, it can be observed that a swirl number of 1.0 displays superior flame stability in the presence of the CO₂ diluent, with blowout happening at higher CO₂ concentrations in the O₂/CO₂ oxidizer mixture. This is also evident in Figure 4.18, in which the oxidizer Reynolds number at blowout is comparatively higher in the case of a swirl number of 1.0. The wider stability window observed in the case of a swirl number of 1.0 compared to swirl numbers 0.6 and 1.5 can be attributed to better mixing conditions attained in the combustor at that swirl number. A lower vortex strength resulting from a lower swirl of 0.6 swirl number will reduce mixing in the combustor,

hence explaining the comparatively narrower stability window recorded with that swirler. For the 1.5 swirl number, the lower stability range can be attributed to the effect of excessive swirl. This is because while swirl is said to entrain hot gases and enhance stability, excessive swirl comes with excessive vortex strength that can create an entrained cold, CO₂-rich oxidizer mixture, resulting in cooling and local extinction within the flame. Furthermore, excessive swirl can increase the rate of strain imposed on the flame by flow and exposes the flame to a velocity gradient that convectively cools the flame.

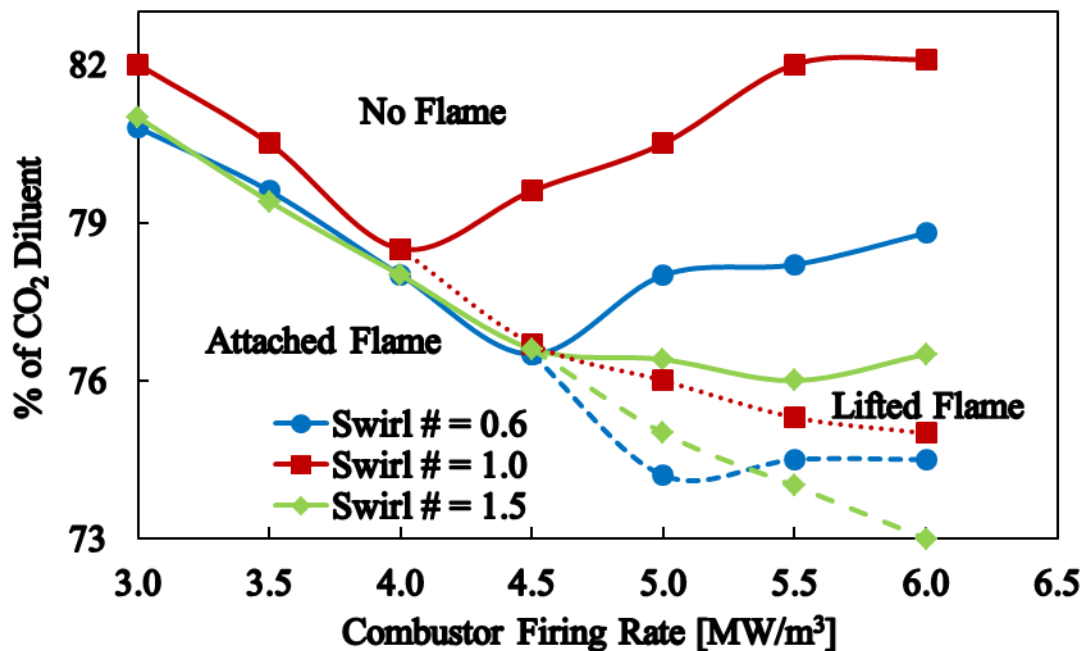


Figure 4.17: Stability map for oxyfuel flames at different swirl numbers, CO₂ dilution level, and at $\Phi = 1.0$

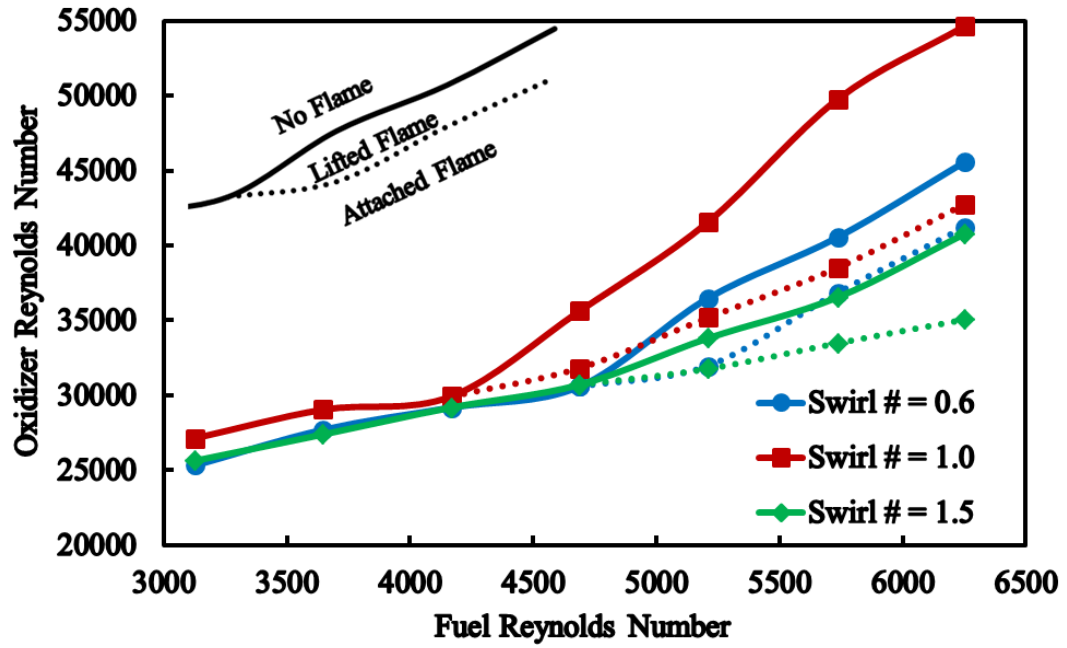


Figure 4.18: Stability map depicting blowout Reynolds number for fuel and oxidizer for oxyfuel flames at $\Phi = 1.0$ and different swirl numbers

CHAPTER 5

NUMERICAL STUDY OF THE COMBUSTION

CHARACTERISTICS OF PROPANE-OXYFUEL

FLAMES WITH CO₂ DILUTION

In this chapter, results from the numerical study of the effect of CO₂ dilution level on propane-oxyfuel flames in terms of the flame's macrostructure, temperature, and emissions are presented.

5.1 Overview

The use of computational fluid dynamics (CFD) in combustion studies is vital because of the tool's relatively lower cost compared with experimental studies, its use in optimization, and its ability to be used in the developmental phase of plants to reduce time. Modeling combustion requires the use of appropriate mathematical models for flow, heat transfer, as well as the chemistry. While it is known that modeling combustion is more accurate in 3D geometries, 2D axisymmetric geometries give reasonable accuracy at a relatively cheaper computational cost [159, 160]. The accurate prediction of flame macrostructure, temperature, and resulting species concentration from combustion

all depend on the reaction mechanism used during modeling among other things. The most accurate of such predictions can be achieved by the use of a detailed chemical mechanism which is computationally very expensive. Ultimately, it is a common practice in CFD to use reduced and global chemical mechanisms which are comparatively less expensive and give a reasonable degree of accuracy [161, 162]. Some of the global mechanisms modified for oxyfuel combustion reported in the literature include the work of Stefan et al. [163], Frassoldati et al. [164], and Andersen et al. [165].

There have been some numerical studies focusing on oxyfuel combustion in the literature. These include a study using detailed combustion mechanism, and thermodynamics analysis on oxyfuel combustion characteristics in gas turbine modes [166], study on the roles combustion chemistry and radiation heat transfer play in oxyfuel combustion modeling [167], and study on combustion and heat transfer properties in a retrofitted 600MW utility boiler [168]. Xie et al. [169] studied the effect of high CO₂ dilution on the oxy-combustion laminar flame in terms of stability, chemical reaction, and flame radiation. It is reported that the laminar burning velocity decreases with the increase in the CO₂ diluent. Only a few numbers of studies are available on the numerical analysis of oxyfuel combustion in the literature. These include the study by Krieger et al. [170] in which two oxyfuel mixtures and air were studied in a gas turbine model combustor using chemical equilibrium combustion model. Al-Abbas et al. [171] also studied two oxyfuel oxidizer mixtures and air-propane flames. They reported 8 times higher CO₂ concentration in the oxyfuel cases compared to air combustion products and lower CO concentrations for lower CO₂ diluent cases. To the best of our knowledge, no

numerical study regarding the effect of CO₂ dilution on the oxyfuel combustion of propane is reported.

In this study, a 2D axisymmetric geometry is used to approximate the cylindrical, swirl-stabilized, gas turbine model combustor. The schematic of the computational domain is shown in Figure 5.1. About 260,000 structured, non-uniform grid meshes are used in the domain, with denser mesh used in regions having high properties gradient like the inlets. The maximum aspect ratio in the mesh is about 10 with 95% of the mesh having values less than 4.

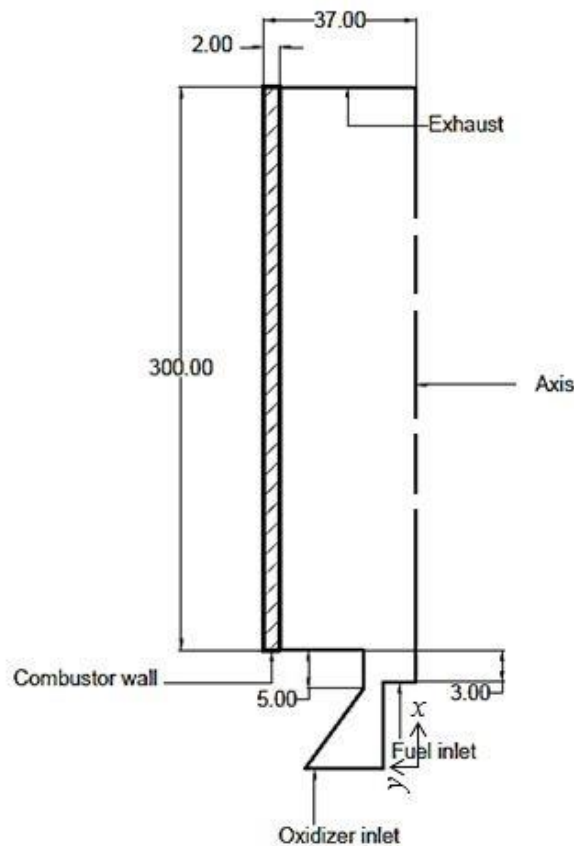


Figure 5.1: The schematic of the computational domain (all dimensions are in mm)

5.2 Chemical Reaction Modeling

The chemistry is modeled using the Eddy Dissipation Concept (EDC) suitable for turbulent reacting flows that assumes that reaction occurs in fine scales of turbulent structures. Unlike the eddy-dissipation model, that assumes the same turbulent rate for all reaction and, therefore, limited to modeling only one-step reaction (valid for chemical equilibrium and very fast chemistry scenario), EDC can be used to model detailed chemical mechanism that involves intermediate radicals. The source term for the reaction in EDC is computed using:

$$R_l = \frac{\rho(\varepsilon^*)^2}{\tau^*[1-(\varepsilon^*)^3]} (Y_l^* - Y_l) \quad (5.1)$$

Where Y_l^* is the small scale mass fraction corresponding to a reaction that proceeds over the time scale τ^* and fine length scale fraction ε^* obtained by directly integrating their respective Equations (5.2) and (5.3):

$$\tau^* = C_\tau \left[\frac{\nu}{\varepsilon} \right]^{\frac{1}{2}} \quad (5.2)$$

$$\varepsilon^* = C_\varepsilon \left[\frac{\nu \varepsilon}{k^2} \right]^{\frac{1}{4}} \quad (5.3)$$

Where C_τ and C_ε are the time scale and volume fraction empirical constants having values of 0.4082 and 2.1377 respectively [172].

The constants for reaction rates are calculated using the Arrhenius equation given as:

$$k(T) = AT^b \exp\left(-\frac{E_a}{RT}\right) \quad (5.4)$$

Where E_a is the activation energy of the reaction with the ones used in this study given in Table 5.1, b is the exponent for temperature T , R is the universal gas constant, and A is the pre-exponential factor whose adopted values for this study is also given in Table 5.1. Table 5.2 shows the Chemkin code input file for the three-step Jones-Lindstedt mechanism used in this study. The input file was implemented using the appropriate keywords and units utilized by Fluent software. It is noteworthy that the fourth and fifth reactions in the table do not involve H_2O ; hence, we use zero stoichiometric coefficients for it. However, the forward rate exponent of H_2O (having a value of 0.5) needs to be included as it affects the reaction due to H_2O presence in the combustion mixture [164, 165]. Also, the rate exponent of the H_2O is used in the calculation of the pre-exponential factor, A , in proper units for importing it into the Fluent software. The mechanism is adopted from the work of Hjartstam et al. [163] where the dissociation reactions were modified from the original Jones-Lindstedt [162] to account for changes in Oxy-fuel combustion.

Table 5.1: Three Steps Jones-Lindstedt Propane Oxy-Combustion Arrhenius Rate Constants with reaction orders adopted from Stefan Hjartstam et al. [163] in units of Kg, m, s, Kcal, mol

Reaction	Reaction Order	A	b	E_a
$C_3H_8 + 1.5O_2 \Rightarrow 3CO + 4H_2$	$[C_3H_8]^{0.5}[O_2]^{1.25}$	4×10^{11}	0	30.0
$H_2 + 0.5O_2 \Rightarrow H_2O$	$[H_2][O_2]^{0.5}$	1.8×10^{13}	0	35.1
$H_2O \Rightarrow H_2 + 0.5O_2$	$[H_2O]$	5.337×10^{16}	-0.5	94.3
$CO + 0.5O_2 + 0H_2O \Rightarrow CO_2$	$[CO][O_2]^{0.5}[H_2O]^{0.5}$	1.3×10^{11}	0	30.0
$CO_2 + 0H_2O \Rightarrow CO + 0.5O_2$	$[CO_2][H_2O]^{0.5}$	1.213×10^{16}	-0.5	97.1

Table 5.2: The Three Steps Jones-Lindstedt [162] adopted from Stefan Hjartstan et al. [163] Propane Oxy-Combustion Chemkin code in units of cm, s, cal, mol, and K:

ELEMENTS		
C H O		
END		
SPECIES		
C3H8 O2 H2O CO2 CO H2		
END		
REACTIONS		
C3H8 + 1.5O2 => 3CO + 4H2	7.113E+130.0	30000
FORD/C3H8 0.5/		
FORD/O2 1.25/		
H2 + 0.5O2 => H2O	5.69E+14 0.0	35100
FORD/H2 1/		
FORD/O2 0.5/		
H2O => H2 + 0.5O2	5.337E+16-0.5	94300
FORD/H2O 1.0/		
CO + 0.5O2 + 0H2O => CO2	1.30E+14 0.0	30000
FORD/CO 1.0/		
FORD/O2 0.5/		
FORD/H2O 0.5/		
CO2 + 0H2O => CO + 0.5O2	3.836E+17-0.5	97100
FORD/CO2 1.0/		
FORD/H2O 0.5/		
END		

5.3 Boundary Conditions

Mass-flow-inlet boundary conditions are used at the fuel as well as the oxidizer inlets with axial ($\cos \theta$) and tangential ($\sin \theta$) components of flow direction specified based on the swirl number (swirl number of 1.0 is used throughout the study in this chapter). The inlet fuel and oxidizer conditions are provided based on the desired operating conditions of the combustor in terms of firing rate, equivalence ratio, and CO₂ dilution level. The temperature of the reactants (fuel and oxidizer) is fixed at 300 K at their respective inlets. The exhaust from the combustor is modeled to discharge to surroundings at standard

atmospheric conditions. Conjugate heat transfer (fluid-solid interface heat transfer) is considered within the inner walls of the combustor with a condition of no species flux normal to the wall surface. The conjugate heat transfer solves the Navier-Stokes and energy equations, first in the fluid domain, before solving for the heat transfer across the solid boundary. For the non-adiabatic combustor, heat losses by conduction through the combustor wall, as well as mixed (convection and radiation) heat transfer on the outer side of the combustor are considered. An average estimated value of the convection heat transfer coefficient of $20 \text{ W/m}^2\text{K}$ is used for the ambient air.

5.4 Solution Procedure

The partial differential equations of the conservation laws, together with radiative heat transfer equation are solved subject to appropriate boundary conditions, using the commercial code ANSYS FLUENT 16.2. The semi-implicit method for pressure-linked equations (SIMPLE) algorithm is employed for pressure-velocity coupling. The pressure equation is discretized using the pressure staggering option (PRESTO), deemed more appropriate with high swirl number flows. All other equations including that of species conservation and momentum are discretized using a second-order upwinding scheme. The convergence criteria used is when the maximum residuals of continuity, momentum, turbulent kinetic energy, and turbulent dissipation rate are less than 10^{-4} . Residuals used for energy and radiation equations are less than 10^{-6} . Also, CO and temperature were monitored in the combustor through their changes until a constant value is achieved. The

solvers used are pressure-based with axisymmetric swirl used in the 2D space under steady state conditions.

5.5 Results

In subsequent sections, the results obtained from the developed numerical model will be presented and discussed.

5.5.1 Flame Macrostructure

The flames macrostructures, which are time-averaged flame shapes represented by the calculated temperature field and experimentally recorded images at different CO₂ dilution level, are shown in Figure 5.2. The CO₂ dilution level was varied from 0 to 69% at a fixed global equivalence ratio of stoichiometry and firing rate of 5 MW/m³ while monitoring the flame transition. Images shown in the figure are selected among others to represent visibly contrasting structures from their counterparts during dilution. From the figure, the similarity between experimental and numerical flame structures is evident giving credence to the validation of the numerical model used. Without any CO₂ dilution (at 0% CO₂), as can be seen from the figure, the flame exhibits a jet-like appearance of a simple jet flame, suggesting that the annular-fuel-jet dominated the flame because of large jet momentum relative to vortex-induced momentum. This jet-flame-like appearance continued with the addition of the diluent until 45% when the flame transits

into a V-shaped flame. The wide V-shaped flame suggests high vortex strength momentum relative to fuel-jet momentum. Further addition of the diluent makes the V-shaped flame more compact and wider as can be seen from the figure. The annular-fuel-jet dominated flame has an extended reaction zone evident from the comparatively wider region of propane consumption in the combustor as shown in Figure 5.3. From the figure, one can observe that the increase in CO₂ dilution level increases the consumption rate of propane, happening within a comparatively shorter distance in the combustor. This is because increasing the diluent increases the oxidizer Reynolds number and hence the turbulent mixing in the combustor. With enhanced mixing in the combustor, the reaction becomes more efficient owing to more contacts between the reactants. We stopped the dilution at 69% because at that percentage, and at stoichiometry, the oxidizer mixture is estimated to have the same adiabatic flame temperature as that of propane-air mixture. Also at higher dilution levels, the flame's static stability window will be exceeded at a certain point leading to flame liftup and subsequent blowout.

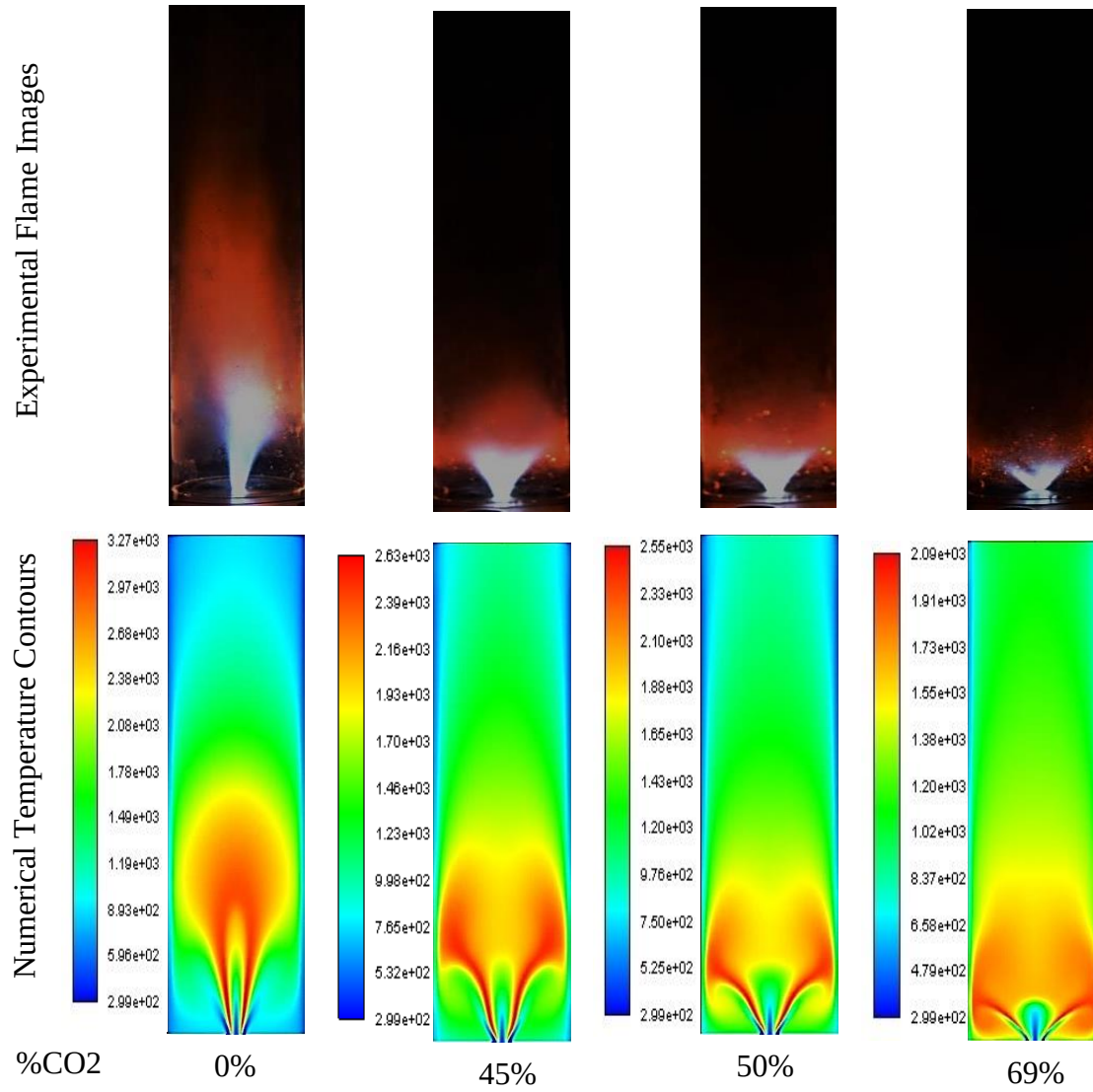


Figure 5.2: Experimental and numerical flames macrostructure obtained at different dilution levels, the firing rate of 5MW/m³, and $\Phi = 1.0$

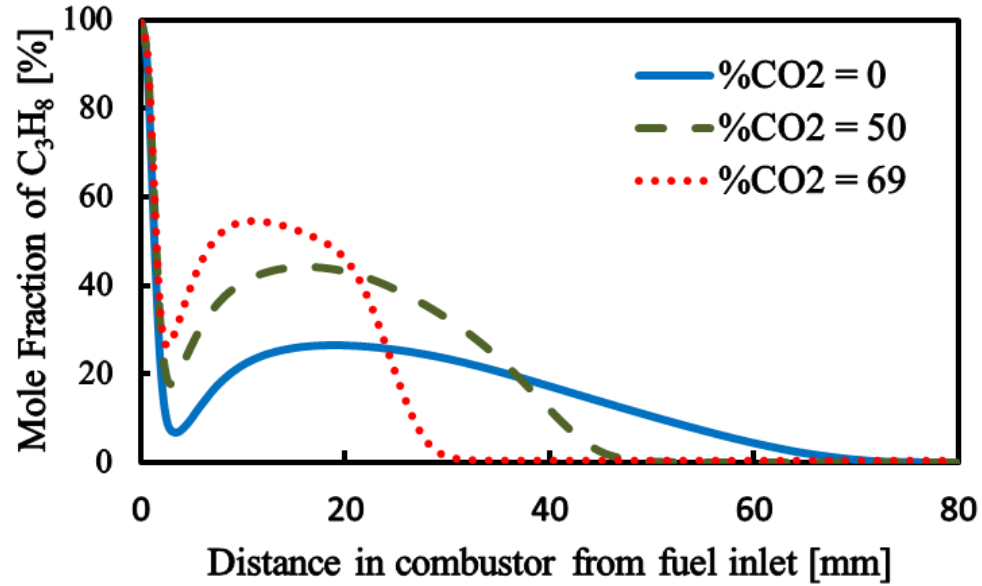


Figure 5.3: Propane mole fraction distribution from the combustor's inlet at different dilution levels obtained at $\Phi = 1.0$, and the firing rate of 5MW/m^3 .

The flame transitions resulting from increased dilution level discussed above was observed to result in different anchoring position of the flames, with different nature of coherent structures formed in the flow. This can be seen in Figure 5.4 in which we overlaid the computed flow stream function onto the kinetic rate of the hydrocarbon oxidation reaction for the same CO_2 dilution level points between 0 and 69%. It is observed that the fuel-jet dominated flame manifesting at zero and low CO_2 dilution level is anchored between the outer recirculation zones (ORZ) formed by the sudden expansion of flow, either side of the central annular fuel jet, into the combustor, downstream of its dump plane. It is reported in the literature that relation between fuel jet momentum and vortex strength momentum determines the structure exhibited by swirl-stabilized non-premixed flames [57]. At zero and CO_2 dilution level lower than 45%, the fuel-jet momentum is high relative to vortex strength momentum causing the fuel-jet to penetrate

the recirculation zone, in contrast to the V-shaped flame where the fuel-jet does not penetrate the recirculation zone.

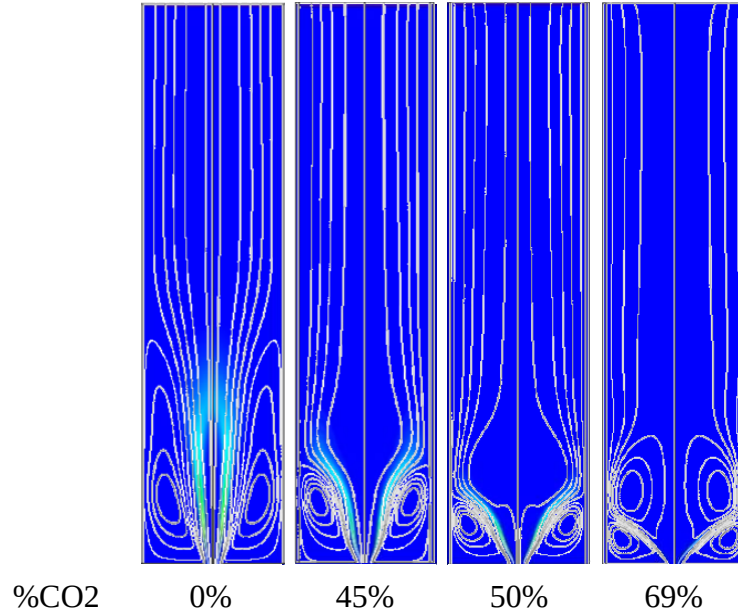


Figure 5.4: Flow stream function overlaid onto the kinetic rate of the hydrocarbon oxidation reaction at different dilution levels obtained at $\Phi = 1.0$ and the firing rate of 5MW/m^3

The vortex strength, as reported in the literature, can be directly increased by increasing the velocity of the flow into the swirler as it is linearly related to the velocity of the recirculating flow, or by increasing the swirl number. As the vortex strength grows with the increase in flow due to higher CO_2 dilution level, for the fixed fuel jet momentum and swirl number, vortex breakdown occurs resulting into the formation of vortex-breakdown-induced recirculation zone which forms the inner recirculation zone (IRZ). Consequently, the V-shaped flame is anchored in-between ORZ and IRZ in the inner shear layer. In Figure 5.5, the non-dimensional vortex strength (I^*) is presented as a

function of the CO₂ dilution level at stoichiometric equivalence ratio and firing rate of 5 MW/m³ (constant jet momentum). The vortex strength (Γ) used to compute Γ^* was obtained by defining a custom field in Fluent by dividing stream function (units of kg/s) by density (kg/m³) so that Γ is obtained in m³/s, which is equivalent to m²/s in the 2D field. From the figure, it can be observed that at dilution levels between 0 and 40%, Γ^* remains almost constant at 0.2. Beyond this range, which coincides with the transition point from jet to V-shaped flame at 45% CO₂ diluent, Γ^* suddenly begins to increase. This fact can be utilized to predict the flame transition or target a specific flame's macrostructure by controlling the jet momentum and the strength of the vortex created by the swirling flow. The closer the non-dimensional vortex strength is to zero, the more jet-like flame structure becomes, while higher values signify a more compact flame.

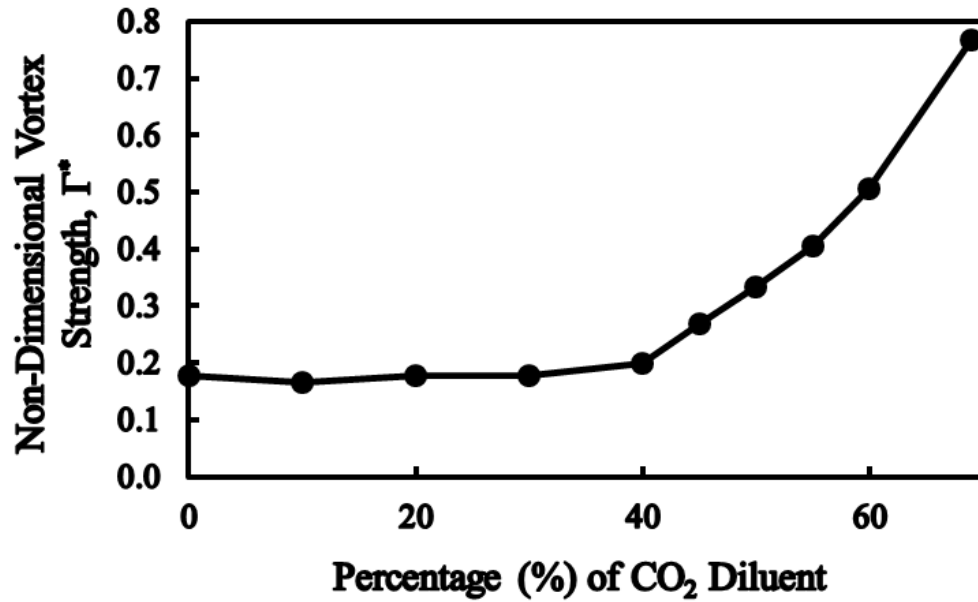


Figure 5.5: Non-dimensional vortex strength as a function of CO₂ dilution level obtained at $\Phi = 1.0$ and the firing rate of 5MW/m³.

5.5.2 Effect of CO₂ dilution on mixing and chemical reaction time

As we have discussed in Chapter 2 of this dissertation, the static stability of the non-premixed combustor can be scaled by the ratio of mixing to chemical reaction time scales. While the numerical model developed cannot be used to ascertain the blowout limit (the 2D, steady, RANS model only captures stable range of operation), we can employ it to look into the mixing and chemical reaction time scales characteristics prior to flame liftup and eventual blowout. The mixing time is defined as the ratio of length scale to reference velocity. Using our model, we can estimate the mixing time to be the time the combustion gases took in the combustor (the ratio of the combustor length to the velocity at the exhaust). The chemical time, on the other hand, can be estimated by the ratio of thermal diffusivity to the square of laminar flame speed. By defining a custom field in Fluent, thermal diffusivity is calculated using Equation 5.5. Laminar flame speed, on the other hand, can be obtained using Equation 5.6.

$$\alpha = \frac{K}{\rho c_p} \quad (5.5)$$

$$S_L = \left[\alpha \dot{w} \frac{T_F - T_{ig}}{T_{ig} - T_o} \right]^{1/2} \quad (5.6)$$

Where K is the coefficient of thermal conductivity, ρ is the density, $\dot{w}$ is the reaction rate in $\text{Kgmol/m}^3\text{-s}$, T_F is the flame temperature, and T_{ig} is the ignition temperature. Using an assumption that $T_F - T_{ig} \cong T_{ig} - T_o$, the laminar flame speed obtained from the model is shown in Figure 5.6 as a function of CO₂ dilution. The variation of thermal diffusivity as a function of CO₂ dilution is also shown in Figure 5.7. From the figures, it can be

observed that both flame speed and thermal diffusivity decreases with increase in CO₂ dilution. Subsequently, the chemical reaction time decrease with increase in CO₂ diluent (Figure 5.8), signifying slower chemistry at higher diluent concentrations. In literature, propane/air laminar flame speed was reported to have an average maximum value of 0.4 m/s at STP [173, 174]. This value falls between 50 to 60% CO₂ (estimated flame speeds of 0.57 to 0.34m/s) dilution level for the oxyfuel mixtures studied. The decrease in flame speed with an increase in CO₂ dilution is understandable due to the high thermal capacity of CO₂ that takes away heat and because of low CO₂ molecular diffusivity compared to O₂ (0.16cm²/s for CO₂ in air versus 0.176cm²/s for O₂ in air).

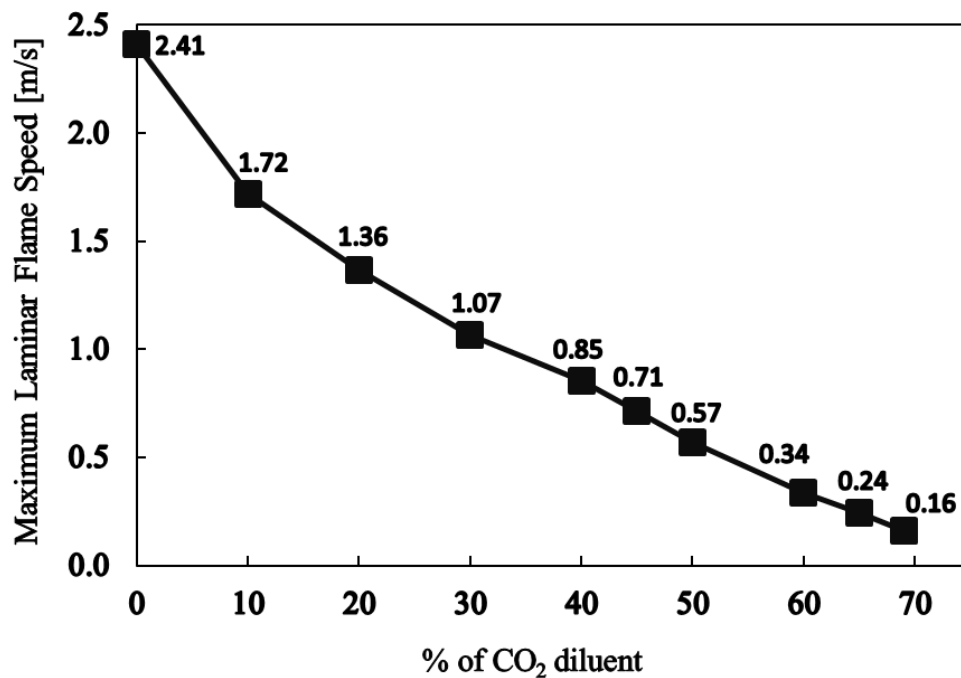


Figure 5.6: Maximum laminar flame speed as a function of CO₂ dilution level obtained at $\Phi = 1.0$ and the firing rate of 5MW/m³.

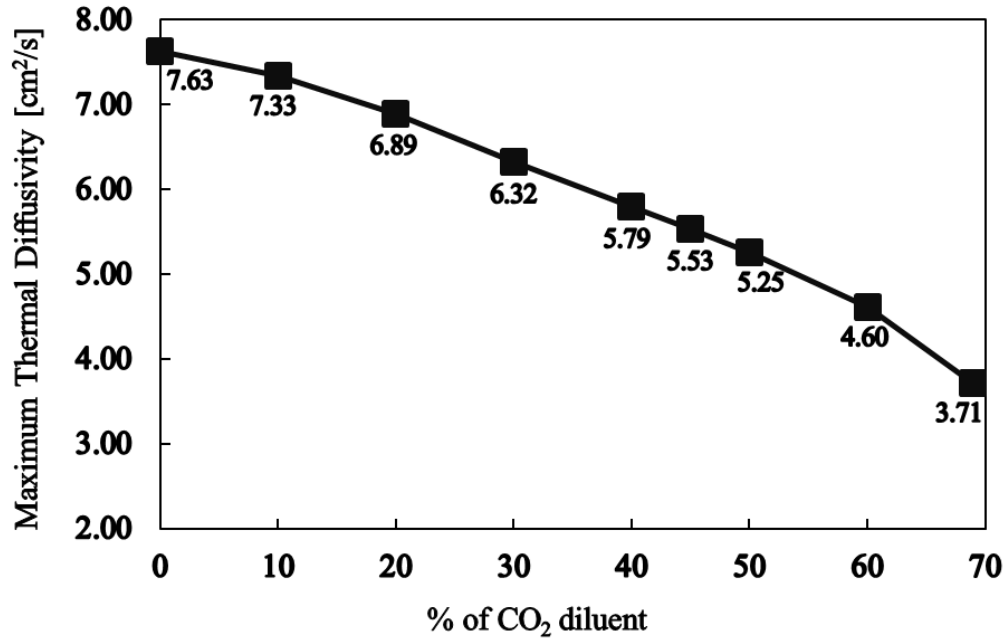


Figure 5.7: Maximum thermal diffusivity as a function of CO₂ dilution level obtained at $\Phi = 1.0$ and the firing rate of 5MW/m³.

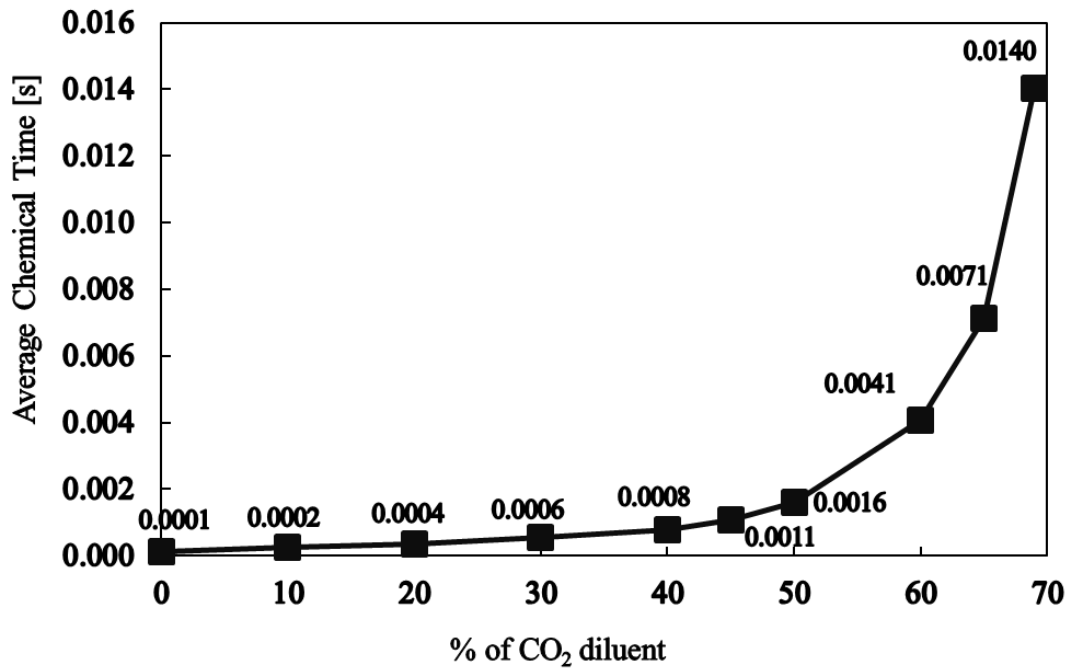


Figure 5.8: Average chemical reaction time as a function of CO₂ dilution level obtained at $\Phi = 1.0$ and the firing rate of 5MW/m³.

The effect of CO₂ dilution on the Damkohler number can be seen in Figure 5.9. From the figure, it is clear that increasing the dilution level decreases the Damkohler number. The maximum value of 4,430 is obtained for Damkohler number at zero CO₂ dilution (pure oxygen) compared with the value of 15 obtained at 69% CO₂ diluent. High Damkohler number entails closeness of chemical reaction to chemical equilibrium (fast chemistry), whereas lower values signify an increased departure from chemical equilibrium (slow chemistry that is comparatively more susceptible to flame extinction). Subsequently, the lower the Damkohler number, the closer the flame is from blowout, which happens at a certain critical Damkohler number. The results shown here are all for attached flames, it is, however, clear that increasing the CO₂ dilution level beyond these reported values will eventually lead to flame blowout as we have seen in the experimental results discussed in Chapter 4. From the previous chapter's results, the CO₂ dilution level at blowout is about 79% for the stoichiometric equivalence ratio and firing rate of 5 MW/m³.

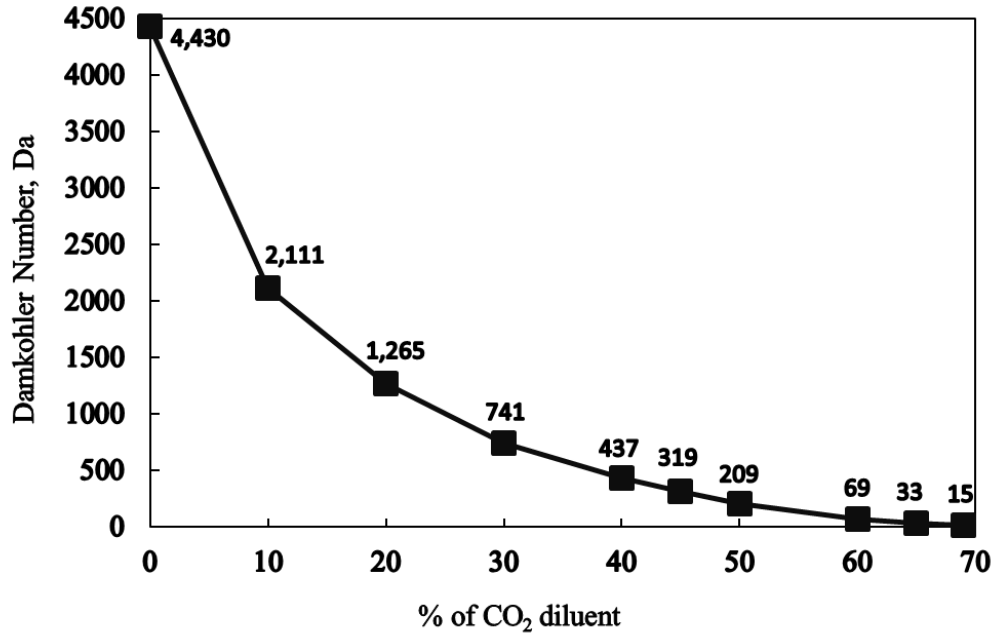


Figure 5.9: Damkohler number as a function of CO₂ dilution level obtained at $\Phi = 1.0$ and the firing rate of 5MW/m³

Apart from the chemical effect of CO₂ dilution, increased dilution also contributes to increased strain on the flame. Figure 5.10 shows the effect of CO₂ dilution on strain rate at stoichiometric global equivalence ratio and firing rate of 5MW/m³. From the figure, it can be observed that increasing the dilution level is accompanied by an increase in the rate of strain. Consequently, flames having higher CO₂ dilution level are more susceptible to blowout. It is, therefore, evident that flame blowout for the oxyfuel flames diluted with CO₂ occurs as a consequence of both chemical effect of CO₂ and the strain imposed on the flame by higher flow at high CO₂ dilution. By fixing the flow, therefore, one can limit the effect of CO₂ dilution to only chemical effects.

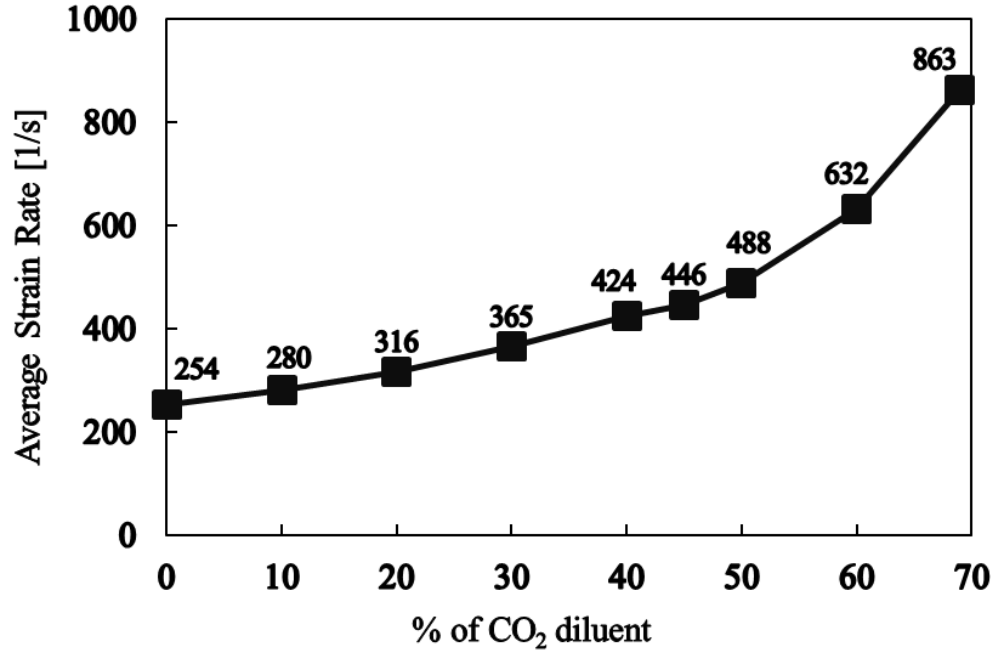


Figure 5.10: Strain rate as a function of CO₂ dilution level obtained at $\Phi = 1.0$ and the firing rate of 5MW/m³

5.5.3 Temperature Distribution

Figure 5.11 shows the temperature distribution along the center of the combustor at the distance of 150mm to 250mm from the dump plane of the combustor. The two profiles are experimental measurement and numerical estimation at a fixed firing rate of 5 MW/m³, stoichiometric global equivalence ratio, and CO₂ dilution level of 69%. From the figure, as expected, the temperature in both cases decreases downstream of the combustor, as the combustion gases losses their heat by convection and radiation moving toward the exit. The numerically estimated temperatures are slightly higher than the corresponding experimental measurements with a maximum deviation of 15%.

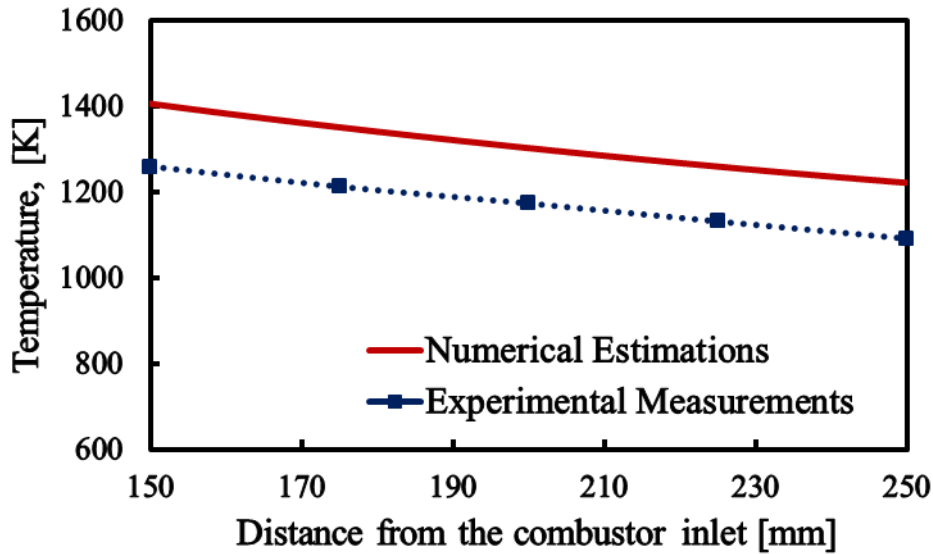


Figure 5.11: Experimental and numerical temperature distribution of combustion gases obtained at 69% CO₂ dilution level, $\Phi = 1.0$, and the firing rate of 5MW/m³.

The effect of CO₂ dilution level on numerically obtained temperature distribution in the combustor is shown in Figure 5.12. At the fixed firing rate of 5 MW/m³ and stoichiometric global equivalence ratio, the profiles depict the temperature variation from near the fuel inlet ($y = 3.175\text{mm}$) to the combustor exit. The cooling effect of the CO₂ diluent is evident from the figure with the peak of temperature varying from 3250 K when no diluent was added to about 1900 K at 69% CO₂ dilution level. The peak of the temperature decreases with each increase in the diluent. First and the second peaks in the temperature profiles signify the beginning and the end of the flame region. The drops in temperature profiles after the first peaks represent a nonflame, hot gases region at the flame core; annular space inside the fuel jet for the jet-like flame and IRZ for the V-shaped flame (see Figure 5.2 and Figure 5.4). Shorter distances between the first and the

second peaks at high CO₂ dilution levels as depicted in Figure 5.12 attest to the compactness of the flame at high dilution level as discussed in the previous section. Toward the exit of the combustor, the difference in temperature between these profiles becomes narrower irrespective of the amount of diluent, suggesting an increased heat transfer by the highly radiative, CO₂-rich, combustion products. Figure 5.13, shows the effect of CO₂ diluent on the maximum temperature in the combustor. The figure compliments what was discussed previously with regards the decrease in temperature with increased CO₂ dilution.

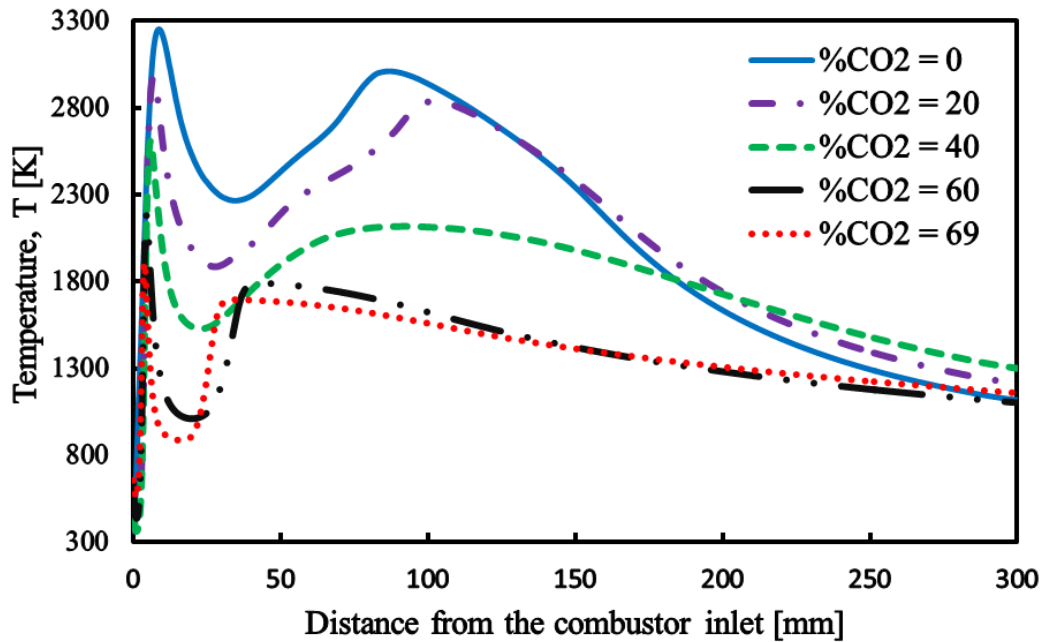


Figure 5.12: Temperature distribution in the combustor from inlet to exit at different CO₂ dilution levels, $\Phi = 1.0$, and the firing rate of 5MW/m³

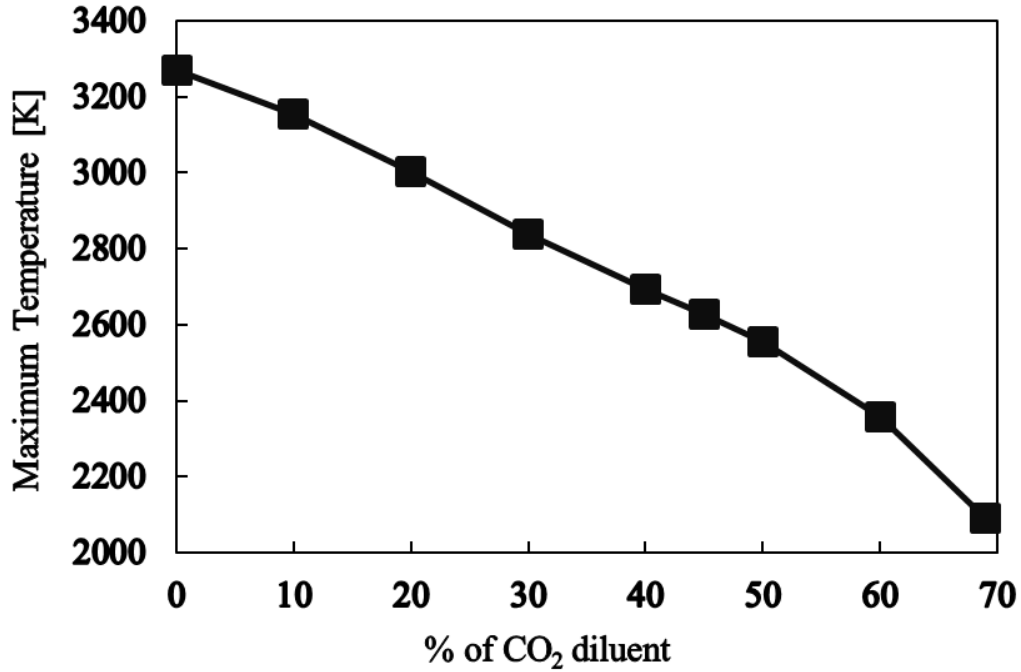


Figure 5.13: Maximum combustor temperature at different CO₂ dilution levels, $\Phi = 1.0$, and the firing rate of 5MW/m³

5.5.4 CO Emission

The effect of CO₂ dilution level on average CO emission at the combustor exit is shown in Figure 5.14. The profiles were obtained at a constant firing rate of 5MW/m³ and three global equivalence ratios of 1.0, 0.98, and 0.95. It is noteworthy that the equivalence ratio sweep conducted here is near stoichiometry to avoid the excessive use of oxygen, typically produced using expensive separation techniques. Lowering the equivalence ratio lowers the amount of CO produced due to more oxygen available for the conversion of CO to CO₂. The effect of equivalence ratio on the average CO emission is more pronounced at low dilution levels as depicted, at high dilution levels greater than 60%,

the effect of equivalence ratio shrinks. From the figure, we can see that the amount of CO in the exhaust gases increases with the increase in CO₂ diluent up to 55% beyond which the amount of CO begins to decrease irrespective of the equivalence ratio. This decrease is attributable to the cooling effect of the diluent that hinders the dissociation of CO₂ at low temperatures corresponding to the high amount of diluent and higher mixing time produced by the transited V-shaped flame. As a consequence of the decrease in temperature due to dilution, CO₂ dissociation reaction can be seen to diminish in Figure 5.15 in which represent the kinetic rate of CO₂ dissociation reaction as a function of the amount of diluent. From the figure, high peaks can be observed for zero and low dilution level. Also, the presence of a second peak, downstream of the combustor, can be observed, which demonstrates an elongated reaction zone. This is against the flattened line recorded at 69% CO₂ dilution level that signifies almost zero dissociation for the compact flame. Consequently, this could suggest CO₂ diluent participation in the reaction at higher temperatures.

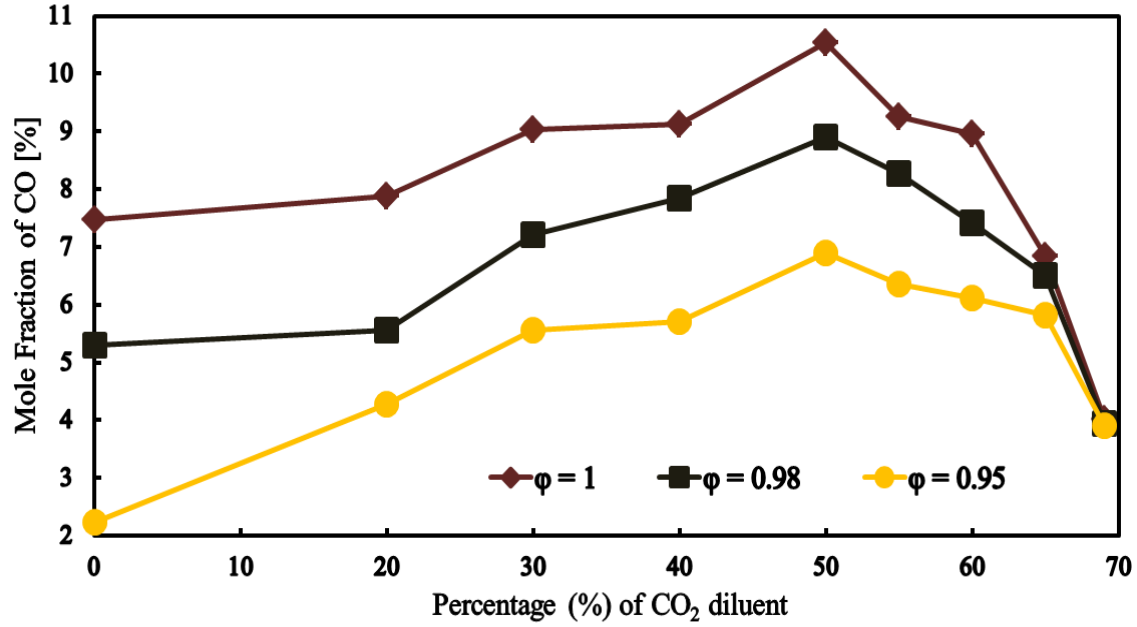


Figure 5.14: Effect of CO₂ dilution level on average CO emission obtained at three different global equivalence ratios, and firing rate of 5MW/m³.

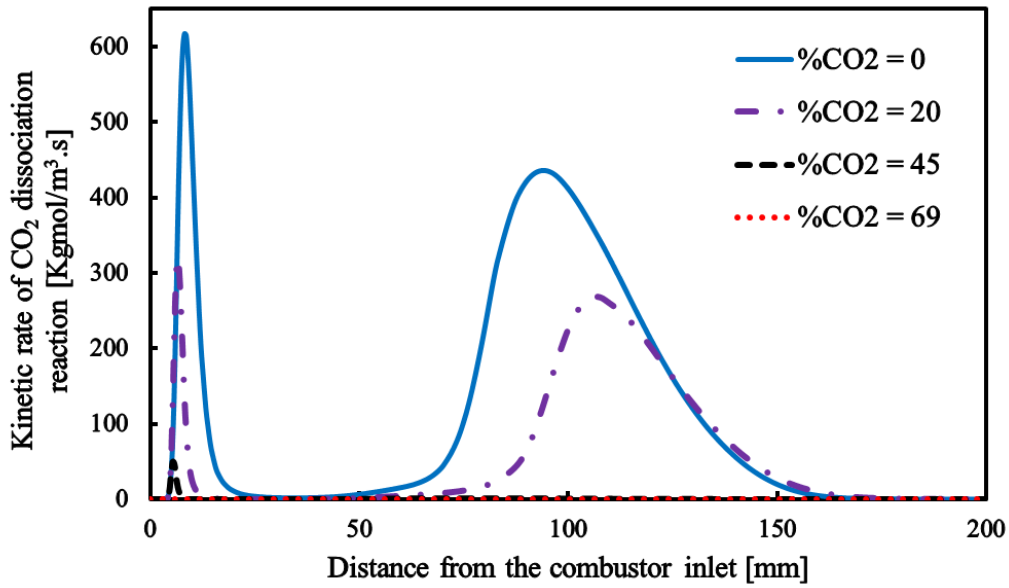


Figure 5.15: The kinetic rate of CO₂ dissociation reaction with distance in the combustor at different dilution level obtained at $\Phi = 1.0$, and the firing rate of 5MW/m³.

Apart from CO₂ dissociation at high temperatures, the increase in CO level in the exhaust gases at higher dilution levels is also related to lower residence time in the combustor resulting from increased flow due to the CO₂ dilution. Lower residence time at high dilution level will hinder recombination of the dissociated CO₂. That could explain the continued increase in the amount of CO at the exhaust despite the increase in the diluent between 0 and 55%. Figure 5.16 illustrates the distribution of mole fraction of CO from inlet to the exit of the combustor drawn at the combustor axis. The profiles complimented what was previously discussed using the average mole fraction of CO at the combustor's exit.

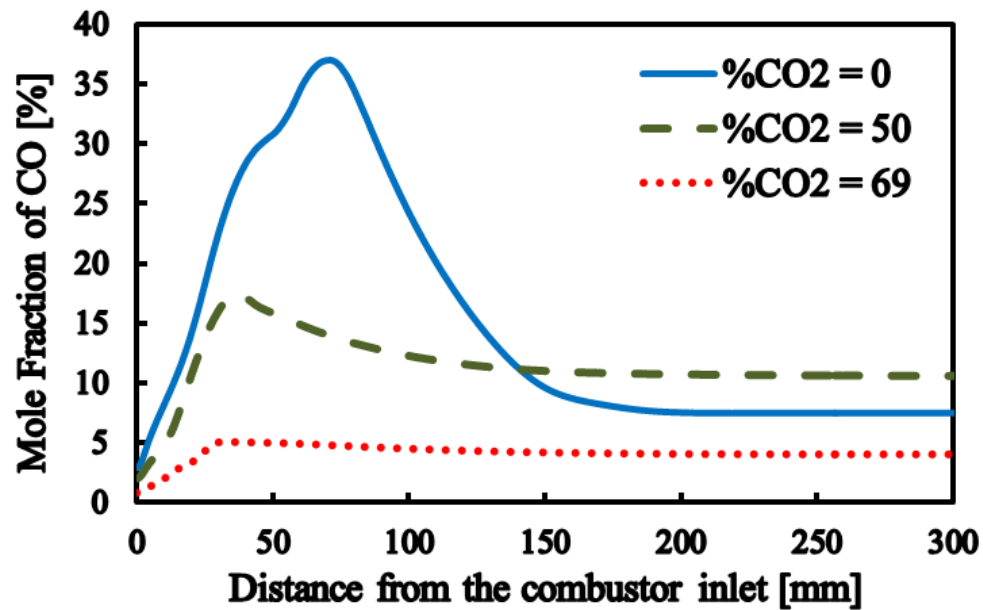


Figure 5.16: Mole fraction of CO at the center of the combustor with distance at different dilution level obtained at $\Phi = 1.0$, and the firing rate of 5MW/m³.

5.5.5 CO₂ Emission

The distribution of CO₂ mole fraction in the combustor at different dilution levels, as well as the average CO₂ mole fraction at the combustor's exit, are shown in Figure 5.17 and Figure 5.18 respectively. The profiles were obtained at a stoichiometric global equivalence ratio and firing rate of 5 MW/m³. In Figure 5.17, the CO₂ mole fraction at the combustor's axis was plotted as a function of distance in the combustor. From the figure, the increase in the amount of CO₂ with increased dilution level can be observed. At higher dilution levels, the change in the CO₂ mole fraction terminates within shorter distance in the combustor, signifying a more compact and shorter flame, resulting from enhanced mixing, caused by the added diluent. For the case of zero dilution level, the decrease in CO₂ mole fraction observed at about 65 mm into the combustor could be attributed to dissociation of the CO₂ at the high temperature associated with the propane-oxyfuel flame having no diluent added. At the highest dilution level studied, the amount of CO₂ by volume in the exhaust reaches the average of 68% with H₂O reaching 27% meaning about 95% of the gases consist of CO₂ and H₂O; good candidates for carbon capture and sequestration. The remaining 5% of the gases consists of about 4% CO and traces of hydrogen and unburnt hydrocarbon. In Figure 5.18, it can be seen that the average mole fraction of CO₂ at the combustor exit increases with an increase in the dilution level. Lower equivalence ratios are associated with higher CO₂ at the exhaust owing to more available oxygen for CO conversion into CO₂. This effect, however, dampens at higher dilution levels as the cooling effect of the diluent dominates.

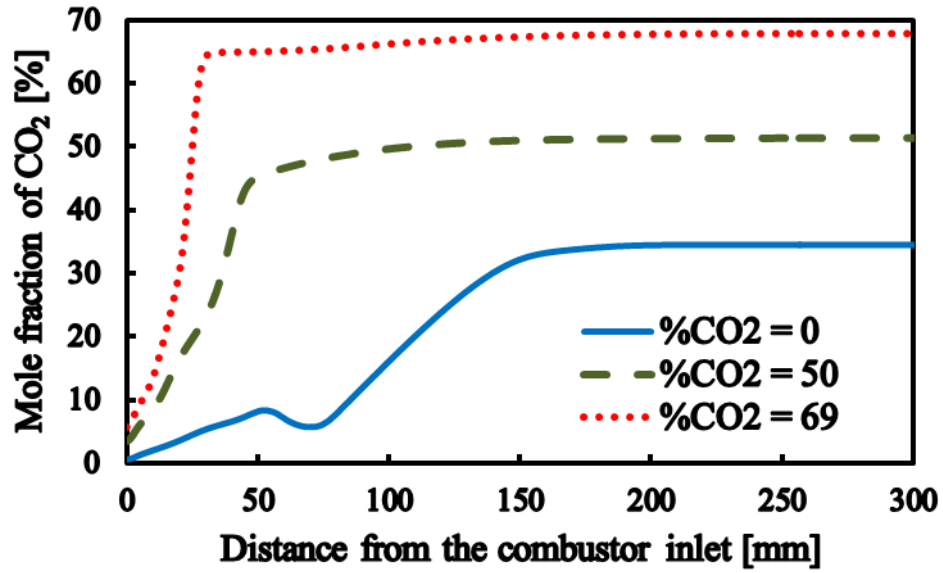


Figure 5.17: Mole fraction of CO₂ at the center of the combustor with distance at different dilution level obtained at $\Phi = 1.0$, and the firing rate of 5MW/m³.

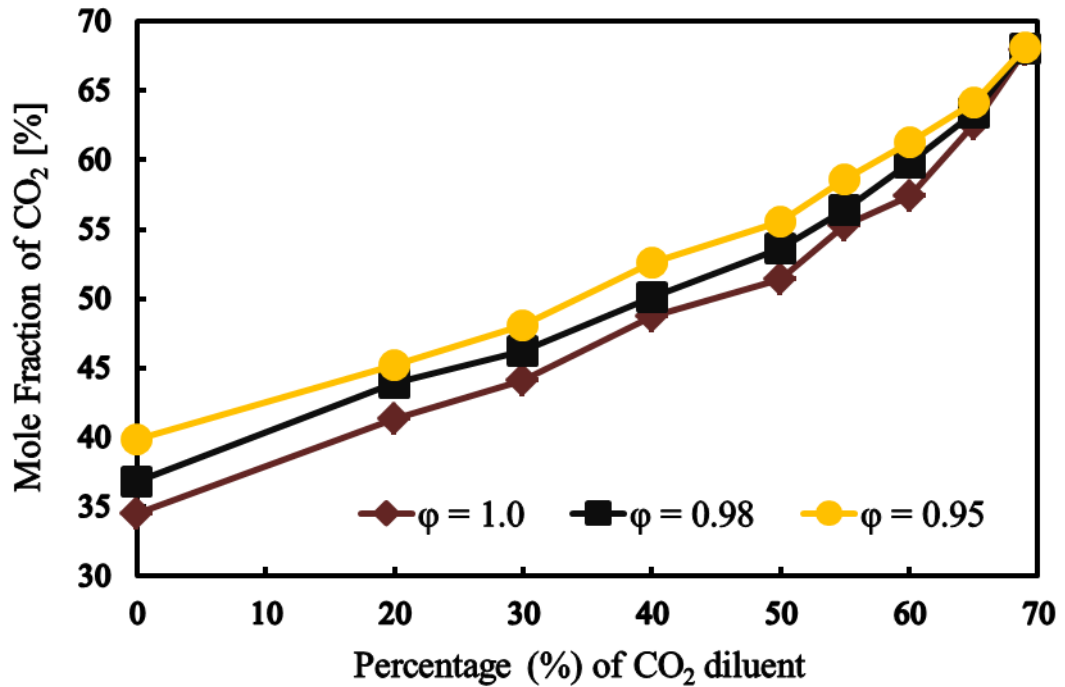


Figure 5.18: Effect of CO₂ dilution level on average CO₂ emission obtained at three different global equivalence ratios, and firing rate of 5MW/m³.

CHAPTER 6

EXPERIMENTAL AND NUMERICAL STUDY OF NON- PREMIXED OXY-COMBUSTION OF HYDROGEN- ENRICHED PROPANE

In this chapter, results from the experimental study focusing on the effect of adding hydrogen on the blowout limit of propane oxyfuel combustion with carbon dioxide dilution are presented and discussed. The study was conducted in a non-premixed, swirl-stabilized combustor under steady state and close to global stoichiometric conditions. Furthermore, a numerical model to study the effect of hydrogen enrichment on the combustion thermo-chemical scalars such as temperature and emissions under fixed oxyfuel oxidizer mixture was developed. Results obtained from the numerical model are also presented and discussed. Non-premixed combustion model that solves transport equation for mixture fraction was used in modeling the chemistry as no reduced chemical reaction mechanism concerning hydrogen-enriched oxyfuel flames was reported in the literature.

6.1 Overview

As discussed in greater detail in Chapter 2, flame blowout occurs when the local fuel and oxidizer mechanical mixing rate is shorter than the characteristic local reaction rate. At that critical condition, the chemical reaction time is too long to allow for flame propagation even if the reactants attain stoichiometric mixture fraction at localized spots. In other words, flame blowout occurs when the characteristic chemical time exceeds the characteristic mixing time in combustion systems [29]. The mixing time can be quantified as the time available for “backmixing” by large-scale flow structures of hot products with the incoming mixture of reactants [56]. Another mechanism through which flame blowout can be explained is when the rate of heat loss from the combustor becomes higher than the rate of heat liberation from the chemical reaction [113]. CO₂ dilution, in oxyfuel flames, causes cooling and lowers the flame speed. Consequently, at a certain concentration in the oxyfuel oxidizer mixture, CO₂ will cause flame blowout.

Hydrocarbon fuels are commonly enriched with hydrogen to alter their combustion dynamics particularly with respect to static stability [175]. Apart from stability, the emission characteristic from hydrogen-enriched fuels combustion is also affected. In hydrogen enriched fuels, the major role with regard to flame blowout is played by the hydrogen concentration in the fuel mixture. Hydrogen-containing fuels, depending on the concentration of hydrogen, are characterized by relatively higher flame speeds, which play a major role in establishing the flames blowout limit. Almost all the literature dealing with the use of hydrogen to enhance blowout limits of hydrocarbon fuels combustion focuses on extending lean blowout limit in air combustion for low NO_x.

Literature regarding hydrogen enrichment of oxyfuel flames are few and focus on methane rather than propane fuel which have higher carbon content (a good attribute for oxyfuel combustion with CCS) [10]. A study focusing on H₂ enrichment onto propane-oxy-combustion flames with CO₂ dilution, however, is not reported in the literature.

6.2 Hydrogen-Enriched Oxycombustion; Experimental Study

Using the experimental set-up and conditions discussed in Chapters 3 of this thesis, experiments were conducted to determine the blowout limit of hydrogen-enriched, propane oxyfuel flames under CO₂ dilution. The results from these experiments are presented and discussed in the following section.

6.2.1 Static Stability of propane-oxyfuel flames with hydrogen enrichment

Figure 6.1 and Figure 6.2 depict the stability map with attached and no-flame regions in terms of CO₂ dilution level and Reynolds number of the oxidizer respectively. The blowout points were obtained at stoichiometric global equivalence ratio ($\Phi = 1$) and different hydrogen concentration in propane fuel. It is evident in Figure 6.1 that adding hydrogen to the propane fuel extends the flame's blowout limit under the influence of CO₂ dilution as the flame withstands higher CO₂ concentration in the oxyfuel oxidizer mixture. An average increase of 2.5% in CO₂ diluent concentration in O₂/CO₂ oxidizer mixture was recorded when the hydrogen concentration in propane was increased from 0

to 30% at different combustor firing rates. The calculated uncertainty of about 0.8% was recorded for the CO₂ dilution. We can also observe from Figure 6.1 that an increase in the firing rate decreases the concentration of CO₂ in the oxidizer at blowout by about 4% from the firing rate of 2 to 3 MW/m³. This is because an increase in firing rate entails increasing the fuel flow rate which will necessitate a corresponding increase in oxygen flow rate to maintain the stoichiometric equivalence ratio constant. Consequently, the percentage of CO₂ in the oxidizer mixture decreases. However, at high firing rate, due to the consequent increase in local flame temperature, higher CO₂ flow rate was endured by the flame at blowout so that the increase in oxygen does not lower its percent concentration in the oxidizer mixture. Furthermore, as we have seen in the previous chapter, increasing firing rate increases the level of strain on the flame by the flow, and hence, it reduces its resistance to blowout under CO₂ dilution.

In Figure 6.2, one can observe an increase in oxidizer Reynolds number at blowout with an increase in the combustor firing rate. An average increase of 7000 in Reynolds number was recorded when the combustor firing rate increases from 2 to 3.5 MW/m³ at different hydrogen concentrations in the fuel mixture. Also, from the figure, one can observe enhanced flame stability with an increase in hydrogen concentration in the fuel. An average increase of 3200 in oxidizer Reynolds number at flame blowout was recorded when the hydrogen composition was increased from 0 to 30% at different firing rates. This is because when in a mixture, hydrogen can alter the local equivalence ratio as a result of its high molecular diffusivity and accordingly increases the local flame speed [128]. As a consequence of this increase in local flame speed, the flame's resistance to extinction gets enhanced.

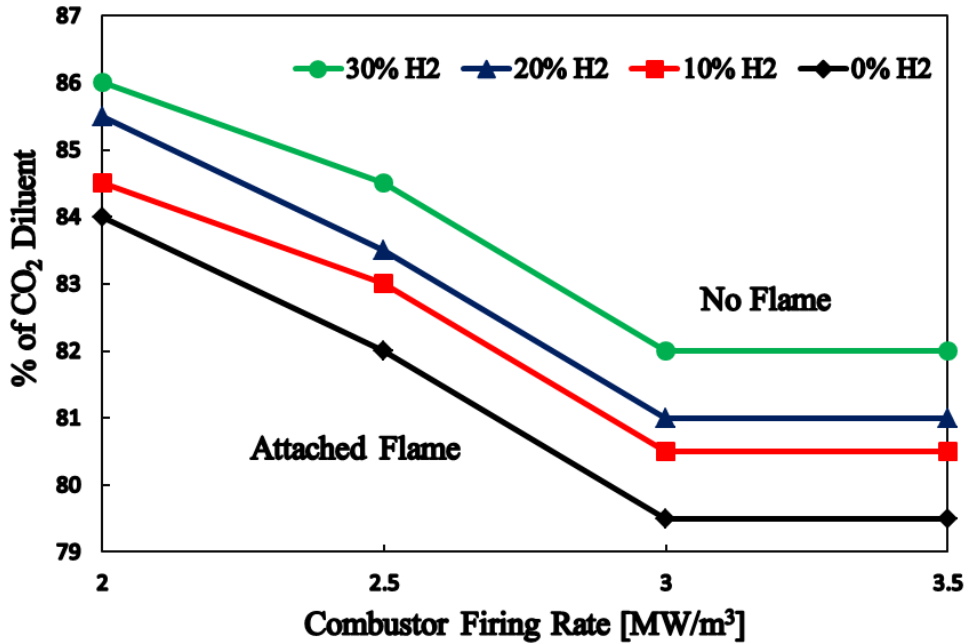


Figure 6.1: Stability map showing blowout points in oxyfuel flames with CO₂ dilution at $\Phi = 1$ and different H₂ concentration in the fuel

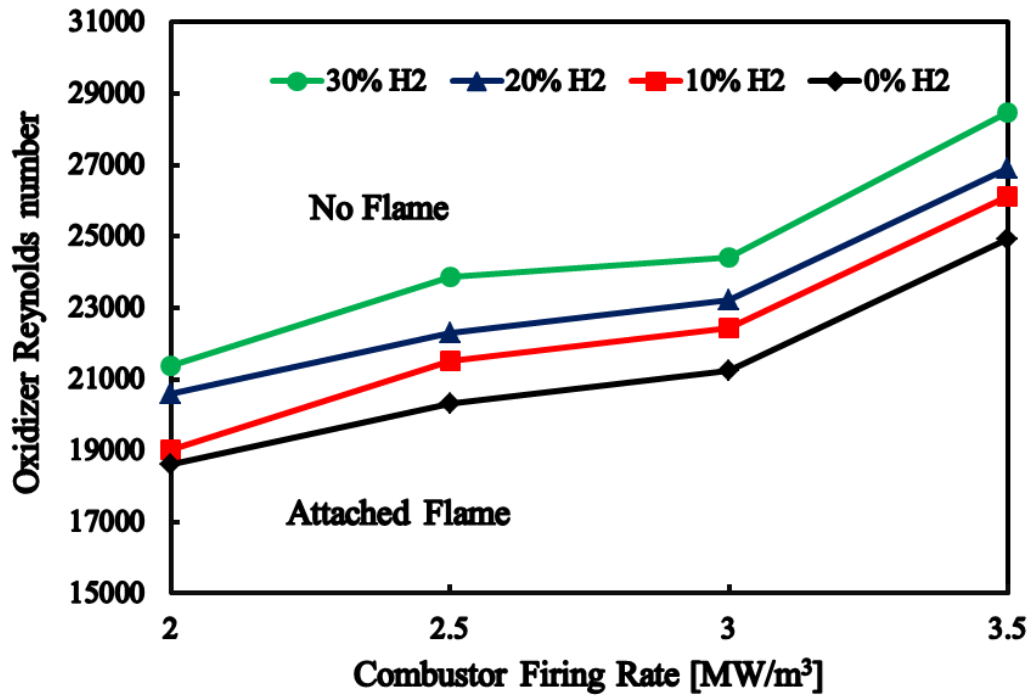


Figure 6.2: Stability (blowout) map in terms of oxidizer Reynolds number for oxyfuel flames with CO₂ dilution at $\Phi = 1$ and different H₂ concentration in the fuel

The effect of equivalence ratio on the stability of the oxyfuel flames under CO₂ dilution is shown in Figure 6.3. At different global equivalence ratios all near stoichiometry (1.0, 0.95, and 0.9), CO₂ mass flow rate was increased until flame blowout occurs. Uncertainty in the equivalence ratio is about 3%. These equivalence ratios were selected near stoichiometry to avoid excessive oxygen utilization in oxyfuel combustion because of the high cost of its separation. From the figure, it can be observed that a higher equivalence ratio leads to a wider flame stability region with the flames withstanding higher CO₂ diluent concentrations. An average increase of 1.5% in CO₂ concentration was observed between global equivalence ratio of 0.9 and 1.0. The weaker stability at lower equivalence ratios can be attributed to the cooling effect that lowers the flame's resistance to extinction. Subsequently, operating the combustor at stoichiometry as against leaner equivalence ratios is beneficial not only in lowering the amount of costly oxygen usage but also in enhancing flame stability under the influence of the diluent.

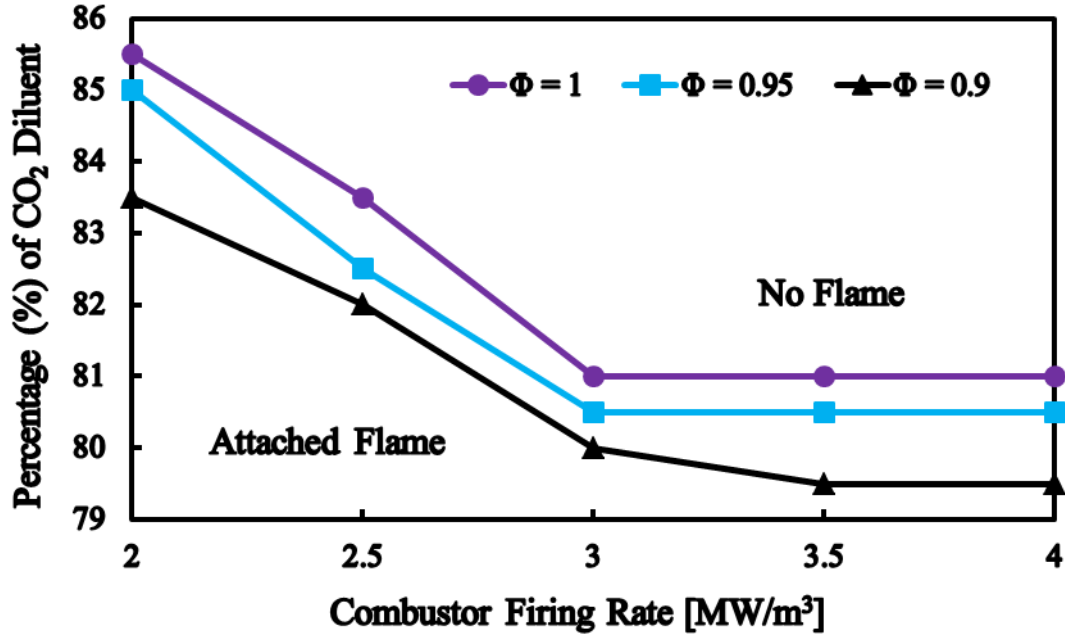


Figure 6.3: Stability map showing blowout points for oxyfuel flames with CO₂ dilution at 20% H₂ and different global equivalence ratios

6.3 Hydrogen-Enriched Oxycombustion; Numerical Study

In addition to the transport equations discussed in Chapter 3 (Continuity, Momentum, Energy, RTE, Turbulent Kinetic Energy and Turbulent Dissipation Rate Equations), to model a reacting flow, the chemical reaction needs to be modeled as well.

6.3.1 Chemical Reaction Modeling; the Non-Premixed Combustion Model

The non-premixed combustion (NPC) model used in this study to model the chemistry employs the assumption of chemical equilibrium where reactions proceed till chemical

equilibrium. This fact, together with the Reynolds-Averaged Navier-Stokes (RANS) equations employed for the turbulent flow makes it impossible to carry out flame stability studies with the numerical model. Consequently, the numerical study was used to determine combustion characteristics such as temperature and emissions. Previous studies reported the adequacy of the NPC model with RANS in predicting the temperature and other combustion parameters for turbulent reacting flows [170, 176]. Non-premixed combustion is characterized by fuel and oxidizer entering the reaction zone in distinct streams. Such combustion in turbulent reacting flows can be modeled using the chemical equilibrium model with mixture fraction transport equation [177, 178]. For an elemental mass fraction Z_i of element i , with subscripts, ox and $fuel$ denoting values at oxidizer and fuel streams, respectively, mixture fraction f can be generally defined as in equation (6.1).

$$f = \frac{Z_i - Z_{i,ox}}{Z_{i,fuel} - Z_{i,ox}} \quad (6.1)$$

Under the assumption of equal diffusivities for all species, f defined in equation (6.1) simply becomes the elemental mass fraction that originated from the fuel stream. Consequently, for an infinitesimally small volume, f is simply defined as the ratio of the mass of material that originated from fuel stream to the mass of the mixture in the control volume. Hence, f is unity at the side of fuel stream, zero at the oxidizer side, and takes in values from zero to one in regions where the two streams mix in the combustion zone and beyond.

The transport equation for f can be obtained from the well-known species conservation equation under the assumption of equal diffusivities of the species. Under such assumption, the reaction source terms in the species conservation equations (series of

equations for each of the species) will cancel out when the equations are added together. What will remain is a source-less species conservation equation that can be easily written in terms of f . Consequently, thermo-chemistry can be reduced to a single parameter called the mixture fraction, effectively reducing the combustion process to a mixing problem, and avoiding the difficulties that come with using reaction rates [177]. NPC model, therefore, does not solve equations for individual combustion species. Rather, the chemistry is modeled by the transport equations of f . While the assumption of equal diffusivities is invalid for laminar reacting flows, highly turbulent flows can be assumed to have equal diffusivities of species in the flow where turbulent convection outweighs molecular diffusion. The density-averaged (Favre mean) mixture fraction ($\bar{f}$) transport equation is given as;

$$\nabla \cdot (\rho \vec{u} \bar{f}) = \nabla \cdot \left(\frac{\mu_l + \mu_t}{\sigma_t} \nabla \bar{f} \right) \quad (6.2)$$

Where μ_l and μ_t are the laminar and turbulent viscosities, respectively, σ_t is the turbulent Prandtl number, ρ is density, and $\vec{u}$ is the velocity vector.

The next aspect of modeling using the NPC is that the turbulent-chemistry interaction needs to be fully accounted for in the turbulent reacting flow. A conservation equation for mixture fraction variance ($\overline{f'^2}$) that accounts for turbulent-chemistry interaction [179] is given as:

$$\nabla \cdot (\rho \vec{u} \overline{f'^2}) = \nabla \cdot \left(\frac{\mu_l + \mu_t}{\sigma_t} \nabla \overline{f'^2} \right) + C_g \mu_t \cdot (\nabla \bar{f})^2 C_d \rho \frac{\varepsilon}{k} \overline{f'^2} \quad (6.3)$$

Where: $f' = f - \bar{f}$, C_g and C_d are empirical constants having default values of 2.86 and 2.0, respectively [155], k is the turbulent kinetic energy, and ε is the dissipation of that energy.

For non-adiabatic combustion systems, heat transfer affects the thermochemical parameters such as temperature and species mass fraction. Mean enthalpy transport equation (Equation (6.4)) derived using the concept of conserved scalar [179] was used to account for the heat transfer effect in the non-adiabatic system. Subsequently, each thermochemical scalar (Φ_i) was determined using state relationship as a function of f and $\bar{H}$, developed under the assumption of chemical equilibrium, so that the instantaneous value of the scalar $\Phi_i = \Phi_i(f, \bar{H})$. Finally, a closure model that relates the instantaneous scalars with their respective average values is needed. NPC uses an assumed-shape probability density function (PDF); $p(f)$ as such a model. The shape of the PDF is generally developed from experimental data that predicted such a shape in a combustion system. The β -function assumed PDF given in equation (6.5) was used in this study. Prior to the start of the solution for the transport equations, a table is generated containing the thermochemical scalars as functions of the predicted mixture fractions, its variance, and mean enthalpy. These calculated PDF tables are stored and used as look-up tables during the solution by table interpolation. $p(f)$ is used as a weighting function in the determination of the mean values of the scalars as represented in equation (6.6). Note that in equation (6.6), it is assumed that heat transfer does not affect enthalpy fluctuations in a significant manner. Therefore, $p(f)$ was used as the weighing function in the determination of the average thermochemical scalars instead of computing another PDF that is a function of both f and H ; $p(f, H)$.

The mean enthalpy ($\bar{H}$) transport equation is given as:

$$\nabla \cdot (\rho \vec{u} \bar{H}) = \nabla \cdot \left(\frac{k_t}{c_p} \nabla \bar{H} \right) + S_h \quad (6.4)$$

Where c_p is the specific heat capacity, k_t is the turbulent thermal conductivity, and S_h is a source term which accounts for heat transfer due to radiation. The β -function assumed PDF is given as:

$$p(f) = \frac{f^{\alpha-1}(1-f)^{\beta-1}}{\int f^{\alpha-1}(1-f)^{\beta-1} df} \quad (6.5)$$

$$\text{Where } \alpha = \bar{f} \left[\frac{\bar{f}(1-\bar{f})}{\bar{f}^2} - 1 \right], \text{ and } \beta = (1 - \bar{f}) \left[\frac{\bar{f}(1-\bar{f})}{\bar{f}^2} - 1 \right]$$

The equation for the average value of a scalar ($\bar{\Phi}_i$) is given as:

$$\bar{\Phi}_i = \int_0^1 \Phi_i(f, \bar{H}) p(f) df \quad (6.6)$$

The assumption of chemical equilibrium used in the NPC model is a good one for fast chemistry combustion, where reactions proceed to form the products instantaneously at a point where fuel and oxygen exist. In other words, the chemical equilibrium assumption is good for reactions with a very high Damkohler number like reactions involving hydrogen fuel [180]. Where non-equilibrium exists due to the slower reaction, the equilibrium model will fail to accurately predict the thermochemical state of the combustion system. To accommodate chemical non-equilibrium in the NPC model, rich flammability limit (RFL) option is used with the model in this study. The RFL option suspends the chemical equilibrium calculation in fuel-rich regions where the fuel is not allowed to burn and is passed on in the mixture. That way, only leaner mixtures will burn

under equilibrium. Six (6) species (O_2 , CO_2 , C_3H_8 , CO , H_2O , and H_2) and two (2) radical species (OH and O) making the total of eight (8) species are considered in the NPC model for this study.

6.3.2 Transport Properties

The model used for chemistry makes an assumption of equal molecular diffusivities for all the species as will be discussed in the next section. However, other molecular transport properties are important, and therefore, are considered. For instance, flow Reynolds number is a function of viscosity making it an important property to account for. The variation of dynamic viscosity as well as thermal conductivity (K) with temperature, in the combustion gases, was calculated using a fourth order polynomial fitted from a data set developed by Poferl et al. [181] for natural gas combustion in air. The fitted data together with the polynomial equations used for the dynamic viscosity and thermal conductivity is shown in Figure 6.4 and Figure 6.5, respectively. The R^2 values for the correlations are 1.0 and 0.9998 for the dynamic viscosity and thermal conductivity, respectively, as displayed in the figures. Mixing law was used in the determination of the specific heat ($c_{p,i}$).

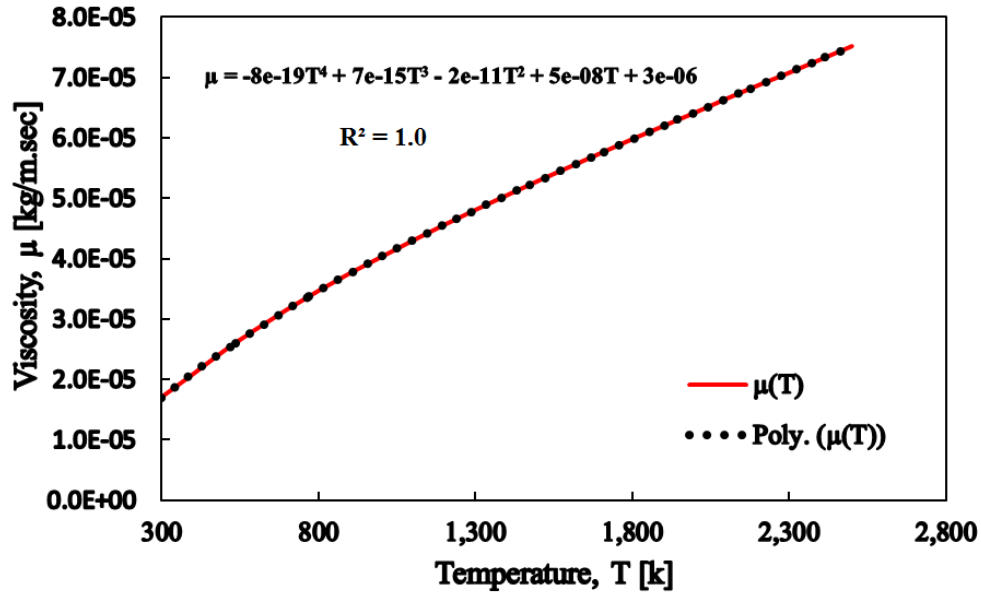


Figure 6.4: Variation of fitted experimental data and polynomial function of dynamic viscosity with temperature for combustion gases

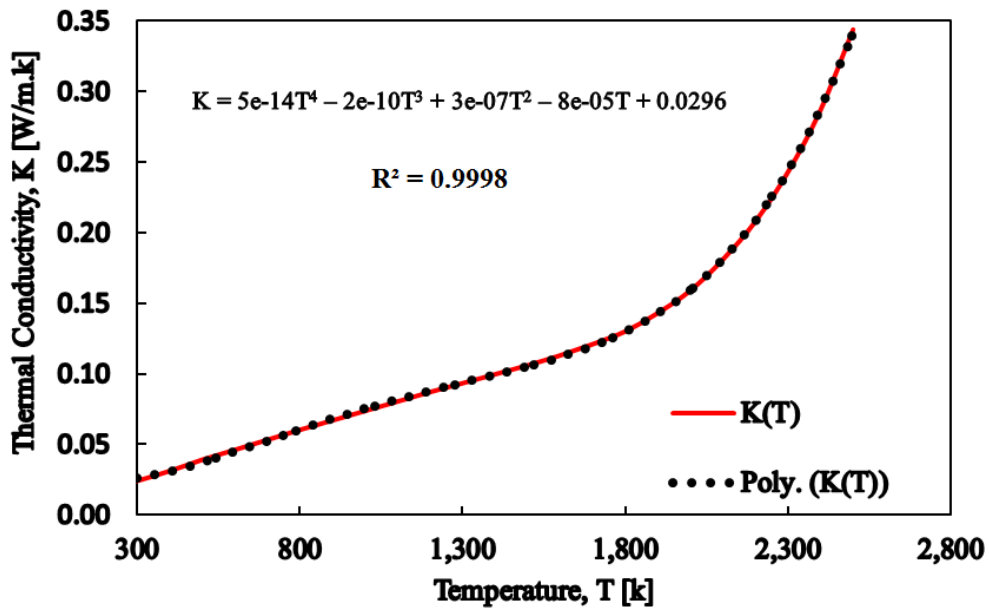


Figure 6.5: Variation of fitted experimental data and polynomial function of thermal conductivity with temperature for combustion gases

6.3.3 Numerical Modeling and Solution Procedure

The solution to the governing equations was obtained using a commercial computational fluid dynamics (CFD) code based on the finite volume scheme called ANSYS FLUENT 16.2. The set of governing equations together with appropriate boundary conditions were solved in a meshed domain. The computational domain used was presented in Figure 5.1 in the previous chapter of this dissertation. We assumed axisymmetric conditions, and so, all the cases studied were solved using the 2-D axisymmetric swirl option in FLUENT. Swirl factor of 0.1 was used for the swirl dominated flow in this study after some tuning because, at that value, we obtain the closest agreement between our experimental and numerical temperature values as well as the flame's mean structure. The solvers used were pressure-based, hence, for pressure-velocity coupling, the semi-implicit method for pressure-linked equations (SIMPLE) algorithm was used. All the cases were solved under steady state conditions.

Pressure staggering option (PRESTO) was used in discretizing the pressure equation because of its superiority compared to other pressure equation discretization schemes for swirl-dominated flows [182]. The second-order upwind scheme was used in discretizing all the remaining transport equations including the transports equations for the conservation of mass, momentum, and mixture fraction. The maximum residual for continuity, momentum, turbulent kinetic energy and turbulent dissipation rate used as convergence criteria was 10^{-4} . For energy, mean mixture fraction, and radiation equations, the maximum residual used was 10^{-6} . Also, as an additional convergence

criterion, we monitor the mean mixture fraction and CO mole fraction at the exhaust until constant values were reached.

6.3.4 Boundary Conditions

The boundary conditions used for both oxidizer and fuel was mass flow inlet, which is more appropriate for swirling flow than velocity boundary condition as it allows for pressure fluctuation according to the solution. At the oxidizer inlet, the flow direction has equal axial and tangential components because of the 45-degree swirler used, those components were set accordingly, while the mean mixture fraction was set to zero. For the fuel inlet, the flow direction was set normal to the boundary, while the mean mixture fraction was set to unity. The reactants were supplied at a fixed temperature of 297 K and based on the chosen equivalence ratio and combustor firing rate. Pressure outlet boundary condition was used at the exit to the combustor as the gauge pressure was set to zero. The heat transfer from the inner combustor wall was modeled as coupled, while conduction heat loss was considered through the combustor thickness. For the combustor outer wall, we used mixed heat transfer boundary condition in which both convection and radiation heat transfer are modeled. Free stream temperature of 298 K, an estimated convection heat transfer coefficient of $25 \text{ W/m}^2\text{K}$, and emissivity 0.85 were used as inputs for the mixed heat transfer boundary condition.

6.3.5 Mesh Description

GAMBIT 2.4 software was used to create the simple 2-D mesh with the assumption of axisymmetric condition. A mesh size of more than 22,000 cells having structured and non-uniform grids were used after results were found to be reasonably independent of this mesh size. The non-uniformity in the mesh was utilized to allocate denser mesh at locations with a tendency of high property gradient like the inlets. Table 6.1 shows the results for the mesh independence test carried out for four different mesh sizes. Mass-weighted averages of temperature, velocity, and mole fraction of CO were compared with their respective values using the 43,000 mesh size. The results were obtained numerically at stoichiometric equivalence ratio, the combustor firing rate of 5MW/m^3 , and oxygen oxidizer diluted with 69% CO_2 . As can be seen from the table, almost similar results were obtained with the 22,000 and 33,000 mesh sizes with small changes in the results when the mesh size was increased to 43,000. Therefore, the mesh with 22,000 cells was adopted in the study. Figure 6.6 shows the meshed computational domain used with (6.6a) showing the entire domain while (6.6b) depicts an enlarged section of the burner head and the beginning part of the combustion chamber.

Table 6.1: Mesh independence test results at different mesh sizes; all values were taken as mass-weighted average at the combustor exit.

Mesh Size [Number of Cells]	Temperature [K]	Percentage Difference [%]	Velocity [m/s]	Percentage Difference [%]	CO Emission [ppm]	Percentage Difference [%]
10,000	1057	2.5	1.256	4.9	544.0	1.7
22,000	1075	0.8	1.290	2.3	550.8	0.5
33,000	1075	0.8	1.301	1.5	550.3	0.5
43,000	1084	-	1.321	-	553.6	-

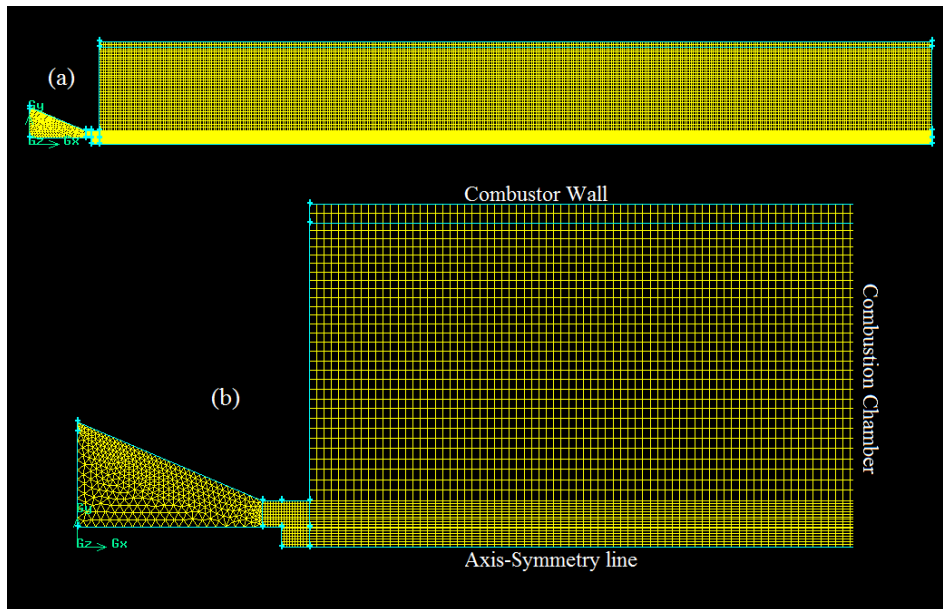


Figure 6.6: Meshed computational domain

6.3.6 Model Validation

The combustion model used in this study was validated with some experimental measurements. For the purpose of this validation, experiments were conducted using the combustion system described in Chapters 3. Flame Images representing the mean flame structure, temperature profile, and CO emission were taken experimentally at certain conditions, and these were respectively compared to their counterparts predicted by the numerical model. Figure 6.7 and Figure 6.8 depict the comparison between experimental and numerical flame macrostructures obtained using pure oxygen (100% oxygen) as oxidizer and oxygen oxidizer diluted with 69% CO₂ (by volume) respectively. Both figures were obtained at the global equivalence ratio of stoichiometry and combustor firing rate of 5MW/m³. Computed contours of OH radicals and static temperature were used to depict the time-averaged structure of the flame and were compared with flame images obtained experimentally.

Both OH and temperature contours can be used to depict the active reaction zone where the flame is located and when averaged, each can depict the mean flame structure comparable to an image obtained at steady state condition. As can be observed from the figures, there is a good agreement between the calculated and experimentally acquired flame shapes owing to their macrostructures. With no CO₂ dilution (Figure 6.7), the oxyfuel flame is jet-like having elongated shape despite the swirl-induced flow. Diluting the oxidizer with CO₂ lowers the oxyfuel combustion temperature and shortens the reaction zone (Figure 6.8) changing the mean structure of the flame from jet-like to a V-shaped. This transition in the mean structure of the flame with dilution is a result of

increased flow and hence turbulence in the combustor that enhances mixing (as we have seen in Chapter 5) [57].

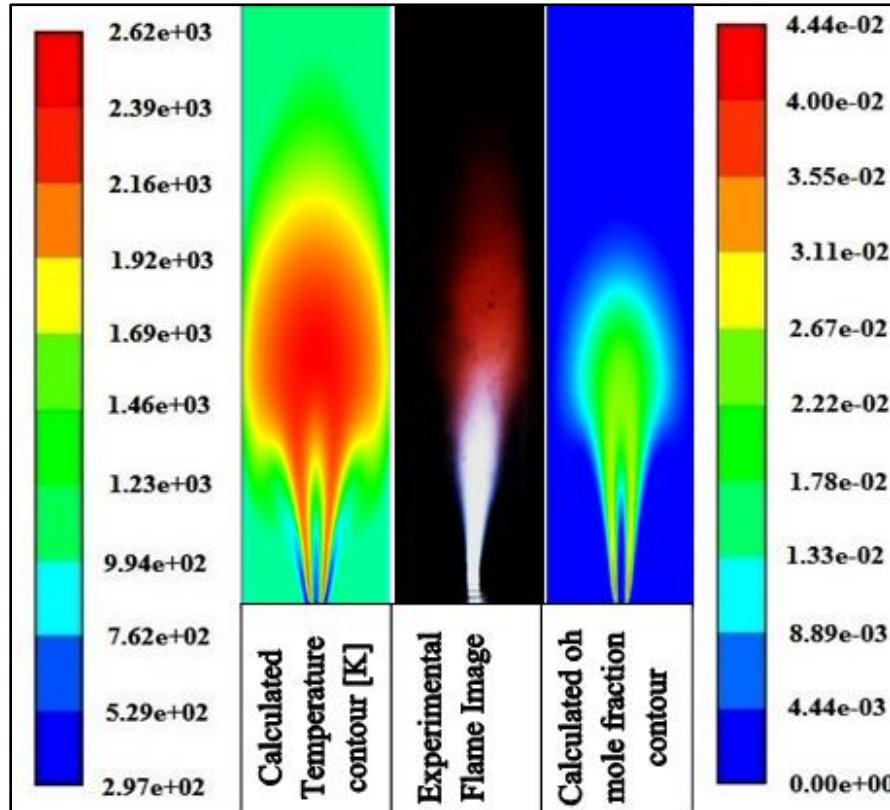


Figure 6.7: Experimental and numerical (calculated OH and temperature fields) flame macrostructure at $\Phi = 1$, the firing rate of 5 MW/m^3 , and 100% O_2 in oxidizer

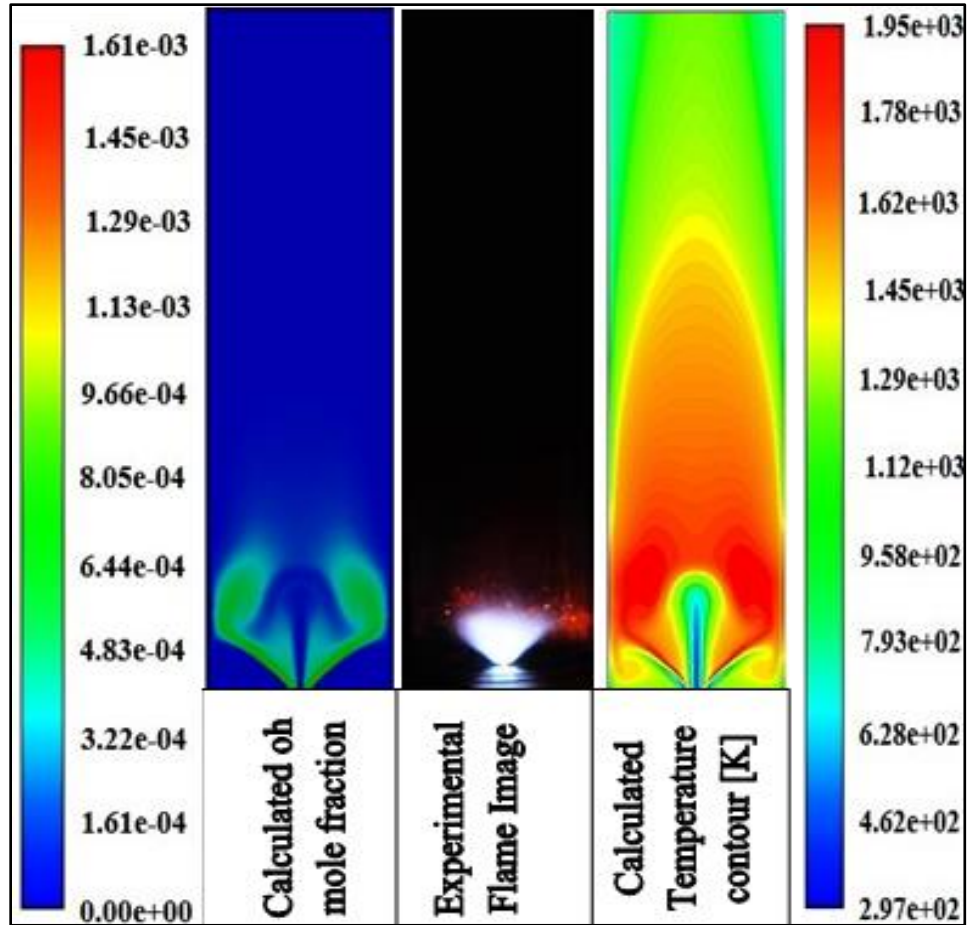


Figure 6.8: Experimental and numerical (calculated OH and temperature fields) flame macrostructure at $\Phi = 1$, the firing rate of 5 MW/m^3 , and 31/69: O_2/CO_2 oxidizer.

Figure 6.9 and Figure 6.10 depict the comparison between experimentally measured and numerically obtained temperature and CO profiles, respectively. The temperature measurements were carried out at axial locations in the combustor from 150mm to 250mm in 25mm increments while the CO was measured close to the exit of the combustor at its axis. Propane enriched with 20% hydrogen, stoichiometric equivalence ratio, the combustor firing rate of 5 MW/m^3 , and oxygen oxidizer diluted with 69% CO_2 are the combustion conditions at which the temperature profiles were obtained. The

locations of the experimental measurements were chosen away from the flame zone characterized by high temperatures due to the limitation in temperature the thermocouple can withstand and accurately measure. From Figure 6.9, it can be seen that slightly higher temperatures were predicted numerically compared to the experimental values but the trends were quite similar as the temperature decreases with axial distance in both cases. A maximum deviation of 12% was recorded between the numerical prediction and experimental measurements. The equilibrium model with RFL has been previously reported to over-predict temperature [183].

The CO emission was obtained at stoichiometric equivalence ratio, and at different combustor firing rates for propane combustion in pure oxygen (no CO₂ added). An attempt was made to measure CO experimentally at different conditions and locations, but for the oxyfuel combustion mixtures with H₂ enrichment, high levels of CO beyond the limit of our measuring device (1000 ppm) were encountered. This is particularly severe in cases where CO₂ dilution was used with the oxidizer. Consequently, only limited measurements were presented for validation purposes. While such measurements were not sufficient to validate a model targeting to map out the CO distribution in the combustion chamber including the flame region, it can satisfactorily estimate the CO emissions at the exhaust which is the focus of this study in terms of CO emissions. It can be observed from Figure 6.10 that lower values of CO were obtained with the numerical model. A maximum deviation of 16.5% was recorded between the numerical prediction and experimental measurements of CO.

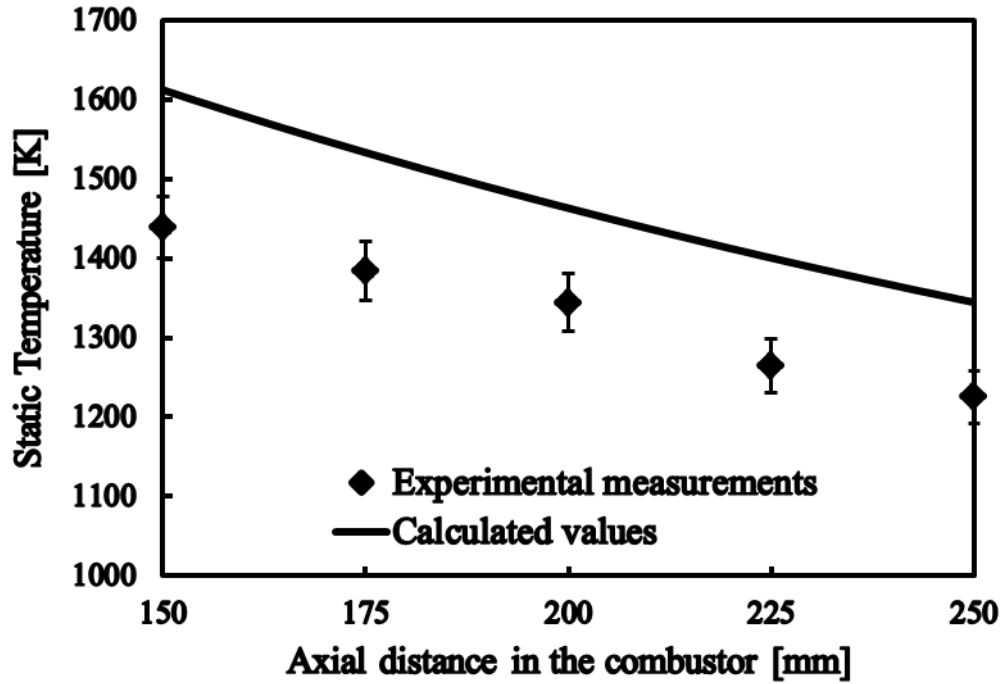


Figure 6.9: Experimental and numerical temperature profiles at 20% H₂ in propane, $\Phi = 1$, the firing rate of 5 MW/m³, and 31/69: O₂/CO₂ oxidizer.

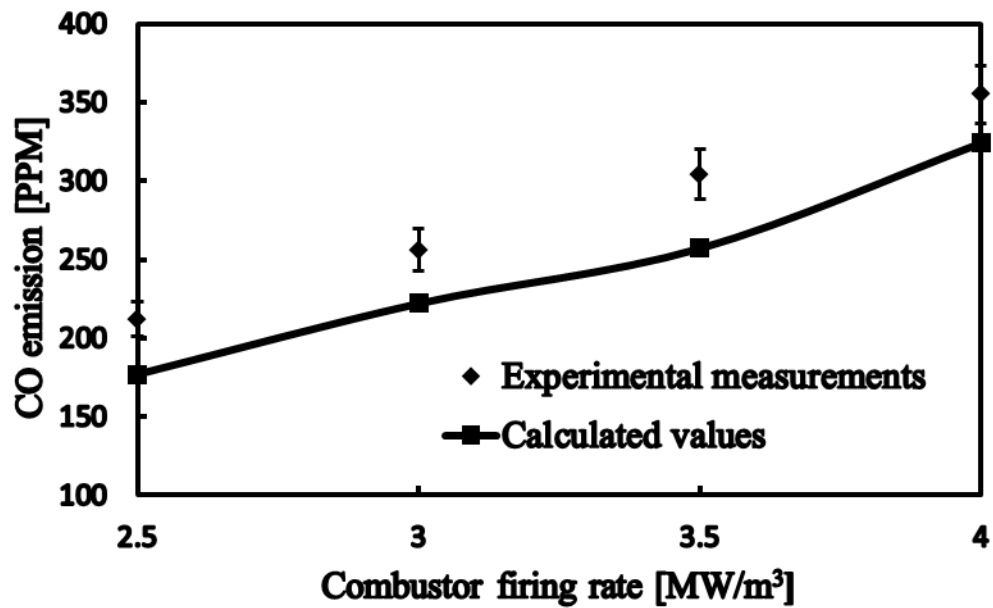


Figure 6.10: Experimental and numerical CO emission profiles for propane oxyfuel combustion (100% oxygen) at $\Phi = 0.9$

6.3.7 Effect of H₂ enrichment on oxyfuel temperature and velocity profiles

Figure 6.11 and Figure 6.12 depict axial and radial temperature profiles, respectively, in the combustor at different hydrogen concentration. In Figure 6.11, the axial temperature profiles were plotted at the combustor axis from the middle of its section to its exit at fixed conditions of stoichiometric global equivalence ratio and firing rate of 5MW/m³. From the figure, it can be seen that an increase in hydrogen concentration in the fuel increases the temperature as expected. The temperature at the exit of the combustor increased by 90 K when hydrogen concentration was increased from 0 to 40%. This increase in temperature can be attributable to higher reactivity and adiabatic flame temperature of hydrogen in comparison to propane from [184]. In all the profiles, the temperature decrease with distance towards the combustor exit as a result of combined heat loss by convection and radiation.

The radial temperature distributions depicted in Figure 6.12 also reveal the same effect of hydrogen enrichment towards an increase in temperature. From the figure, we can also observe that temperature decreases radially from the peak value at the center of the combustor towards the combustor walls. The pattern factor defined in equation (8.7) can be employed to establish temperature uniformity at the exhaust of the combustor [170]. Good temperature homogeneity is desirable in exhaust gases particularly in turbines operation and the closer the pattern factor is to unity, the more uniform the exhaust gas temperature distribution. For the profiles in Fig. 15, the calculated pattern factors are 1.50, 1.57, and 1.60, respectively at hydrogen concentrations of 0, 30, and 40%. The non-

uniformity in exhaust gas temperature distribution increases with an increase in hydrogen concentration in the propane fuel.

$$Pattern\ Factor = \frac{T_{out,max} - T_{in}}{T_{out,ave} - T_{in}} \quad (6.7)$$

Where $T_{out, max}$ is the exhaust maximum temperature, $T_{out, ave}$ is the average temperature at the combustor exit, and T_{in} is the oxidizer inlet temperature.

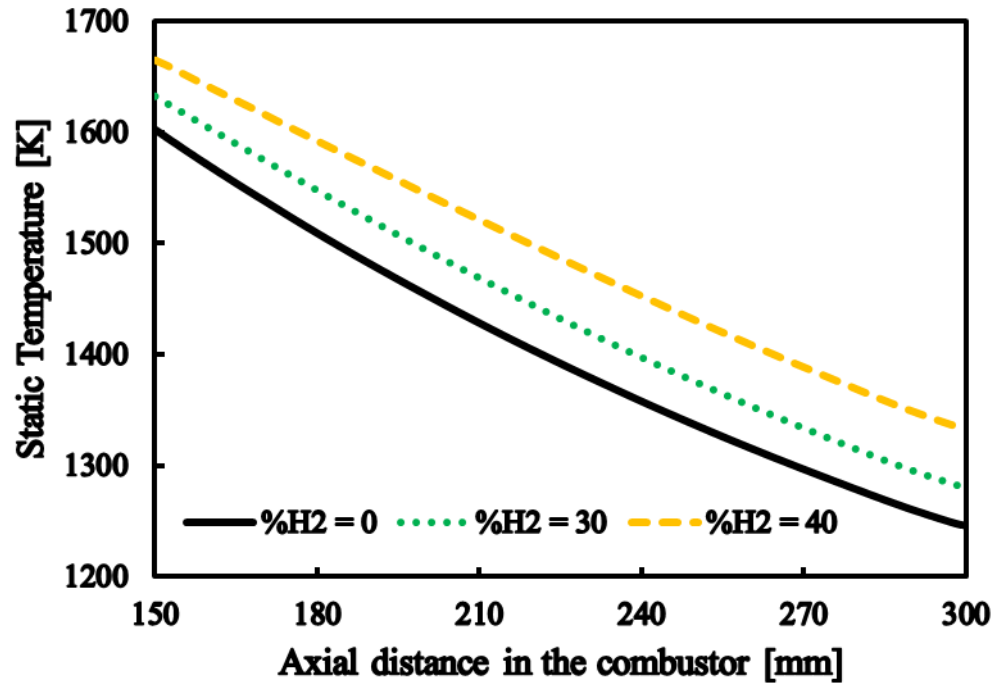


Figure 6.11: Axial temperature distribution from the middle of the combustor to its exit (150-300 mm) at the axis for different H₂ concentration, at $\Phi = 1$ and firing rate of 5 MW/m³

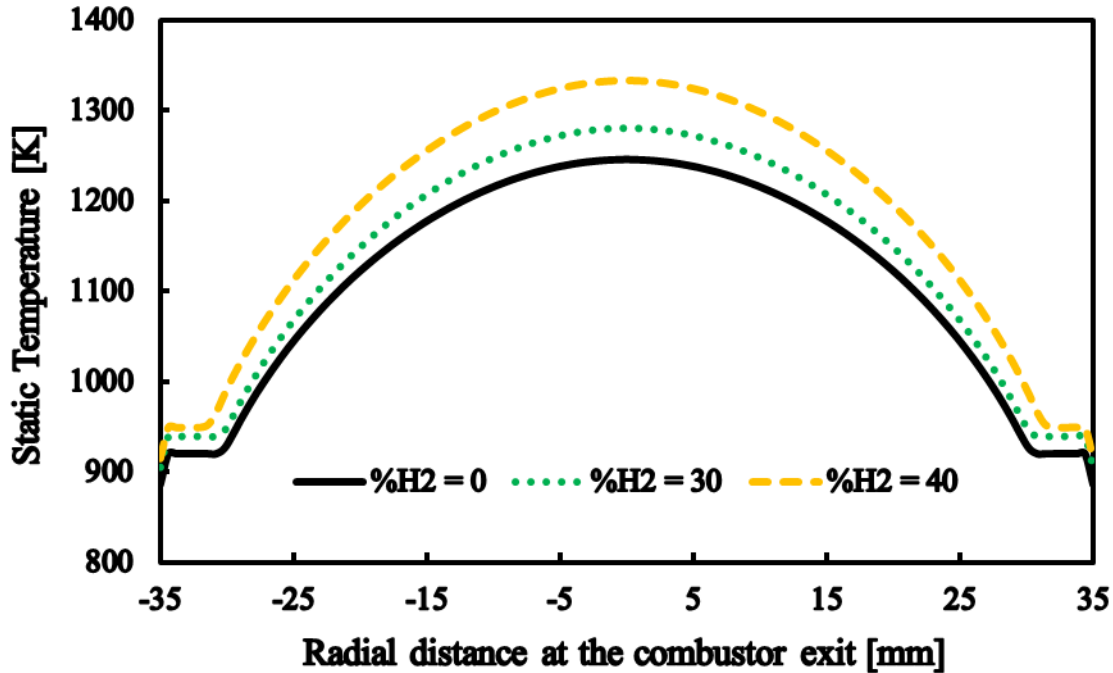


Figure 6.12: Radial temperature distribution from the combustor axis to the wall (0-35 mm) at the exhaust for different H₂ concentration, at $\Phi = 1$ and firing rate of 5 MW/m³

Velocity variation along the axis of the combustor is shown in Figure 6.13 as a function of axial distance. The profiles were obtained for different hydrogen concentrations at a fixed stoichiometric global equivalence ratio and firing rate of 5 MW/m³. It can be observed from the figure that the axial velocity increases with an increase in hydrogen concentration in the fuel. The peak axial velocity increases by 9.5 m/s when hydrogen concentration was increased from 0 to 30%. This increase in velocity entails that in the cases where the fuel is hydrogen-enriched, the combustion mixture will not have enough residence time in the combustor. In all the profiles, the axial velocity continues to decrease downstream in the combustor due to the combined effect of the chemical reaction and the vortices formed by the swirling flow. The vortices formed by the swirling flow are the outer recirculation zones (ORZ) formed by the flow's sudden

expansion at it enters the larger diameter combustor and the inner recirculation zone (IRZ) that forms as a result of vortex breakdown about the fuel annular jet (Figure 6.14). Consequently, flames in swirl-stabilized combustors are anchored in-between these flow structures. The location of the IRZ can be pin-pointed from Figure 6.13 to have a leading edge at around 60mm downstream of the combustor inlet where we observed negative axial velocity due to flow separation. This negative axial velocity weakens in adversity with an increase in hydrogen concentration in the fuel. Consequently, a weaker vortex strength of the IRZ with its core shifting further away from the combustor axis is associated with higher hydrogen concentration in the fuel mixture. This weak vortex strength together with lower residence time resulting from higher velocity is attributable to the higher values for mixture fraction observed beyond the primary flame zone with an increase in hydrogen concentration (Figure 6.15). The weaker the vortex strength, the lower the amount of hot gases recycled into the fresh combustion charge and, therefore, the lower the combustion intensity. Mixture fraction is a mass fraction originating from the fuel stream; consequently, more un-burnt fuel species are present in the hydrogen-enriched cases compared to pure propane combustion.

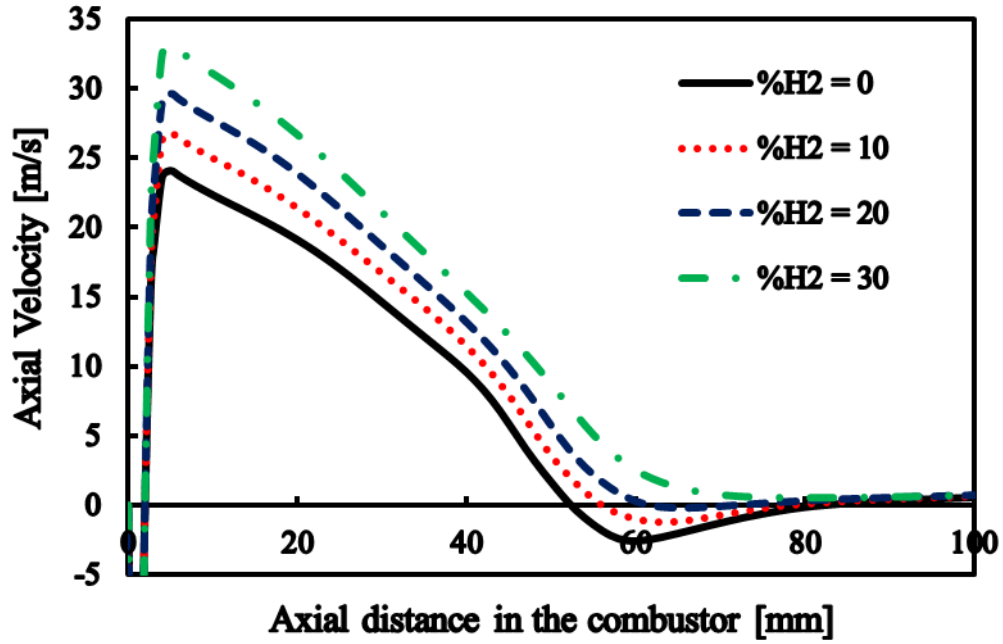


Figure 6.13: Axial velocity distribution at the combustor axis from inlet to 100mm downstream for different H₂ concentration, at $\Phi = 1$ and firing rate of 5 MW/m³

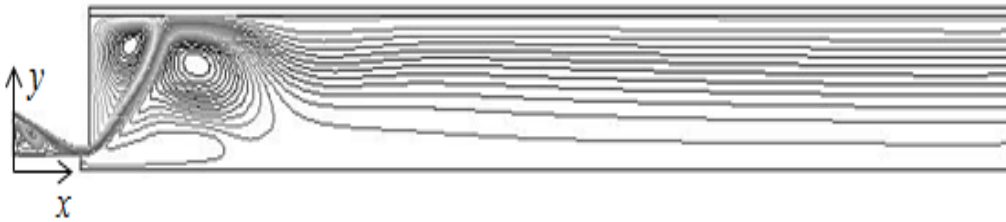


Figure 6.14: Contour of stream function depicting the ORZ and IRZ for the swirl-stabilized combustor

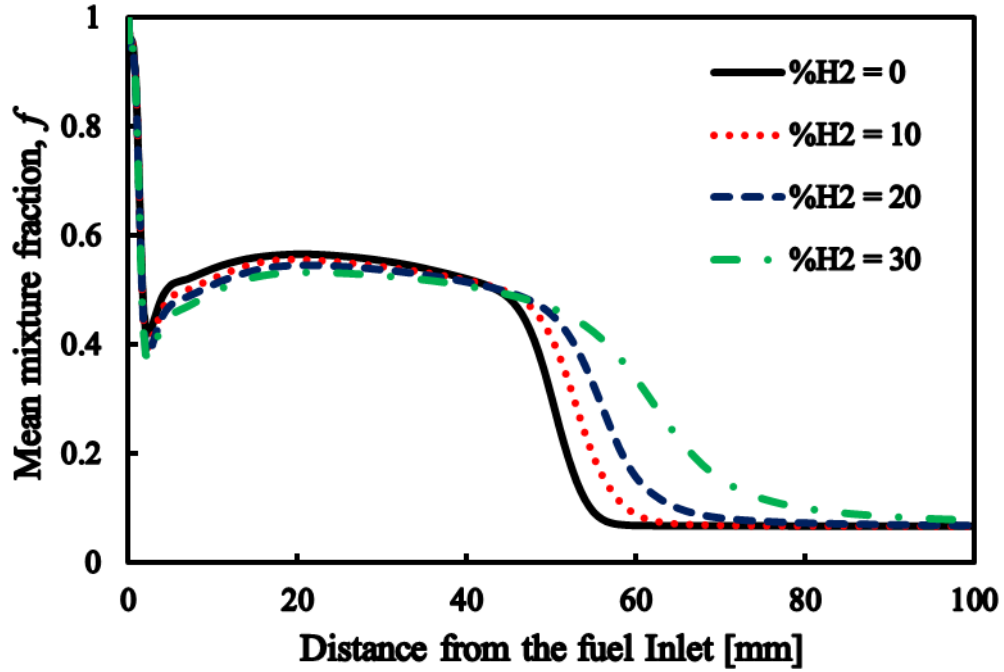


Figure 6.15: Mean mixture fraction from the fuel inlet to a distance 100mm downstream in the combustor for different H₂ concentration, at $\Phi = 1$ and firing rate of 5 MW/m³

6.3.8 Effect of hydrogen enrichment on CO and CO₂ emissions

The effect of hydrogen enrichment on CO and CO₂ emissions for the propane oxyfuel flames is shown in Figure 6.16. Near stoichiometric equivalence ratio and fixed firing rate of 5MW/m³, the percentage of hydrogen in propane was varied from zero to 40%. From the figure, it can be seen that an increase in hydrogen content in the fuel is associated with higher CO emission (dry). An opposite trend to the CO was observed in case of CO₂ emission where an increase in H₂ content is associated with a decrease in CO₂ emission (dry) as seen in the figure. The minimum amount of CO₂ emission (97.33%) corresponds to the maximum CO emission (1.93%) on a dry basis at the

hydrogen concentration of 40%. Oxyfuel combustion targeting CCS seeks combustion products that are mainly CO₂ and H₂O. This is because after the H₂O is condensed, the purer the resulting CO₂ stream the better in terms of its transportation and ultimate sequestration. Consequently, increased CO emission at the detriment of reduced CO₂ emission is not suitable for oxyfuel combustion with CCS. At 1.93%, the CO emission from the combustor obtained at 40% hydrogen composition in propane is already higher than the reported limit of 0.1% pegged to prevent reactions and formation of pentacarbonyls in some CCS CO₂ transport pipelines standards [55].

The increase in CO emission with an increase in hydrogen concentration could be attributed in part to the lower residence time exhibited by the gases in the combustor at higher hydrogen concentration as we have seen in the previous section. The increase in CO emission with increased hydrogen concentration could also be explained using the water-gas shift reaction (WGSR); an exothermic reversible reaction of CO and water vapor (H₂O) that produces CO₂ and H₂.

WGSR is written as; $\text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{CO}_2 + \text{H}_2$

The WGSR is a temperature dependent reaction with the reaction rate that increases with an increase in temperature, while reactants conversion to products becomes less favorable. Conversely, the conversion of CO to CO₂ is encouraged at lower temperatures [185]. In other words, due to exothermic nature and temperature sensitivity of WGSR, higher CO conversion is encouraged at lower temperatures while at higher temperatures, the shift in the equilibrium constant swings towards the reactants [186]. As we have seen in the previous section, an increase in hydrogen concentration increases the temperature

and, therefore, encourages more of the reactants formation in WGSR which can explain the corresponding higher CO concentration observed.

Another reason for the increase in CO emission with hydrogen enrichment is the nature of the fuel mixture and its effect on the chemical reaction. Because of higher reactivity and adiabatic flame temperature of hydrogen in comparison to hydrocarbon fuels, hydrogen-enriched fuel mixtures are expected to combust more efficiently. High temperatures (below CO₂ dissociation threshold) in hydrocarbon combustion are also reported to encourage CO conversion and hence results in more complete combustion and lower CO emission [184]. But despite all that, the competition for oxygen between the highly reactive hydrogen and propane in a globally stoichiometric, non-premixed mixture of the oxyfuel oxidizer can encourage more CO emission. In other words, the hydrogen can be said to inhibit the oxidation of propane and its fuel intermediaries (CO) in the oxygen-limited environment embodied by the non-premixed system at stoichiometry (inhibit CO conversion to CO₂).

The effect of the hydrogen enrichment on the chemical reaction activity can be seen in the scalar dissipation plot of Figure 6.17 where an increase in scalar dissipation rate for each increase in hydrogen concentration in the fuel mixture can be observed. Scalar dissipation (χ) represents the rate of mixing at the molecular level which means for fast chemistry it is proportional to the rate of chemical reaction [187]. Subsequently, for a non-premixed, turbulent, fast chemistry conditions the instantaneous rate of chemical reaction per unit volume $\dot{w}_i$ (Equation (6.8)) is directly related to the rate of scalar dissipation defined in Equation 6.9 based on the conserved scalar f [188]. Therefore, the

higher dissipation rate recorded for the hydrogen-enriched mixtures attests to their enhanced reaction rates.

$$\dot{w}_i = \rho a_i(f) \chi \quad (6.8)$$

$$\chi \equiv \mathcal{D} \nabla f \cdot \nabla f \quad (6.9)$$

Where ρ is the density, $\mathcal{D}$ is molecular diffusivity, and $a_i(f)$ is a chemistry-dependent parameter.

The leading edge of the IRZ earlier determined to be around 60 mm using Figure 6.13 in section 6.3.7 is further reinforced by Figure 6.18 in which we observe three peaks of scalar dissipation rate. The first, second, and the third peaks represent the trailing edge, the core, and the leading edge of the IRZ respectively. The trailing edge of the IRZ represented by the first peak in Figure 6.18 shares axial (x) location with ORZ as observed previously in Figure 6.14 under section 6.3.7. From Figure 6.18, the core of the IRZ can be estimated to be around 32mm downstream in the combustor while the trailing edge is estimated to be around 4 mm.

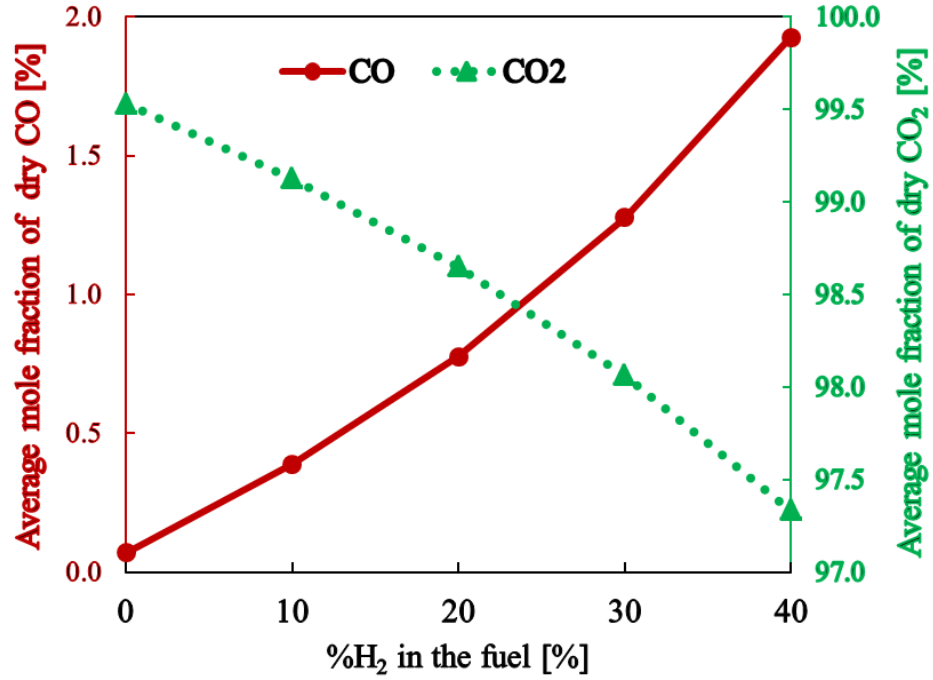


Figure 6.16: CO and CO₂ emissions at the combustor exhaust for different H₂ concentration at $\Phi = 1.03$ and firing rate of 5 MW/m³

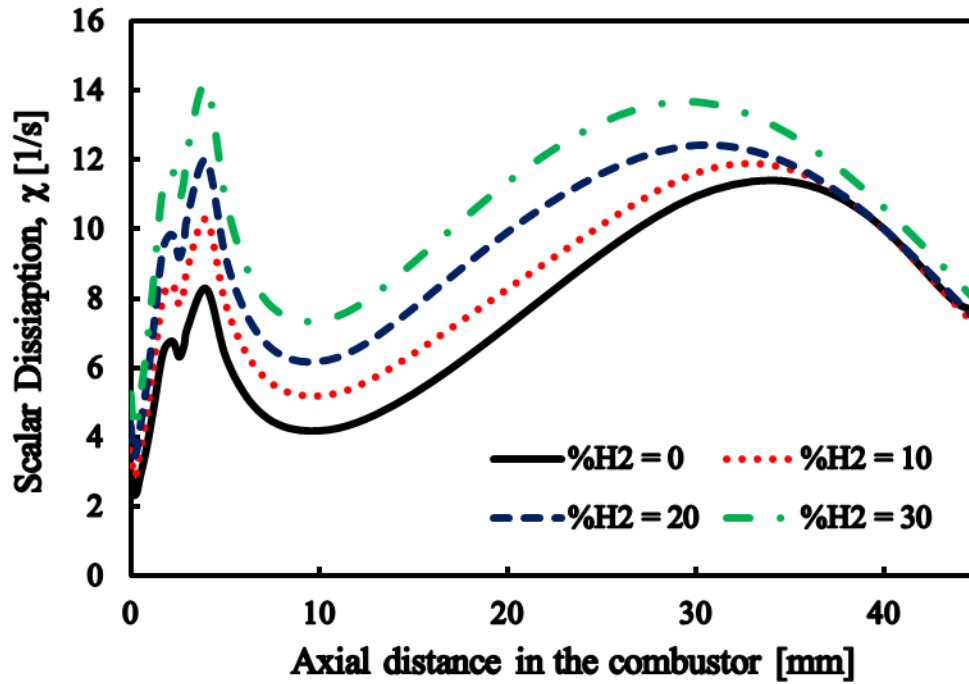


Figure 6.17: Scalar dissipation at the combustor axis from its inlet to 45 mm downstream for different H₂ concentration, at $\Phi = 1$ and firing rate of 5 MW/m³

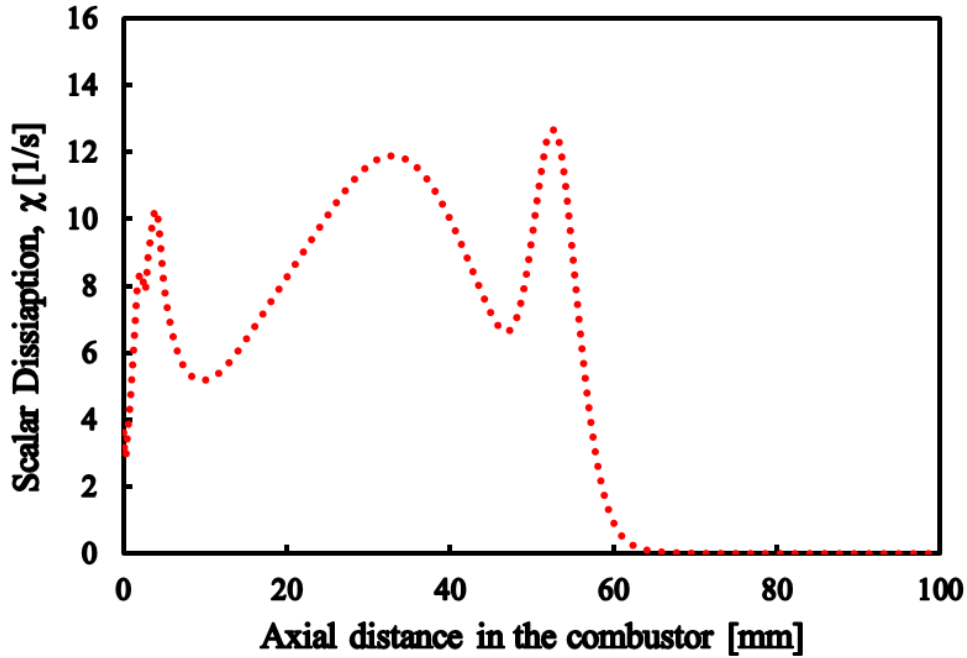


Figure 6.18: Scalar dissipation at the combustor axis from its inlet to 100 mm downstream at H₂ concentration of 10%, $\Phi = 1$ and firing rate of 5 MW/m³

Equivalence ratio sweep near stoichiometry that makes oxygen more available to the hydrogen-enriched fuel mixture showed a significant reduction in CO emission as can be seen in Figure 6.19. The figure was obtained at 20% H₂ and a firing rate of 5 MW/m³ as the equivalence ratio was varied from 1.03 to 0.93. A sharp drop in CO emission from near 8000 ppm at $\Phi = 1.03$ to less than 1 ppm at $\Phi = 0.93$ was observed. The decrease in CO emission, accompanied by the increase in CO₂ emission with a decrease in global equivalence ratio is a result of extra oxidizer available for more complete combustion. This is evident in the higher scalar dissipation, and hence, enhanced chemical reaction activity observed at lower equivalence ratio as shown in Figure 6.20. From the figure, it is can be observed that in the IRZ (signified by the second and the third peaks in the figure), the lower equivalence ratio is associated with higher scalar dissipation rate.

Furthermore, Figure 6.21 shows the variation of mixture fraction as a function of global equivalence ratio obtained at 20% H₂ concentration and a firing rate of 5MW/m³. It can be observed from the figure that a higher value of mixture fraction is associated with higher global equivalence ratio which reinforces the observed higher CO emissions.

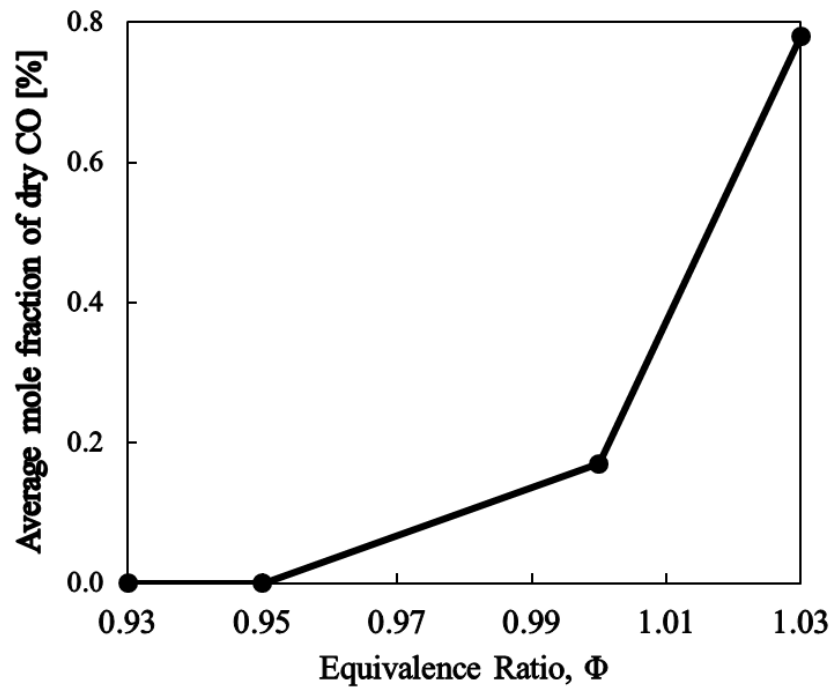


Figure 6.19: CO emissions at the combustor exhaust for different equivalence ratios at 20% H₂ and firing rate of 5 MW/m³

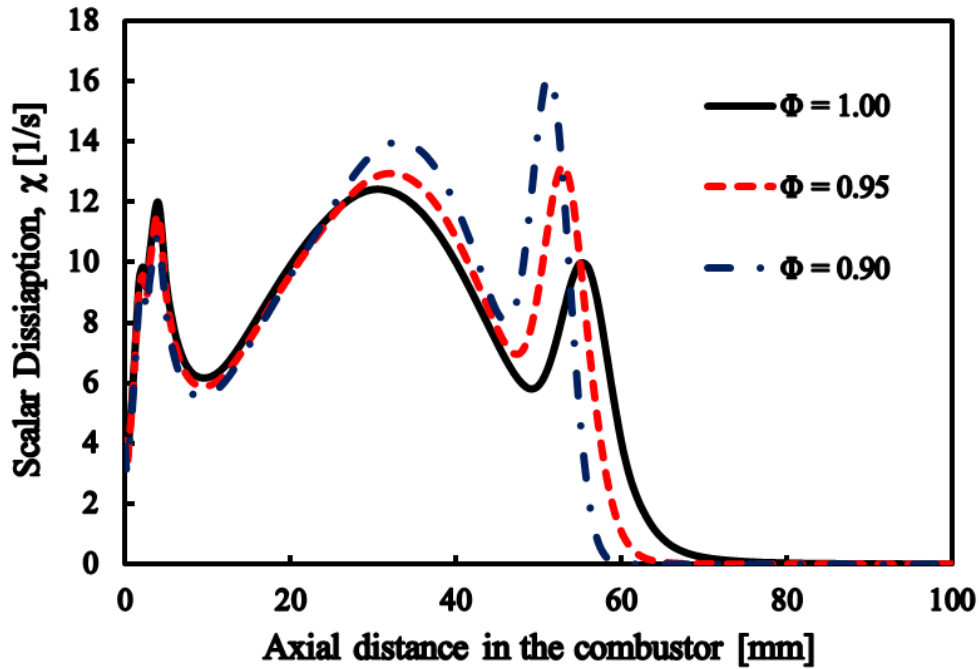


Figure 6.20: Scalar dissipation at the combustor axis from its inlet to 100 mm downstream at different equivalence ratios, 20% H₂ and firing rate of 5 MW/m³

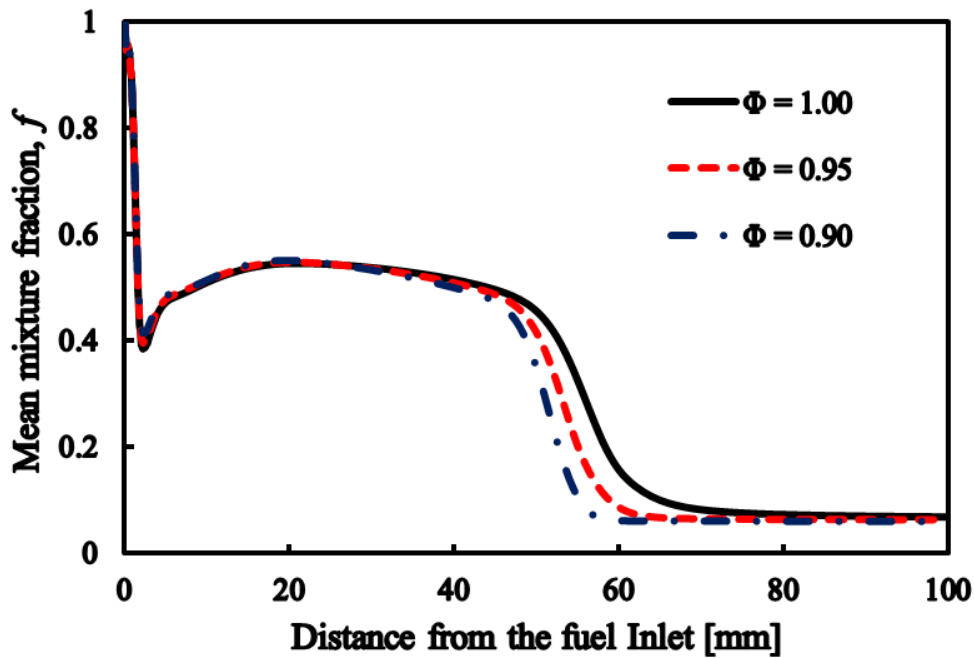


Figure 6.21: Mean mixture fraction distribution from the fuel inlet to a distance 100mm downstream in the combustor at different equivalence ratios, 20% H₂ and firing rate of 5 MW/m³

A decrease in CO emission, albeit less drastic compared to the case in which equivalence ratio was decreased, was also achieved by increasing the residence time of the gases through lowering the combustor firing rate as shown in Figure 6.22. Geometric modification to the combustor to achieve longer residence times for combustion mixtures could, therefore, help lower the CO emission.

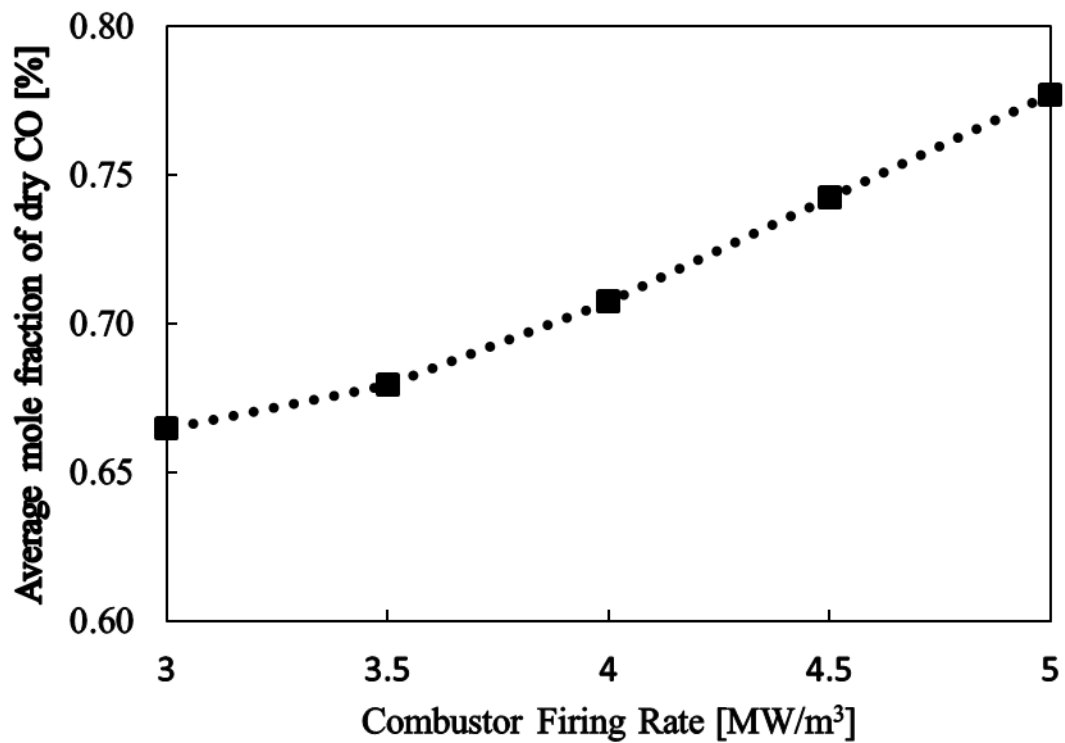


Figure 6.22: CO emission at the combustor exhaust for different firing rates at 20% H₂ and $\Phi = 1$

Figure 6.23 shows O₂ emission as a function of equivalence ratio. It can be observed from the figure that decreasing the equivalence ratio from 1.03 to 0.93 increase O₂ emission from 0 to about 1.74% in the exhaust gases on a dry basis. As we have seen earlier, CO emission becomes less than 1 ppm at the low equivalence ratio of 0.93.

Achieving sequesterable exhaust limits is, therefore, a balancing act between low CO emission, high O₂ emission, and cost of excess oxygen usage associated with lean oxy-combustion among other things. High oxygen concentrations in exhaust gases intended for CCS beyond 50 ppm can lead to corrosion in pipelines and reactions in geologic reservoirs containing the sequestered [55].

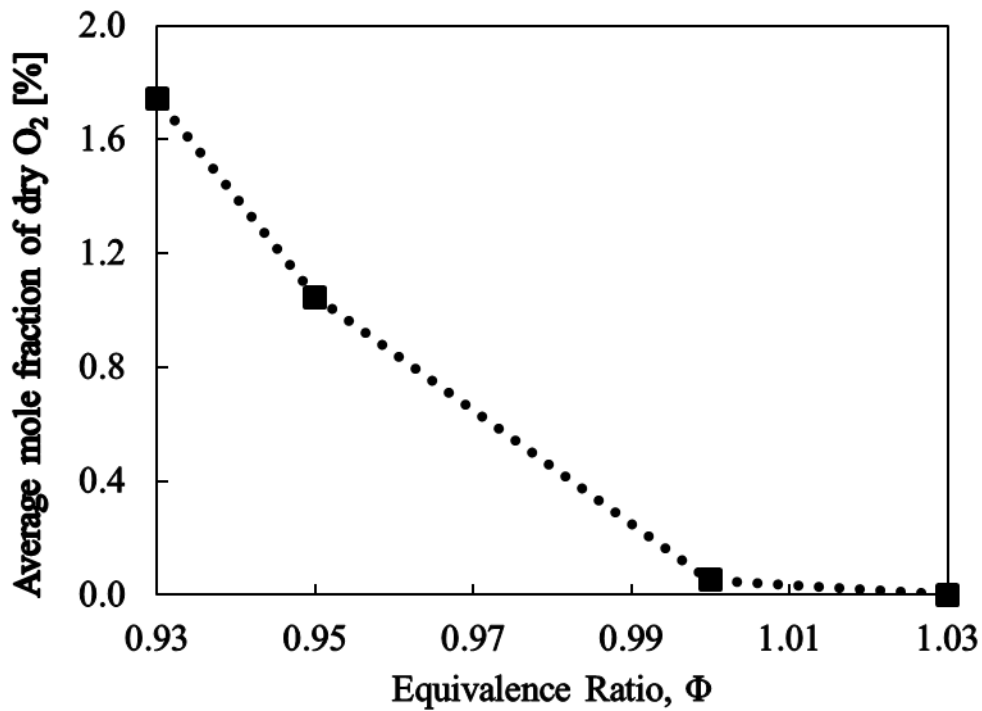


Figure 6.23: O₂ emission at the combustor exhaust for different equivalence ratios at 20% H₂ and firing rate of 5 MW/m³

CHAPTER 7

DYNAMIC COMBUSTION INSTABILITY IN PROPANE-OXYCOMBUSTION WITH CO₂ DILUTION

In this chapter results obtained from an experimental study focusing on dynamic instability of propane-oxy-combustion under the influence of CO₂ dilution are presented and discussed. The study was conducted in the non-premixed, swirl-stabilized combustor discussed in chapters 3. All the results were obtained at global stoichiometric equivalence ratio ($\Phi = 1$) and swirl number of unity.

7.1 Overview

Thermoacoustic instability arises due to the coupling between heat release and pressure oscillations. Such instability in non-premixed flames is mainly due to diffusive-thermal effects underscored by preferential diffusion effects and heat losses, and it can also arise as a result of flame-vortex interaction in swirling stabilized combustors. In the present experimental study, high-intensity microphones are used to obtain sound pressure fluctuations, while a photomultiplier tube with a bandpass filter centered at the wavelength of 307 Nano meters (nm) is used to observe relative heat release fluctuations. At the wavelength of 307 nm, the intermediate radical being targeted is OH. Data from both sensors is obtained at the sampling rate of 10 KHz for 10 seconds. Subsequently, a

total number of 100, 000 data points was acquired for each run all of which were then transformed to the frequency domain for further analysis. Data from both sensors is obtained at the sampling rate of 10 KHz for 10 seconds. Discrete Fourier Transform (DFT) of the data is taken to transform the data from time to frequency domain using the Fast Fourier Transform (FFT) algorithm with LABVIEW software. Also, background noise obtained from the sensors prior to the data capture during experiments is subtracted from the reported signal using LABVIEW software. This was achieved by carrying out an FFT on the recorded data obtained from the sensors prior to the start of the experiments. After the FFT of the background data, the frequency of any peak observed is marked and later subtracted using a bandstop filter from the data obtained during the experiments. A bandstop filter is a type of filter that allows all frequencies but the specified band in the filter. In all the background signals analyzed, a peak at 60 Hz is inherently observed, which can be attributed to electric interference. Figure 7.1 shows the schematic of the main components in the acoustic experiments. The PMT is situated exactly normal to the combustor since any tilt can affect the recorded signal. The high-intensity microphone used is situated upstream of the combustor flange containing the swirler and fuel nozzle. Signal conditioner is used for signal control of factors like overload and gain. The signal from both sensors is obtained using a data acquisition system (DAQ) connected to a personal computer equipped with LABVIEW software.

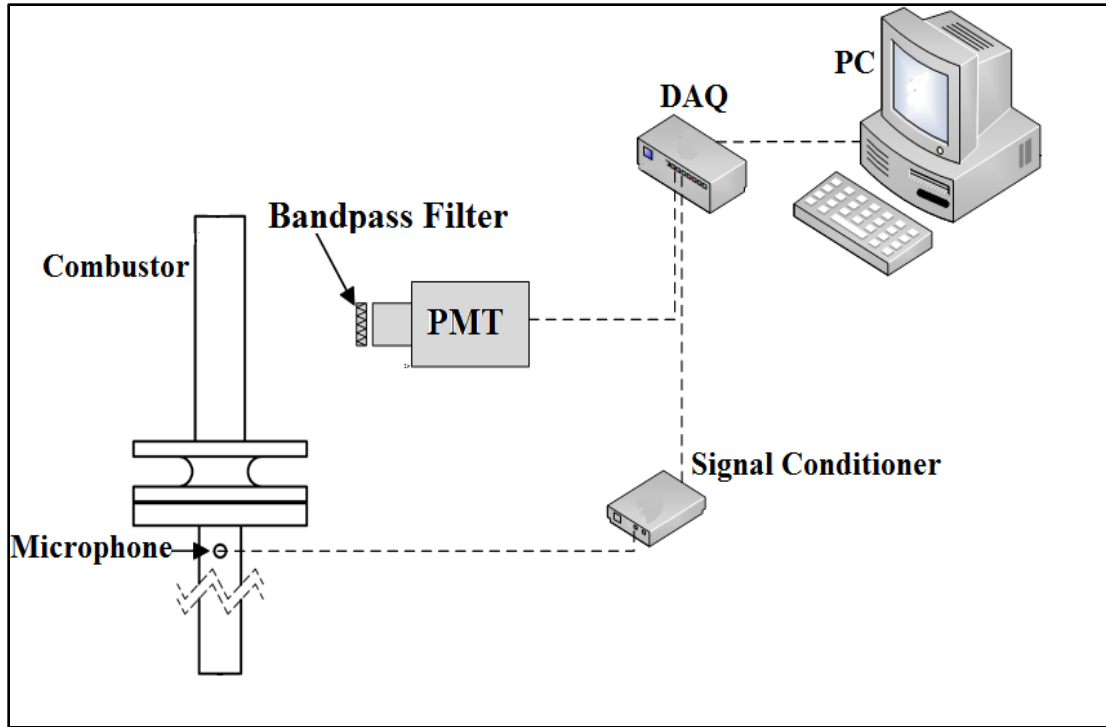


Figure 7.1: Schematic of the main components in acoustic experiments

Table 1 shows the experimental conditions for the thermoacoustic instability study in which the effect of CO₂ dilution on the heat release and acoustic pressure fluctuations in propane oxyfuel flames is studied. Furthermore, the effect of H₂ enrichment and combustor firing rate on the acoustic response of the propane oxyfuel flames under CO₂ dilution is studied. For all the cases studied, initially, the fuel was burnt at a certain firing rate and stoichiometric global equivalence ratio in a stream of pure oxygen. The CO₂ diluent is then added gradually while monitoring its concentration in O₂/CO₂ oxidizer until subsequent flame blowout. A 2% by volume increment of CO₂ concentration in the O₂/CO₂ mixture was used at initial stages of dilution. Beyond 35% CO₂ dilution in the mixture, this increment was further reduced to 0.5% in order to achieve a more gradual

sweep and establish the conditions of coupling between heat release and pressure fluctuations or otherwise.

Table 7.1: Conditions for experimental study into the acoustic response characteristics of propane oxyfuel flames with CO₂ dilution

Study	H ₂ %	Combustor firing rate [MW/m ³ .bar]	Global equivalence ratio; Φ	Oxidizer CO ₂ dilution level
Effect of CO ₂ dilution H ₂	0	4.0	1.00	From 0 % up to the % at flame blowout
Effect of H ₂ enrichment	0	4.0	1.00	
	20			
	40			
Effect of Combustor firing rate	0	3.0	1.00	
		3.5		
		4.0		
		4.5		

7.2 Recap on the effect of CO₂ dilution on the non-premixed flame structure

Flame macrostructures in non-premixed combustors are mainly dominated by the mixing mechanism between fuel and oxidizer streams and, therefore, on the momentum of the respective streams. Vortex-breakdown-induced thermoacoustic instability can be linked to one of the key flame stabilization mechanisms in non-premixed, swirl-stabilized combustor; namely the formation of inner and outer recirculation zones which depends not only on the swirl intensity but on the characteristics of the fuel and oxidizer streams. For oxyfuel combustion with CO₂ dilution (at fixed global equivalence ratio and combustor firing rate), the dilution level affects the oxidizer momentum vis-à-vis the fuel jet momentum and, therefore, the resulting flame structure. It is, therefore, important to begin this section by briefly introducing the effect of varying CO₂ diluent concentration on flames structure; the details of which can be found in Chapter 5 of this dissertation. The burner arrangement which is the same as the present study consists of a central fuel jet surrounded by a swirling oxidizer mixture.

In the numerical study covered in Chapter 5, it is reported that depending on dilution level, the non-premixed oxy-flame transits from an elongated, jet-like structure mainly dominated by the fuel jet momentum at low CO₂ dilution level to a compact, V-shaped flame dominated by the oxidizer momentum at higher CO₂ dilution. At zero dilution level (100% oxygen), the flame is fuel-jet-dominated and is anchored in the outer recirculation zone (ORZ) created by the sudden flow expansion into the combustor. By increasing the CO₂ dilution level, the vortex-driven momentum of the oxidizer mixture will be

enhanced, turbulence will be increased, and the result is an improved mixing giving rise to a shorter, more compact flame. The flame continues to be shorter until eventually, the vortex-driven momentum overwhelms the fuel jet momentum causing flow separation and the formation of inner recirculation zone (IRZ). Consequently, the resulting V-shaped flame at higher CO₂ dilution level is anchored in the shear layer, in-between ORZ and IRZ. This transition which also coincides with flow separation and formation of IRZ is observed to occur at the CO₂ dilution level of 45% as can be seen in Figure 7.2. The figure presents the steady-state structures observed in the combustor at different CO₂ dilution levels. These structures formed at different dilution level have a strong influence on the vortex-breakdown thermoacoustic instability reported in the present study.

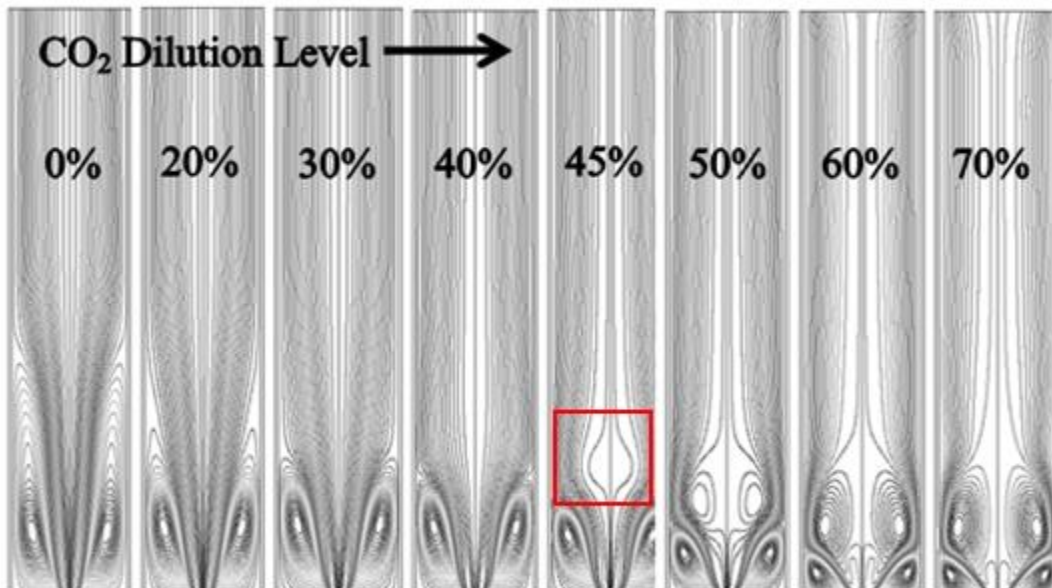


Figure 7.2: Contours of stream function as a function of CO₂ dilution level obtained at $\Phi = 1$

7.3 Effect of CO₂ dilution on the Combustion Dynamics

Figure 7.3, Figure 7.4, and Figure 7.5 depict the fluctuations in sound pressure (acoustic response) and heat release (OH fluctuations) as a function of CO₂ dilution level in the frequency domain. During the experiments, starting with 100% oxygen at stoichiometric global equivalence ratio and firing rate of 4 MW/m³.bar (combustor power of 4.68 kW), CO₂ was added in increasing proportion (varying O₂/CO₂ mixture) while recording the sound pressure and heat release signals, until flame blowout. From Figure 7.3, it can be observed that at zero and low CO₂ dilution level (0-20%), no significant oscillations, nor any dominant peak in both sound pressure and heat release were observed compared to higher CO₂ dilution cases. At 35% CO₂ dilution level, significant oscillations were observed at low frequency (0-200 Hz) in the heat release spectrum with no apparent dominant peak in the fluctuations. This increased heat release fluctuations accompanying an increase in CO₂ dilution level can be linked to improved turbulence associated with a higher momentum of the swirling oxidizer flow at higher CO₂ dilution level. Contrary to the heat release spectrum, at the same CO₂ concentration of 35%, no significant oscillation or dominant peak was observed in the sound pressure spectrum. This suggests that none of the heat release frequency response coupled with any of the natural acoustic modes of the combustor at that CO₂ dilution level.

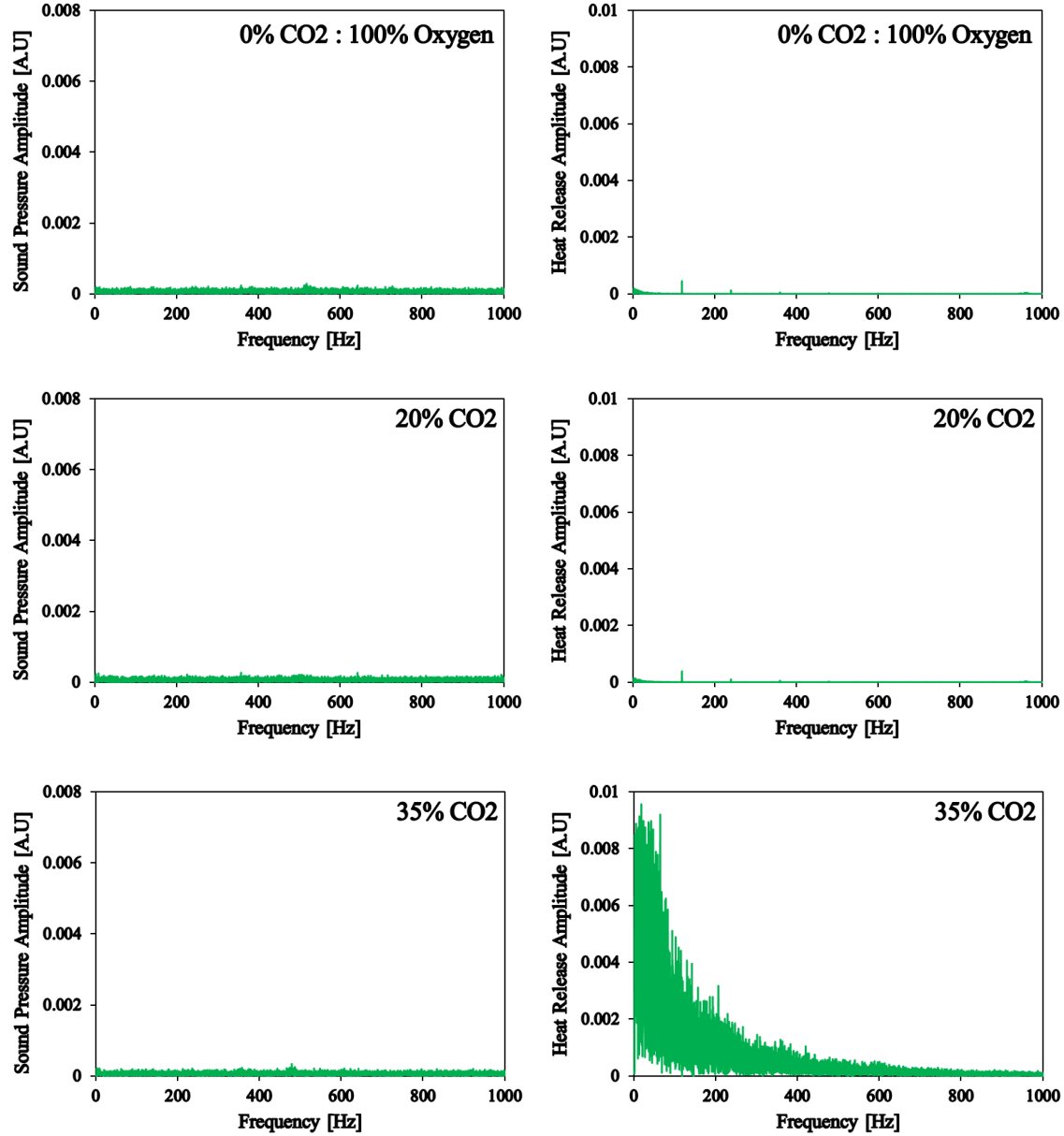


Figure 7.3: Acoustic and heat release frequency responses as a function of CO₂ dilution level at $\Phi = 1$ and firing rate of 4 MW/m³

At CO₂ dilution level of 45% (Figure 7.4), a peak appears at 465 Hz in the acoustic frequency response marking the onset of instability. The appearance of this peak at the CO₂ dilution level of 45% can be attributable to flame transition from a jet-like to V-shaped flame resulting from flow separation and the formation of IRZ which also occurs

at the same CO_2 concentration as discussed earlier. As we have discussed earlier, such flames are anchored in the shear layer, in-between ORZ and IRZ. The amplitude of this acoustic frequency response can be seen to be amplified at 50% CO_2 dilution level (Figure 7.4) while a dominant peak in the heat release fluctuation spectrum appears at the same frequency as the peak in the acoustic frequency response (465 Hz). The appearance of these distinct, high amplitude narrow band, spikes at the same frequency of 465 Hz in both the heat release and acoustic frequency responses is evidence of coupling between the two fluctuations. Consequently, the instability is amplified as a result of this coupling as registered by the increase in the amplitude of the 465 Hz peak in the acoustic frequency response. By our physical observation during the experiments, the sound level during this coupling is distinctively different from the other non-coupled cases as it is comparatively very discomforting. The coupling occurs as the sound pressure oscillation triggered by the flow separation triggers similar oscillation in heat release so that the two oscillations became coupled creating a feedback loop. Subsequently, the coupling mechanism can be characterized as vortex-breakdown-induced thermoacoustic instability. The maximum amplitude for the oscillation in the coupled mode is obtained at 60% CO_2 dilution as can be seen in Figure 7.4. In the coupled mode, the Rayleigh criterion is fulfilled and the energy contained in the oscillation is greater than energy dissipation from the system. Energy dissipation from the oscillation can be originated from one or all of the damping mechanisms that include viscous dissipation, heat transfer, energy transfer to other acoustic modes, and sound convection.

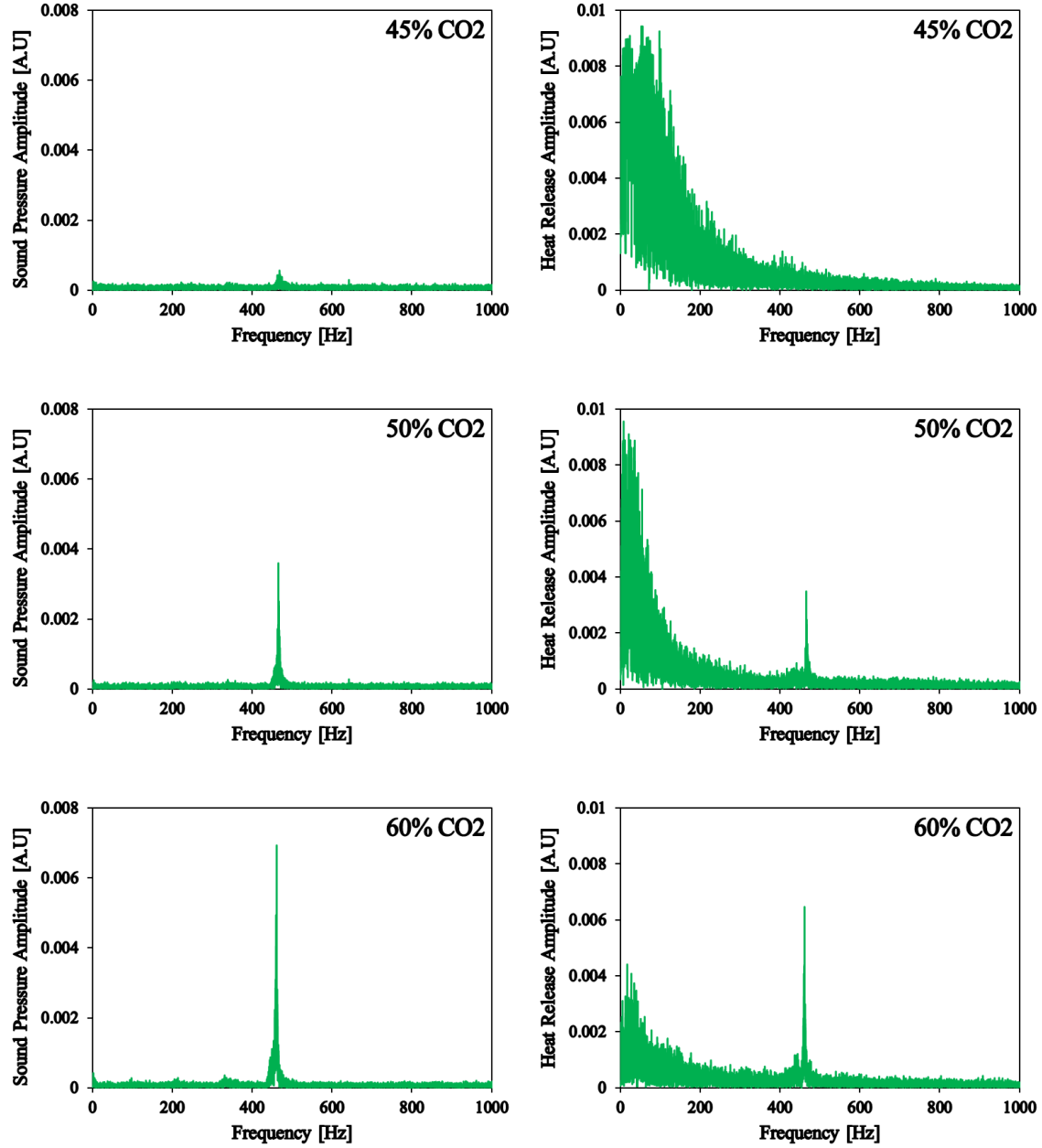


Figure 7.4: Acoustic and heat release frequency responses as a function of CO₂ dilution level at $\Phi = 1$ and firing rate of 4 MW/m³

In Figure 7.5, it can be observed that the amplitude of the frequency responses from both oscillations begins to decrease. The maximum sound pressure amplitude of 0.007 A.U recorded at 60% CO₂ dilution level drops to about 0.003 A.U at 65% CO₂ concentration.

This decrease in the oscillation amplitude can be attributable to damping due to energy dissipation arising from heat loss and viscous dissipation as dilution level increases. At 69% CO₂ level, the 465 Hz peak in the sound pressure spectrum shifted to 446 Hz while other peaks at the frequencies of 322 Hz, 205 Hz, and 94 Hz begin to form. The flame is lifted at the CO₂ dilution level of 77% and the sound pressure spectrum is characterized by multiple low amplitude peaks at the frequencies of 446 Hz, 322 Hz, 205 Hz, and 94 Hz as can be seen in Figure 7.5. These lower frequency peaks are reported in the literature to be excited by coupled convective-acoustic modes that are often encountered near blowout limits [60].

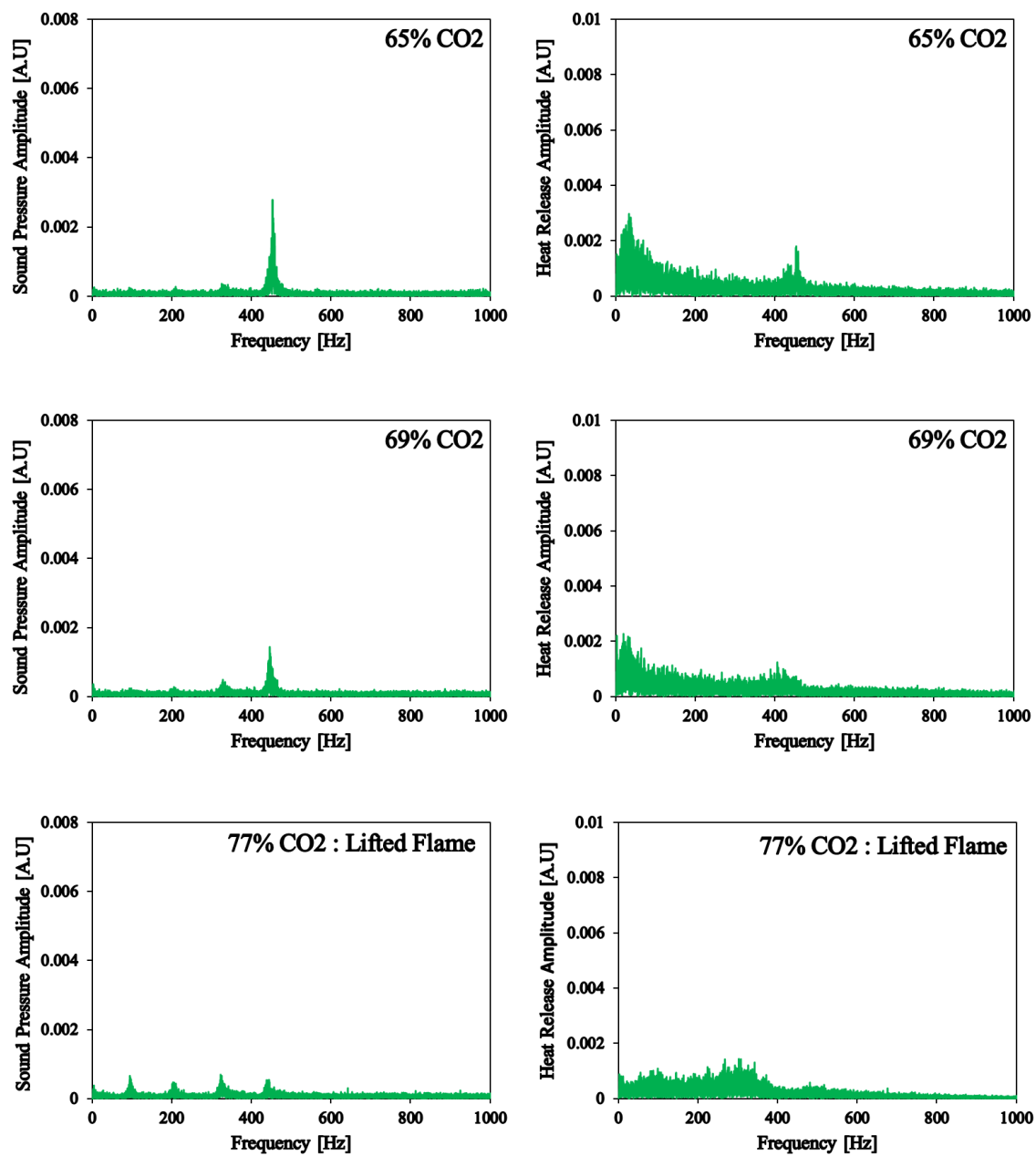


Figure 7.5: Acoustic and heat release frequency responses as a function of CO₂ dilution level at $\Phi = 1$ and firing rate of 4 MW/m³

7.4 Combustion Dynamics of H₂-enriched, CO₂-Diluted Oxy-flames

In the preceding section, we have observed that coupling between heat release and pressure fluctuations leading to thermoacoustic instability occurs at CO₂ dilution level that coincides with flow separation and flame transition into a more compact structure. Our target in this section is to look at the effect of hydrogen (H₂) enrichment on the thermoacoustic instability in the coupled mode. Subsequently, at the established coupled mode at 50% CO₂ dilution level, we vary the H₂ concentration in the fuel (propane) from 0 to 40% at a fixed stoichiometric global equivalence ratio and combustor firing rate of 4 MW/m³.bar.

The acoustic and heat release responses obtained for the CO₂-diluted, propane oxyfuel flames are presented in Figure 7.6 and Figure 7.7 respectively. From these plots, it can be observed that the amplitudes of both oscillations decrease with increase in H₂ concentration in the fuel mixture. In the sound pressure spectrum (Figure 7.6), it can be observed that the amplitude of the 465 Hz oscillations drops from 0.0036 A.U (arbitrary unit) at 0% H₂ to about 0.0006 A.U at 40% H₂ concentration. Similar behavior can be observed for the heat release frequency response shown in Figure 7.7. From the figure, at 40% H₂ concentration, the amplitude of the 465 Hz oscillations is comparatively lower. Moreover, in this case, it loses its distinguishing feature of standing out among the other low amplitude oscillations inherent in the system.

This decrease in amplitude of acoustic and heat release oscillations with an increase in H₂ concentration in the fuel can be attributable to the increase in flame speed (and hence the overall axial velocity) resulting from the added H₂ that can weaken IRZ vortex strength.

It can be recalled based on the results of hydrogen enrichment presented in Chapter 6, that higher hydrogen concentration in the fuel mixture is accompanied by comparatively weaker vortex strength of the leading edge of IRZ. As a consequence of this weaker vortex strength (among other factors), reduced mixing and higher CO emission were recorded at higher hydrogen concentrations. Moreover, due to the reduced mixing, lower scalar dissipation rate (defined in section 6.3.8 in chapter 6 of this dissertation) which entails lower rate of mixing at the molecular level, and hence reduced chemical reaction activity was observed in the IRZ with an increase in hydrogen concentration (Figure 7.8).

Other studies also reported that for fuel having comparatively higher reactivity like hydrogen, due to high flame speed, the vortex may be very small or even not visibly present rendering the flame-vortex coupling unlikely. Therefore, a comparatively lower acoustic amplitude is reported for hydrogen-rich syngas combustion when compared with methane combustion [100, 101]. Consequently, the reduction in acoustic amplitude with the increase in hydrogen concentration observed here can be attributable to the weakened flame-vortex interaction as the amount of H_2 increases in the fuel. It is important to stress here that, while in our preceding discussion we have observed that H_2 addition lowers the acoustic amplitude, energy dissipation from a flame in a thermoacoustically coupled mode, ultimately determines whether the oscillation amplifies or decays.

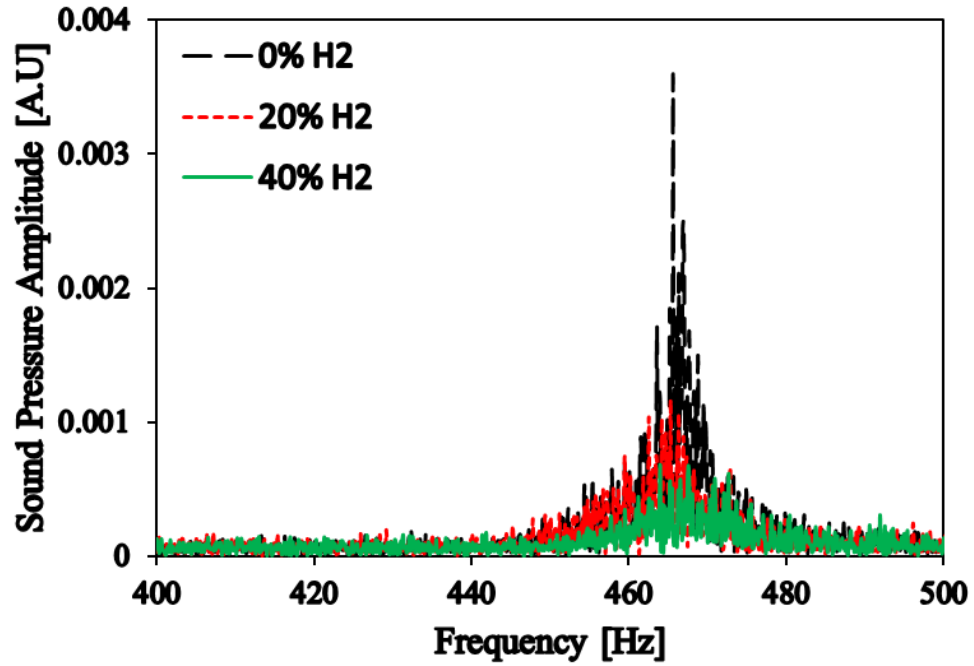


Figure 7.6: Acoustic frequency response as a function of H₂ concentration at 50% CO₂ dilution level, $\Phi = 1$, and firing rate of 4 MW/m³

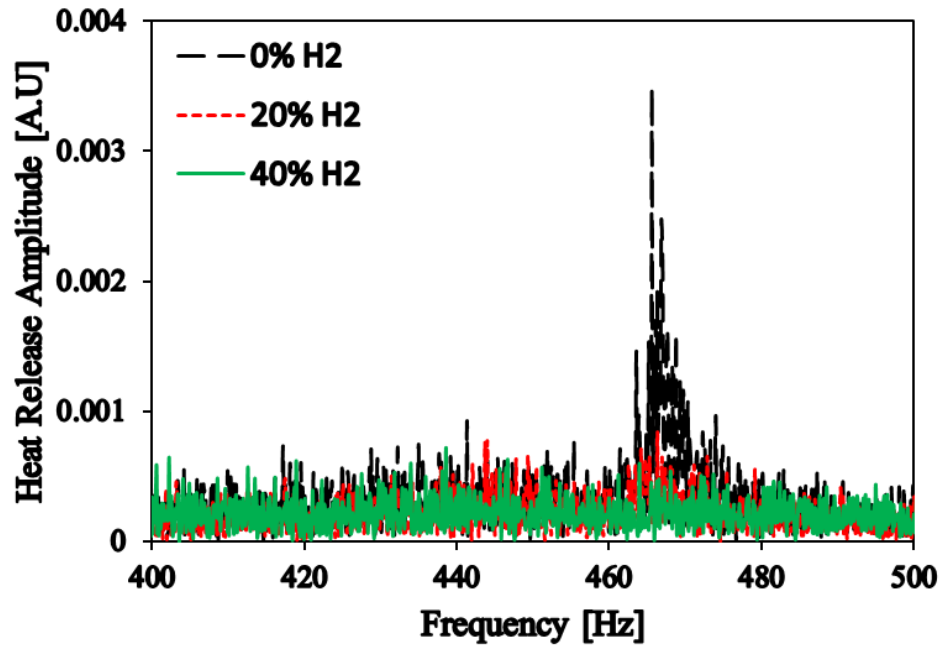


Figure 7.7: Heat release frequency response as a function of H₂ concentration at 50% CO₂ dilution level, $\Phi = 1$, and firing rate of 4 MW/m³

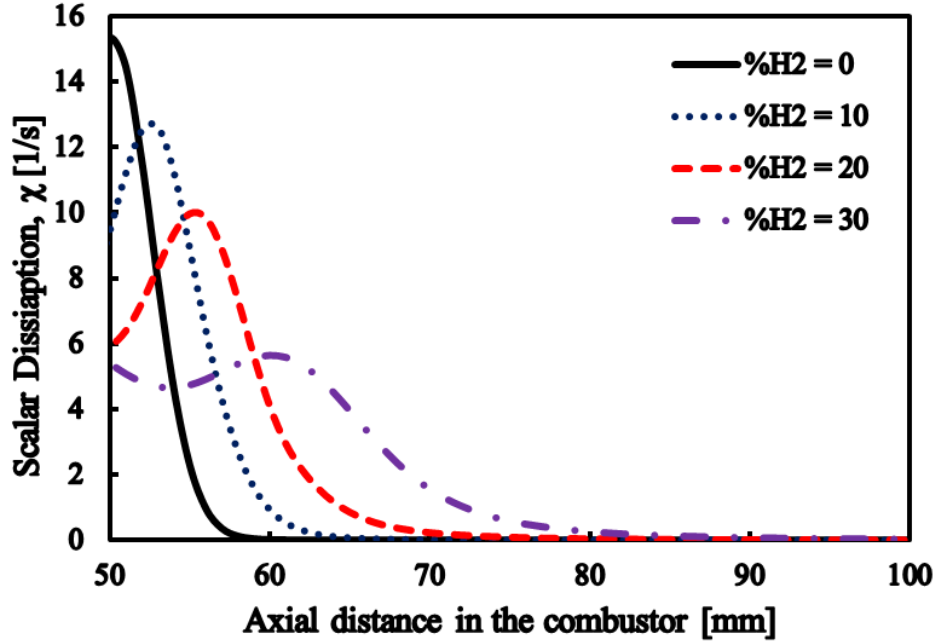


Figure 7.8: Scalar dissipation at the combustor axis from the leading edge of IRZ downstream for different H₂ concentration at $\Phi = 1$

7.5 Effect of Combustor Firing Rate

The results presented so far were all obtained at a fixed stoichiometric global equivalence ratio ($\Phi = 1$) and fixed combustor firing rate of $4 \text{ MW/m}^3 \cdot \text{bar}$. In this section, we discuss the effect of changing the combustor firing rate on thermoacoustic instability for the coupled mode at 50 % CO₂ dilution level and stoichiometric global equivalence ratio. The acoustic and heat release frequency responses obtained at different combustor firing rates are shown in Figure 7.9 and Figure 7.10 respectively. From the figures, it can be observed that both the amplitude and frequency of the oscillations decrease with the decrease in the combustor firing rate. A 60% drop in amplitude of the sound pressure level accompanied by a frequency drop from 470 Hz to 460 Hz is observed when the combustor firing rate was decreased from 4.5 MW/m^3 to 3.5 MW/m^3 .

This shift in frequency suggests that the combustor mode depends on the convective time of the reactants (fuel and oxidizer) and, therefore, their average velocity (and residence time), which decrease with the decrease in the combustor firing rate. The decrease in firing rate lowers the fuel velocity and, consequently, the oxidizer (to maintain the global equivalence ratio) leading to the shift in the frequency of the combustor mode that is triggered. Similar findings were reported by Zinn et al. [31], that depending on the convection time for the reactants, different combustor modes were observed to be triggered. The authors reported that as the convective delay time decreased, the amplitude of the lower-frequency mode drops while that of higher-frequency increases. Increasing combustor firing rate also affects the overall combustor temperature and heat loss, all of which can play an important role in deciding which of the natural acoustic mode of the combustor gets excited.

The results obtained here at different firing rates suggest a comparatively higher frequency and amplitude acoustic response corresponding to higher combustor firing rates. In fact, for the 50 % CO₂ dilution level considered here, at the firing rate of 3.0 MW/m³.bar, no clear coupling between sound pressure and heat release fluctuations can be observed. However, it cannot be stated categorically that at this firing rate, no such coupling exists at different CO₂ dilution level, because, as we have discussed earlier, the coupling depends on flow structures formed as well as the reactants residence time all of which are dependent upon the level of CO₂ dilution. Subsequently, a full and general account of the coupling mechanism leading to acoustic amplification for different firing rate will require a detailed understanding of varying combustors acoustics, the effect of firing rate on chemical reaction and flow characteristics.

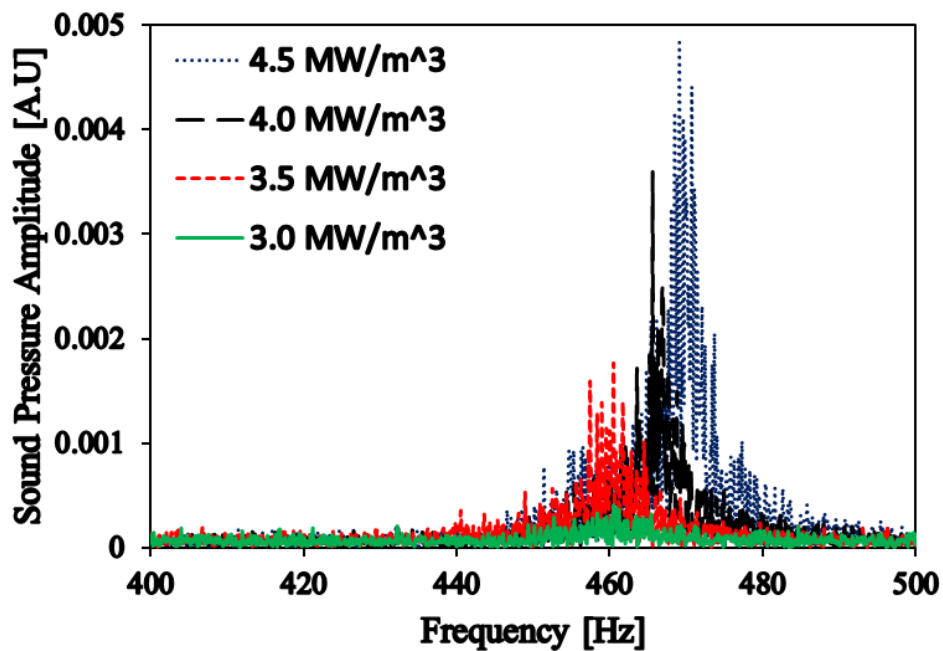


Figure 7.9: Acoustic frequency response as a function of combustor firing rate at 50% CO₂ dilution level and $\Phi = 1$

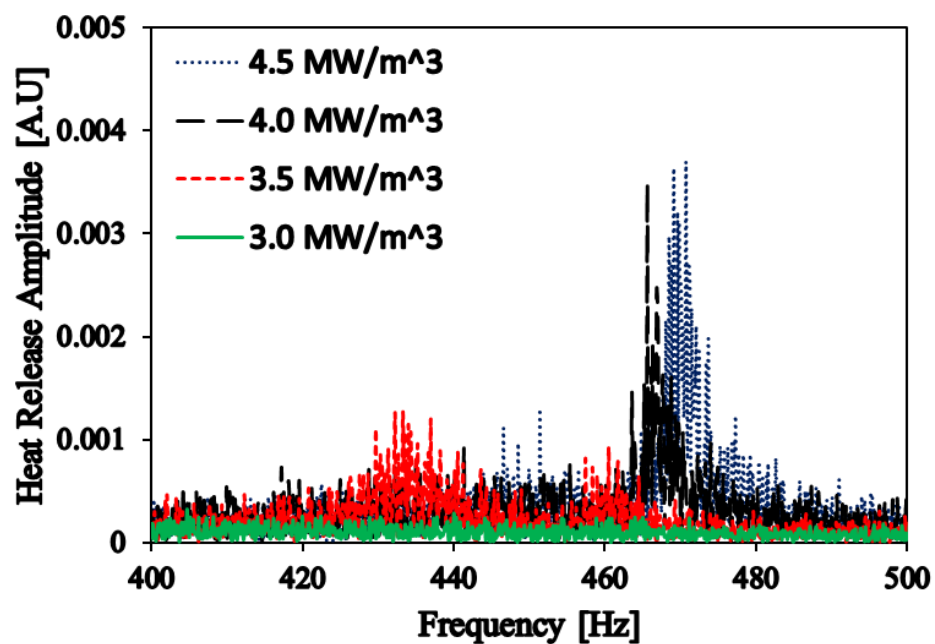


Figure 7.10: Heat release frequency response as a function of combustor firing rate at 50% CO₂ dilution level and $\Phi = 1$

CHAPTER 8

CONCLUSIONS AND RECOMMENDATIONS

Parametric analysis was conducted under different fuel and oxidizer conditions in order to investigate the effect of such conditions on static and dynamic instability, emission, flame structure, and temperature profiles of propane-oxyfuel flames in a non-premixed, swirl-stabilized combustor. In this chapter, the key findings, conclusions as well as recommendations are presented.

8.1 Conclusions

8.1.1 Propane-Oxyfuel Static Stability

The effects of the equivalence ratio, firing rate, swirl number, and oxidizer mixture (air, oxyfuel I, oxyfuel II, and CO₂ dilution level) on the flame static stability were studied. Results show that, for lean mixtures, the propane-air flame transits from the attached flame to lifted flame before subsequent flame extinction, contrary to oxyfuel I and II flames that transit directly from the attached flame to no flame regime at all firing rates considered. Near stoichiometry, however, the oxyfuel flames display distinct flame transitions, including liftup before extinction as a consequence of CO₂ dilution at high firing rates. These flame transitions were observed to be flow-induced. The blowout

characteristic of the flame is, however, controlled by both the flow and flame dynamics. Consequently, a more detailed study is necessary to understand such dynamics. Higher combustor firing rates (at a certain equivalence ratio and swirl number) are seen to enhance flame stability limits. We also observed that oxyfuel flame exhibits a wider stability window under a swirling flow produced by the swirler having a swirl number of 1.0 in comparison to those having 0.6 and 1.5. This suggests that low and excessive swirl conditions can be undesirable in an effort to enhance the stability of swirl-stabilized flames. Finally, while leaner equivalence ratios in air flames result in lower NO_x emissions, low temperatures are associated with high CO emissions in oxyfuel flames. For oxyfuel combustion, therefore, operating the combustor near stoichiometry is beneficial in not only minimizing the costly, excessive oxygen usage in the process but also in targeting exhaust gases suitable for CCS.

8.1.2 CO₂ Dilution and Combustion Characteristics

The effect of dilution level in the O₂/CO₂ oxyfuel oxidizer mixture on the flame's macrostructure, temperature distribution, and emissions was also studied numerically. The interaction between the fuel jet and the vortex created by the swirling flow was found to play a critical role in the flame's anchoring position and consequently its structure. For the fixed fuel jet momentum and swirl number used in the study, increase in CO₂ dilution level in the oxidizer was found to enhance turbulent mixing in the combustor, enhance the vortex strength, resulting into a compact V-shaped flame. This is in contrast to the fuel-jet dominated flame obtained at zero and low dilution levels,

characterized by a longer reaction zone. Non-dimensional vortex strength can be employed to characterize the flames macrostructure and predict or target specific macrostructure by controlling the jet momentum and the vortex strength momentum. Apart from enhanced mixing, the CO_2 diluent lowers the combustion maximum temperature, thermal diffusivity, and the flame speed and, therefore, the diluent lowers the flame's resistance to extinction. Moreover, increased CO_2 dilution increases the strain imposed by the flow on the flame which further lowers the flame's resistance to extinction. The CO and CO_2 emissions from the combustor were found to exhibit an inverse relationship with higher CO concentrations accompanied by lower CO_2 concentrations. The cooling effect of the diluent, residence time of gases in the combustor, and CO_2 dissociation at high temperatures were found to play key roles in CO emissions.

8.1.3 Hydrogen-Enriched Propane Oxycombustion Characteristics

The effect of hydrogen enrichment on the blowout limit of propane oxyfuel flames with CO_2 dilution was analyzed experimentally in a swirl-stabilized, non-premixed combustor. Furthermore, the effect of hydrogen-enrichment on propane oxyfuel flames in terms of combustion thermochemical scalars under fixed oxyfuel oxidizer mixture was studied numerically. Results show that an increase in hydrogen concentration in the fuel extends the blowout limits of the oxyfuel flames under CO_2 dilution. Up to 2.5% increase in CO_2 diluent concentration in O_2/CO_2 oxidizer mixture was recorded when the hydrogen concentration in propane was increased from 0 to 30%. The operating equivalence ratio

and combustor firing rate were also found to extend the blowout limit under CO₂ dilution. An average increase of 1.5% in CO₂ concentration was observed between global equivalence ratio of 0.9 and 1.0. While extending blowout limits of oxyfuel flames under CO₂ dilution, hydrogen enrichment was, however, found to increase CO at the detriment of CO₂ emission. The minimum amount of CO₂ emission on dry basis recorded in this study (97.33%) corresponds to maximum CO emission (1.93%) at the hydrogen concentration of 40%. This increase in CO emission with an increase in hydrogen concentration can be attributed to the low residence time of gasses in the combustor, shift towards reactants in WGSR due to higher temperatures caused by H₂ addition, as well as competition for oxygen between the highly reactive hydrogen and propane in a stoichiometric, non-premixed mixture of the oxyfuel oxidizer. Further study shows a decrease in the CO emission with even slight decrease in equivalence ratio from stoichiometry. A sharp drop in CO emission from near 8000 ppm at $\Phi = 1.03$ to less than 1 ppm at $\Phi = 0.93$ was observed. Leaner equivalence ratios, however, lead to an increase in O₂ concentration at the exhaust; a condition not suitable for oxyfuel combustion targeting CCS beyond a certain limit. To achieve sequesterable exhaust limits for CSS, therefore, a balancing act between CO and O₂ emissions as well as the cost of excess oxygen utilization needs to be undertaken.

8.1.4 Dynamic Instability and CO₂- Diluted Propane Oxycombustion

The effects of CO₂ dilution level, hydrogen addition, and combustor firing rate on thermo-acoustic instability of propane-oxy flames were studied. Results obtained at a

fixed firing rate of $4 \text{ MW/m}^3 \cdot \text{bar}$ and stoichiometric equivalence ratio show that the oxy-flame is stable at zero and low CO_2 dilution level. The onset of thermo-acoustic instability was observed to occur at the CO_2 dilution level of 45%, which coincides with the flame transition from jet-like to V-shaped resulting from flow separation leading to the formation of IRZ. This transition happens when the fuel-jet momentum is overwhelmed by the oxidizer-driven vortex momentum. Subsequent to this onset of instability, at 50% CO_2 dilution level, a coupling between heat release and pressure fluctuations was observed and the instability was amplified. The excited combustor mode is recorded to be at the frequency of 465 Hz and the resulting instability is characterized as vortex-breakdown-induced thermo-acoustic instability. The amplitude of the oscillation decreases beyond CO_2 dilution level of 60% attributable to damping due to energy dissipation arising from heat loss and viscous dissipation as dilution level increases. Lifted flame sound pressure spectrum at the CO_2 dilution level of 77% is characterized by the multiple low amplitude peaks (446 Hz, 322 Hz, 205 Hz, and 94 Hz) excited by coupled convective-acoustic modes encountered near blowout limits. The acoustic amplitude is observed to decrease with increase in H_2 concentration in the propane (C_3H_8) fuel and this can be linked to the higher flame speed associated with H_2 . Furthermore, 60% drop in amplitude of the sound pressure level accompanied by frequency shift from 470 Hz to 460 Hz is observed when the combustor firing rate was decreased from 4.5 MW/m^3 to 3.5 MW/m^3 . This suggests that the combustor mode depends on the convective time of the reactants (fuel and oxidizer) as well as the resulting flow structures corresponding to reactants (and diluent) flow rates.

8.2 Recommendations

In this work, oxyfuel combustion characteristics of propane were experimentally and numerically studied over a range of operating conditions in a swirl-stabilized, non-premixed gas turbine model combustor. Characteristics like static and dynamic stability as well as flames macrostructure and emissions were analyzed. Based on the outcomes of the work, the following possible areas for future work are recommended:

- ✓ The burner design can be enhanced to mirror gas turbine combustor more closely by geometrically ensuring shorter residence time of the reactants (order of magnitude of Milliseconds; 3-25ms). Furthermore, the design should accommodate combustion under pressurized conditions.
- ✓ Laser diagnostic tools can be employed to map out the combustor flow field, temperature field, and emissions to better understand the combustion characteristics and dynamics.
- ✓ Instead of arbitrary sound pressure amplitude of the combustion instability, the overall sound pressure level of the combustor over a wide range of operating conditions can be obtained. This will give quantifiable and useful information about the noise level of the combustor at those conditions. Locating the microphones very close to the flame region will ensure that the sound pressure level resulting from the flame coupling with the combustor acoustic is obtained before significant energy dissipation. Recording the maximum available sound pressure will ensure the determination of the overall sound pressure level of the combustor.

- ✓ Unsteady, 3-dimensional numerical simulations can shed light on the combustion dynamics which were not captured in the steady state conditions employed in this work. Furthermore, a detailed chemical reaction kinetics of the propane fuel should be incorporated in such simulations to fully understand how the reactions progress.
- ✓ As oxyfuel combustion literature is still evolving, even simplified chemical kinetics models are very scarce. Such models can be developed based on experimentations with different fuel and oxidizer conditions to help provide basic research tools on the subject area.
- ✓ The effect of pre-heating the CO₂ diluent can be studied at different pre-heating temperature by incorporating a heating mechanism before mixing the oxidizer and its subsequent supply to the reaction zone. This will help in understanding the combustion dynamics of high temperature recycled CO₂ diluent that could be encountered in real oxyfuel combustion systems.
- ✓ Other types of fuels having wide-ranging applications can be studied under oxyfuel conditions.

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PUBLICATIONS FROM THIS DISSERTATION

1. **Z. Abubakar**, M. R. Shakeel, and E. M. Mokheimer, "*Experimental and Numerical Analysis of non-premixed oxy-combustion of hydrogen-enriched propane in a swirl stabilized combustor*," Energy, vol. Volume 165, Part B pp. 1401-1414, 2018.
2. **Z. Abubakar**, S. Y. Sanusi, and E. M. A. Mokheimer, "*Experimental Analysis of the Stability and Combustion Characteristics of Propane-Oxyfuel and Propane-Air Flames in a Non-premixed, Swirl-Stabilized Combustor*," Energy & Fuels, vol. 32, pp. 8837-8844, 2018/08/16 2018.
3. **Z. Abubakar** and E. M. Mokheimer, "*Numerical study of the combustion characteristics of propane-oxyfuel flames with CO₂ dilution*," Energy & Fuels, 2018.
4. **Z. Abubakar**, S. Sanusi, and E. M. Mokheimer, "*Stability of Propane-air and oxyfuel diffusion flames in a swirl-stabilized combustor; an experimental study*," Energy Procedia, vol. 142, pp. 1552-1557, 2017.
5. **Z. Abubakar**, Esmail M. A. Mokheimer, " *Dynamic Combustion Instability of Propane-Oxycombustion With Co₂ Dilution: Experimental Study (submitted to International Journal of Energy Research)*
6. **Z. Abubakar** and Esmail M. A. Mokheimer, "Review of static and thermoacoustic instabilities in oxyfuel combustion" **(to be submitted)**