

**INVESTIGATION OF COMBUSTION AND EMISSION
CHARACTERISTICS OF OXY-FUEL FLAMES IN SWIRL-
STABILIZED AND MULTI-HOLE TYPE MODEL GAS
TURBINE COMBUSTORS**

BY

MD AZAZUL HAQUE

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This thesis, written by **Md Azazul Haque** under the direction of his thesis advisor and approved by his thesis committee, has been presented and accepted by the Dean of Graduate Studies, in partial fulfillment of the requirements for the degree of **MASTER OF SCIENCE IN MECHANICAL ENGINEERING.**

Med Habib, Jan 4, 2022

Dr. Mohammed A. M. Habib
(Advisor)



Dr. Khaled S. Al-Athel
Department Chairman

Nemhat, Jan 4, 2022

Dr. Medhat A. Nemitallah
(Co-Advisor)



Dr. Suliman S. Al-Homidan
Dean of Graduate Studies



Dr. Syed A. M. Said
(Member)



Dr. Esmail M. A. Mokheimer
(Member)

Date



Dr. Atia E. A. Khalifa
(Member)

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2021

Dedicated to my beloved family

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LIST OF ABBREVIATIONS

ΔP	:	Pressure difference
AEV	:	Advanced environmental vortex burner
APU	:	Auxiliary power unit
ASU	:	Air separation unit
BFB	:	Bubbling Fluidized Bed boiler
CCS	:	Carbon capture and storage
CFB	:	Circulating Fluidized Bed boiler
CFD	:	Computational fluid dynamics
CO	:	Carbon monoxide
CO₂	:	Carbon dioxide
COG	:	Coke over gas
COP21	:	21 st Conference of the Parties
C_p	:	Specific heat at constant pressure
CPU	:	Compression and purification unit
Da	:	Damköhler number
DLE	:	Dry low emissions
DLN	:	Dry low NO _x
DU	:	Demonstration unit
EGR	:	Exhaust gas recirculation

EV	:	Environmental vortex burner
FGR	:	Flue gas recirculation
GCP	:	The Global Carbon Project
GHG	:	Greenhouse gas
Gt	:	Gigaton
GT	:	Gas turbine
HF	:	Hydrogen fraction
HO	:	Heavy oil
HP	:	High pressure
IGCC	:	Integrated gasification combined cycle
IRZ	:	Inner recirculation zone
ITM	:	Ion transport membrane
ITMR	:	Ion transport membrane reactor
KW	:	Kilowatt
LBO	:	Lean blowout limit
LDI	:	Lean direct injection
LES	:	Large Eddy Simulations
LHV	:	Lower heating value
LPG	:	Liquified petroleum gas
LPM	:	Lean premixed
MM	:	Micromixer combustor

Mt	:	Megaton
MW	:	Megawatt
MWI	:	Modified Wobbe index
NG	:	Natural gas
NIST	:	National Institute of Standards and Technology
NO_x	:	Nitrogen Oxides
OEM	:	Original equipment manufacturers
OF	:	Oxygen fraction
ORZ	:	Outer recirculation zone
OSL	:	Outer shear layer
OTMR	:	Oxygen transport membrane reactors
PC	:	Pulverized coal
PF	:	Pattern factor
PFR	:	Product formation fate
PP	:	Pilot plants
ppmvd	:	parts per million by volume, dry
PV	:	Progress variable
RANS	:	Reynolds Averaged Navier-Stokes equations
Re	:	Reynolds Number
SCOC-CC	:	Semi-closed oxy-fuel combustion combined cycle
SEV	:	Sequential environmental vortex burner

S_L	:	Laminar burning velocity
S_T	:	Turbulent burning velocity
T_{ad}	:	Adiabatic flame temperature
TLR	:	Technology readiness level (developed by NASA)
TWh	:	Terawatt-hour
UHC	:	Unburned hydrocarbon
UNFCCC	:	United Nations Framework Convention on Climate Change
WI	:	Wobbe index
ZEPP	:	Zero-emission power plants

Greek Symbols

Ø	:	Equivalence ratio
ρ	:	Density

Subscripts

th	:	Thermal
L	:	Laminar
T	:	Turbulent
ad	:	Adiabatic

Superscripts

tm	:	Trademark
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ABSTRACT

Full Name : Md Azazul Haque

Thesis Title : Investigation of combustion and emission characteristics of oxy-fuel flames in swirl-stabilized and multi-hole type model gas turbine combustors

Major Field : Mechanical Engineering

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Extensive use of fossil fuels increases the pollutants and presence of greenhouse gases (GHG) in the environment and aggravates global warming. The development of sustainable cleaner energy production is to be adopted to reduce the emissions and increase the combustion efficiencies using fossil fuels. Therefore, this thesis work focuses on oxy-combustion methods with different fuels (propane, methane, and syngas) and different burner designs for power generation in gas turbines with CO₂ capture. Combustion, emission, and flame stability characteristics have been investigated numerically and compared for different combustion technologies under fuel/oxidizer-flexible oxy-combustion conditions. Three gaseous fuels (i.e., methane, propane, and syngas) have been examined in two gas turbine burners (swirl-stabilized and multi-hole burner) over wide ranges of operating parameters.

Computational fluid dynamics (CFD) simulations have been developed for two combustor geometries; swirl-stabilized and multi-hole burner. Transient large eddy simulation (LES) have been adopted for the swirl-stabilized combustor. Developed LES model has been validated against experimentally obtained combustor temperatures. On the other hand,

Reynolds-averaged Navier-stokes (RANS) turbulence model have been employed for the multi-hole burner. Numerical combustor temperatures of multi-hole burner have been compared with the corresponding theoretical adiabatic temperatures. Carbon-dioxide is added with the inlet fuel-oxygen stream to imitate the exhaust gas recirculation in gas turbine. The oxy-fuel flames are compared in various mixture compositions by varying the equivalence ratio ($\Phi=0.241-0.597$) and oxygen fraction ($OF=32.4-60\%$). A fixed bulk inlet velocity of 5.2 m/s is considered for the simulation cases under atmospheric condition.

The adiabatic flame temperature (T_{ad} or AFT) has been identified as a dominant parameter in determining flame stability and combustion behaviors. Two separate inner recirculation zones have been observed from the numerical velocity streamlines for oxy-propane flames in swirl-stabilized combustors. The results with LES indicate that the reaction rates for premixed swirl-stabilized CO_2 -diluted oxy-propane ($C_3H_8/O_2/CO_2$) flames increase with the increase of Φ and OF . Flames of the same adiabatic flame temperature (T_{ad}) show similar macro-and flowfield-structures, in terms of flame shape, flow circulation, and temperature, and species distributions, irrespective of the values of Φ and OF . At higher T_{ad} , the flames were observed to be more compact with reduced flame thickness and higher Damköhler number (Da). In all cases, $Da > 1$ were observed, indicating the dominance of reaction rate in oxy-propane flames than the diffusion rate. A secondary IRZ was also observed near the outlet of the combustor. Mixture composition and combustion temperature influence the CO concentration at the combustor exit. The highest CO emission was observed at 0.17 ppm for the flame with highest Φ and T_{ad} , meanwhile no CO emission was seen for flames with high OF and low Φ among the studied cases. Similar behavior was also observed for oxy-methane flames. In comparison, oxy-syngas flames

have demonstrated more uniform temperature distribution at combustor outlet while oxy-methane and oxy-propane flames have shown lower CO emission and higher thermal power, respectively. Compared to the swirl-stabilized counterpart, only outer recirculation zone (ORZ) has been observed for oxy-propane flames in multi-hole combustor. The oxy-propane flames in multi-hole burner obtained with RANS turbulence model demonstrated relatively higher pattern factor and the presence of only ORZ, as compared to that in swirl-stabilized combustor under similar inlet flow condition.

ملخص الرسالة

الاسم الكامل: محمد عزازول حق

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التخصص: الهندسة الميكانيكية

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يزيد الاستخدام المكثف للوقود الأحفوري من الملوثات ووجود الغازات الدفيئة (GHG) في البيئة ويؤدي إلى تفاقم ظاهرة الاحتباس الحراري. يجب تبني تطوير إنتاج مستدام للطاقة النظيفة لتقليل الانبعثات وزيادة كفاءة الاحتراق باستخدام الوقود الأحفوري. لذلك، تركز هذه الأطروحة على طرق الاحتراق بالأوكسجين بأنواع الوقود المختلفة (البروبان والميثان وغاز التخليق) وتصميمات الموقد المختلفة لتوليد الطاقة في توربينات الغاز مع احتجاز ثاني أكسيد الكربون. تم فحص خصائص الاحتراق والانبعثات واستقرار اللهب عددياً ومقارنتها بتقنيات الاحتراق المختلفة في ظل ظروف احتراق الوقود/المؤكسد المرنة. تم فحص ثلاثة أنواع من الوقود الغازي (الميثان، والبروبان، وغاز التخليق) في موقدين للتوربينات الغازية (موقد دوامي وموقد متعدد الفتحات) على مدى واسع من عوامل التشغيل.

تم تطوير محاكاة ديناميكا الموائع الحسابية (CFD) لكل الموقدين، الموقد الدوامي والموقد متعدد الفتحات. تم اعتماد محاكاة الدوامية الكبيرة العابرة (LES) للموقد الدوامي بعد التحقق من صحتها بمقارنة النتائج مع بيانات درجات الحرارة المقاسة معملياً. وعلى الجانب الآخر، تم اعتماد محاكاة المتوسط النظري لمعادلة Navier-stokes (RANS) للموقد متعدد الفتحات. تم التحقق من صحة نتائج المحاكاة للموقد متعدد الفتحات عن طريق مقارنة درجات الحرارة القصوى للخب مع تلك المحسوبة نظرياً. تم إضافة ثاني أكسيد الكربون مع خليط الوقود والأوكسجين الداخل لتقليد إعادة تدوير غاز العادم في التوربينات الغازية. تم مقارنة لهب الوقود والأوكسجين في تركيبات خليط مختلفة عن طريق تغيير نسبة التكافؤ $\phi = 0.241 - \phi$

0.597) ونسبة الأكسجين ($OF = 32.4-60\%$) عند سرعة مدخل ثابتة تبلغ 5.2 م/ث تحت ظروف الضغط الجوي.

تم تحديد درجة حرارة اللهب القصوى (T_{ad} أو AFT) كمعامل سائد في تحديد استقرار اللهب وسلوكيات الاحتراق. وقد لوحظ وجود منطقتين منفصلتين لإعادة الدوران الداخلي من خطوط انسيابية السرعة العددية للهب البروبان والأكسجين في الموقد الدوامي. تشير النتائج بناء على LES إلى أن معدلات التفاعل لألسنة لهب البروبان والأكسجين المخفف بثاني أكسيد الكربون ($C_3H_8/O_2/CO$) المختلط مسبقاً والمستقر دوامياً تزداد مع زيادة Φ و OF . تُظهر ألسنة اللهب ذات نفس قيمة درجة الحرارة القصوى (T_{ad}) هياكل وحقول تدفق متشابهة من حيث شكل اللهب، ودوران التدفق، ودرجة الحرارة، وتوزيع العناصر الكيميائية، بغض النظر عن قيم Φ و OF . عند قيم T_{ad} أعلى، لوحظ أن ألسنة اللهب تكون أكثر إحكاماً مع انخفاض سماكة اللهب وارتفاع رقم $Damkohler (Da)$. في جميع الحالات، تمت ملاحظة $Da > 1$ ، مما يشير إلى هيمنة معدل التفاعل في لهب البروبان والأكسجين عن معدل الانتشار. كما لوحظ وجود منطقة دوران داخلي (IRZ) ثانوية بالقرب من مخرج غرفة الاحتراق. يؤثر تكوين الخليط ودرجة حرارة الاحتراق على تركيز أول أكسيد الكربون عند مخرج المفاعل. لوحظ أعلى انبعاث أول أكسيد الكربون عند 0.17 جزء في المليون للهب مع أعلى قيم Φ و T_{ad} ، وفي الوقت نفسه لم يُلاحظ أي انبعاث لأول أكسيد الكربون للهب مع ارتفاع OF وانخفاض قيم Φ بين الحالات المدروسة. ولوحظ أيضاً سلوك مماثل لهب الميثان والأكسجين. أظهرت المقارنة أن لهب غاز التخليق والأكسجين ينتج عنه توزيعاً أكثر اتساقاً لدرجة الحرارة عند مخرج المفاعل بينما أظهر لهبي الميثان والبروبان مع الأكسجين انبعاث أقل لأول أكسيد الكربون وطاقة حرارية أعلى، على التوالي. مقارنةً بالموقد الدوامي، لوحظ فقط منطقة إعادة تدوير خارجية (ORZ) للهب البروبان والأكسجين في الموقد متعدد الفتحات. أظهر لهب البروبان والأكسجين في الموقد متعدد الفتحات بناء على نموذج RANS عامل نمط أعلى نسبياً ووجود ORZ فقط، مقارنةً بذلك في الموقد الدوامي في ظل حالة تدفق مدخل مماثلة.

CHAPTER 1

INTRODUCTION AND BACKGROUND

1.1 Introduction

Global Warming is one of the main concerns in today's world due to the emissions of greenhouse gases (GHG). Fossil fuel utilization is one of the primary sources that contribute to the rise in GHG emissions, primarily carbon dioxide (CO₂). Power generation plants consume most of the fossil fuels with about 80% [1]. To regulate and reduce the emissions of greenhouse gases, the Paris Agreement was signed in 2015 among the nations in the 21st Conference of the Parties (COP21) at United Nations Framework Convention on Climate Change (UNFCCC) [2]. The main objective of this accord was to work together for global warming issues through holding the increase in the global average temperature to well below 2 °C above the pre-industrial levels. Achieving this target would require the industries as well as the power sectors to use carbon-free fuels for low CO₂ emission. A study by The Global Carbon Project (GCP), **Figure 1.1**, shows the continuous increase in CO₂ emission. Within one year, from 2018 to 2019, the total CO₂ emission has increased by 1.2 %. In 2019, the carbon emission from energy-related applications has risen to a high record of 36.8 Gt of CO₂ [3].

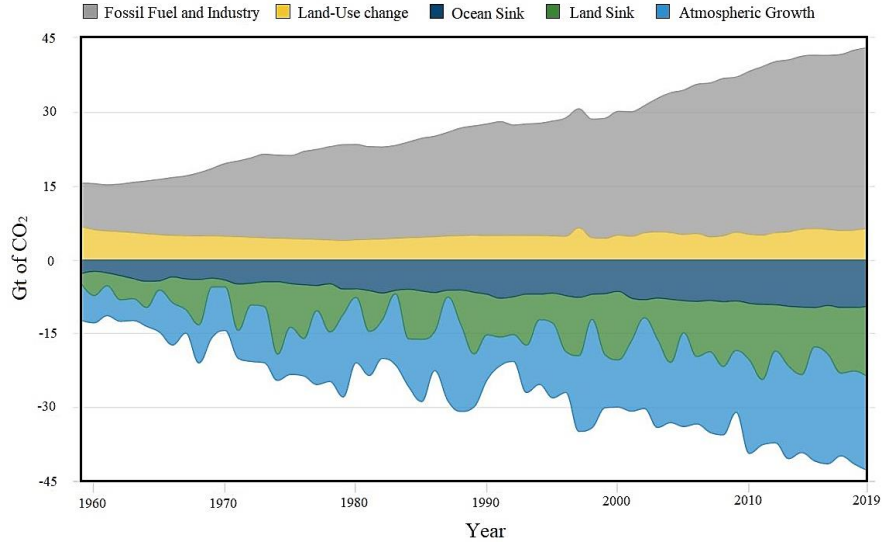


Figure 1.1: Global carbon budget from 1959 to 2019 [3].

Statistics on the energy, fossil fuels, and emissions for different countries in the world are discussed extensively in the ‘Global Energy Statistical yearbook 2020’ prepared by Enerdata [4]. In Saudi Arabia, more than 95% of the electricity has been produced with fossil energy in 2017. The fact that Saudi Arabia is on the world-top-10 list of countries producing electricity (350 TWh in 2019) and generating CO₂ emissions (534.3 Mt of CO₂ in 2019), makes Saudi Arabia the largest user of GTs worldwide. **Figure 1.2** illustrates the annual emission of CO₂ in Saudi Arabia, which is produced from the combustion of fossil fuels. From the year 2000 to 2019, CO₂ emission increased around 4.2 % per year where the increase is 0.9% within a year from 2018 to 2019 [4]. All these highlight the critical need to implement efficient carbon capture and sequestration for GT applications, which is the subject of interest for the present review.

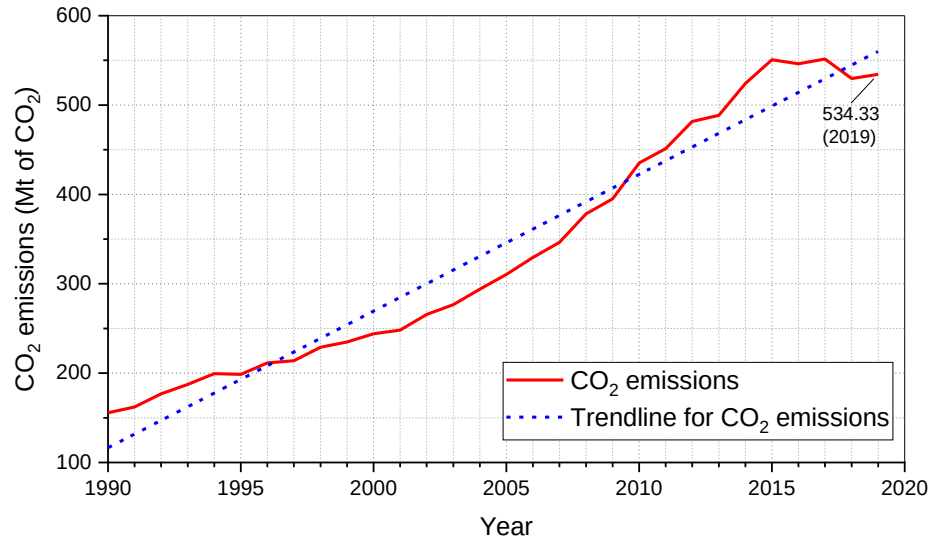


Figure 1.2: Annual CO₂ emission from fossil fuel combustion in KSA from 1990 to 2019 [4].

Carbon emission into the environment can be regulated in several ways, like improving the industrial plant efficiency, minimizing the consumption of fuel, and/or reducing the carbon content in the fuel [5]. Incorporating the carbon capture and storage (CCS) technologies can result in significant reduction in CO₂ emissions. The process of the different CCS technologies consists mainly of three steps, namely capturing, transporting, and storing the CO₂ securely. The first step includes capturing, purifying, and compressing the CO₂ for the next step, transportation [6,7]. Carbon dioxide can be transported using pipelines, road tankers, and/or ships. Lastly, the transported CO₂ can be stored safely in geographical rock deep beneath the surface of the earth, in depleted oil fields for enhanced oil recovery processes, or in deep saline aquifers. Capturing the CO₂ can be done by three methods, pre-, post- and oxy-fuel combustion [8–11]. In the pre-combustion technique, CO₂ is partly captured by converting the fuel into syngas before going into the combustion zone. The post-combustion technique captures CO₂ from the exhaust gas after the combustion

process, through absorption, adsorption, membrane separation, or cryogenic processes [12–15]. The use of air as oxidizer (air-combustion) is, however, not beneficial from a carbon-capture perspective, as unreacted nitrogen from air forms the primary constituent of GT exhaust, which reduces the CO₂ concentration in it, thus complicating the CO₂ separation process and increasing the associated costs of carbon capture. Burning fuel with CO₂-diluted oxygen (instead of air) is termed oxy-combustion. The products of this oxidizer-flexible combustion process are mainly CO₂ and H₂O (vapor) [16], so once the latter is condensed out, the former can readily be captured at the lowest cost.

Over the past five decades, GT manufacturers switched from traditional non-premixed air-combustion to lean premixed (LPM) air-combustion technologies to reduce NO_x (NO + NO₂) emissions. Different companies have developed novel versatile GT combustors for clean and efficient energy generation, including dry low NO_x (DLN) burners, environmental vortex (EV) burners, perforated-plate burners, and recently micromixer (MM) burners. In recent years, several review works have been performed compiling the advances in combustion technologies. Among those, the outlines of the review works related to oxy-combustion are summarized in **Table 1.1**, where the focused areas and main findings are highlighted.

Table 1.1: Overview of recent review studies on oxy-combustion in gas turbines.

Researcher(s) & year	Reviewed areas	Key findings
Nemitallah et al. (2018) [17]	Feasibility of different combustion method in gas turbines	• Environmental vortex (EV) burners can deliver lowest NOx emission with wider flammability limit • Higher cost and energy requirement for oxygen-separation in oxy-fuel combustion is one of the main drawbacks of oxy-combustion
Portillo et al. (2019) [18]	Membrane technology for oxygen separation in oxy-combustion system	• Zero-emission oxy-combustion power system can achieve 0.5-9% and 10.5-17.5% more energy and cost saving than traditional gas turbine combustion

		• The higher oxygen production cost with the cryogenic air separation units (ASU) can be reduced by adopting oxygen-selective membrane technology
Nemitallah et al. (2019) [19]	- Gas turbine combustion techniques - Burner designs for gas turbines	• Premixed oxy-fuel combustion can provide better control over emission and flame stability that the lean premixed (LPM) combustion • H₂-enrichment in combustion zone improves combustion efficiency and provides better fuel economy • Advanced Environmental vortex (AEV) burner has overall widest flame stability while the multi-

		hole burner has demonstrated improved stability near blowout limits.
Khallaghi et al. (2020) [20]	- Production of oxygen, recirculation of exhaust gas and effect of operating pressure in GT oxy-fuel combustion systems - Economics of oxy-combustion with gaseous fuels	• Oxy-combustion cycle (Allam cycle) can achieve around 50% more net efficiency than conventional gas turbine cycle. • Membrane separation can be a viable alternative for O₂ production than ASUs • Lower exhaust gas recirculation ratio results require smaller combustion chamber • Adopting staged combustion can eliminate the requirement for exhaust gas recirculation

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- Higher operating pressure can improve cycle performance with a drawback of higher pressure drop.
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Based on the above discussion and the information in the available literature, this this work aims to investigate and compare the oxy-fuel flames in swirl-stabilized burner. Oxy-fuel flames are further examined in multi-hole type model gas turbine combustor, where a comparison have been presented between the multi-hole and swirl-stabilized burners as well. The oxy-fuel flames have been examined in different mixture compositions ($\phi=0.241-0.597$ and $OF=32.4-60\%$) at a fixed bulk inlet velocity of 5.2 m/s under atmospheric condition. Three-dimensional (3D) numerical simulation has been performed employing both large eddy simulation (LES) and Reynolds-averaged Navier-stokes (RANS) scheme for swirl-stabilized and multi-hole combustor, respectively. The numerical results are supported and validated against some initial experimental findings. This thesis aims to enrich the literature on oxy-fuel combustion studies for gas-turbine applications by presenting emission and combustion characteristics in two separate model gas turbine combustors.

1.2 Research objectives

In order to develop a low-emission fuel-flexible combustion system for gas turbines, three different gaseous fuels (methane, propane, and syngas) are examined in swirl-stabilized combustor. Furthermore, the characteristics of oxy-propane flames are also inspected in a multi hole combustor and compared with those of the swirl-stabilized burner. In summary, the main objectives of the thesis are listed as follows.

- To examine combustion and emission characteristics of premixed oxy-propane flames in a swirl-stabilized gas turbine combustor under atmospheric pressure.
- To examine combustion and emission characteristics of swirl-stabilized premixed oxy-methane flames in gas turbine combustor under atmospheric pressure.
- To compare flame characteristics of propane, methane, and syngas in a fuel/oxidizer-flex swirl-stabilized burner under oxy-combustion conditions.
- To study combustion and stability behaviors of oxy-propane flames in a multi-hole burner and to make a comparison between multi-hole and swirl-stabilized burner.

1.3 Research methodology

The procedure to carry out this thesis work is highlighted in this section.

- A three-dimensional (3-D) large eddy simulation (LES) model is developed based on a lab-scale swirl-stabilized gas turbine to study oxy-fuel flames.
- Developed models are validated against the available experimental data recorded on the same combustor under the same operating conditions to mark the similarity between numerical and experimental results.
- Another 3-D computational fluid dynamics (CFD) model is prepared using the Reynolds-Averaged Navier-Stokes turbulence model to investigate the oxy-fuel flames in multi-hole gas turbine combustor.
- The oxy-combustion flames in different fuels and different combustors are examined in terms of their temperature, velocity, vorticity, Damköhler number, flame thickness, progress variables, product formation rate and CO emissions.

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CHAPTER 2

LITERATURE REVIEW

2.1 Lean premixed (LPM) air-combustion

NO_x emissions are a major concern in combustion applications like GTs. Two primary mechanisms are responsible for NO_x formation during combustion, namely the thermal (Zeldovich) and the prompt (Fennimore) mechanism. In the Zeldovich mechanism, the formation of NO_x is highly temperature dependent, hence the name thermal NO_x, see **Figure 2.1**. In the prompt mechanism, NO_x forms through the reaction of CH radical with N₂ under fuel-rich conditions [21,22]. In the early 1970's, the water-injection technique was introduced to control the formation of NO_x. This water was injected into the combustor to reduce the flame temperature, thus alleviating the thermal NO_x emissions. Later, due to the impact of water injection on system performance, higher CO emission, and higher water/steam requirements, the dry emission control method was introduced, namely LPM combustion [23,24].

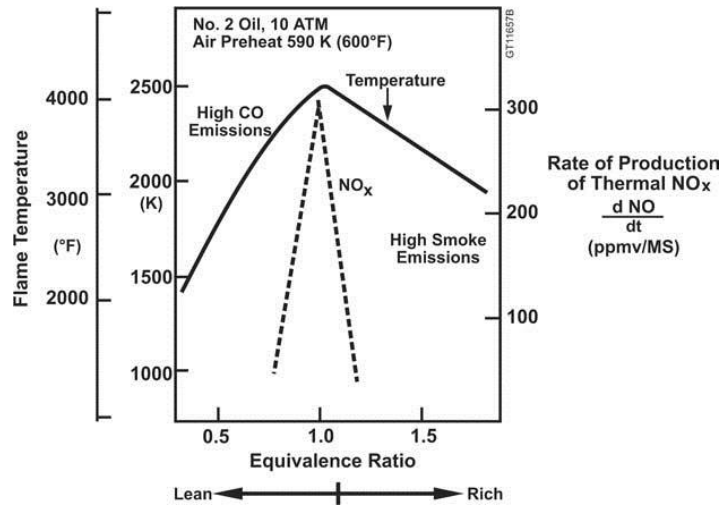


Figure 2.1: Thermal NO_x production rate as function of flame temperature and equivalent ratio [25].

2.1.1 Combustion and emission characteristics of LPM systems

LPM combustors in GTs split the incoming compressed air significantly differently compared to their non-premixed predecessors, see **Figure 2.2**. The latter have a stoichiometric-rich primary flame zone that requires a small portion of the compressor air; the larger portion is thus used as secondary air for liner cooling, combustion completion, and downstream dilution. Non-premixed flames have stoichiometric spots, where the local temperature can be high enough to pave the way for excessive NO_x formation [26,27]. By comparison, LPM combustors feed a greater portion of the compressor air into the flame to make it lean (and thus colder, see **Figure 2.3**), leaving a smaller portion of air for liner cooling. The lower temperature of LPM flame reduces the generation of thermal NO_x [28,29]. However, the lower flame temperatures can also lead to incomplete combustion, resulting in unburned hydrocarbons and CO in the exhaust stream. This tradeoff between

CO and NO_x, shown in Figure 3 above, should be considered while designing a LPM GT combustor and maintained during its operation [26,30]. A comparison between non-premixed and LPM flames is given in **Table 2.1**.

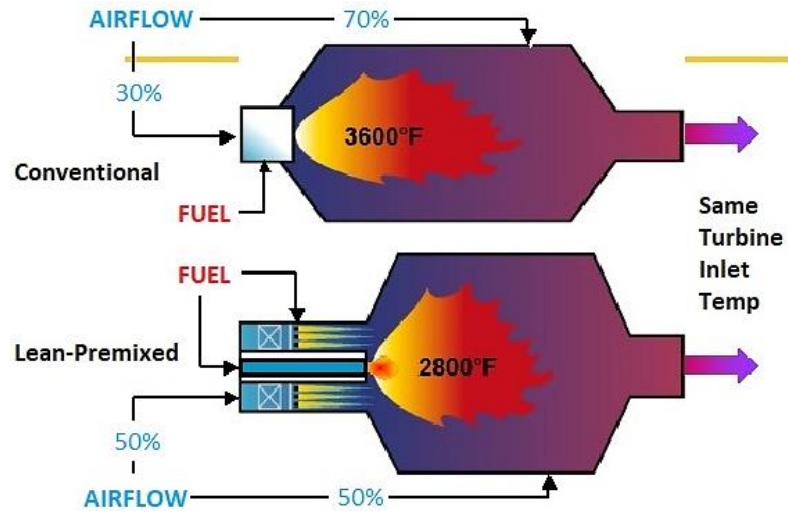


Figure 2.2: Non-premixed vs. lean premixed combustion systems [31].

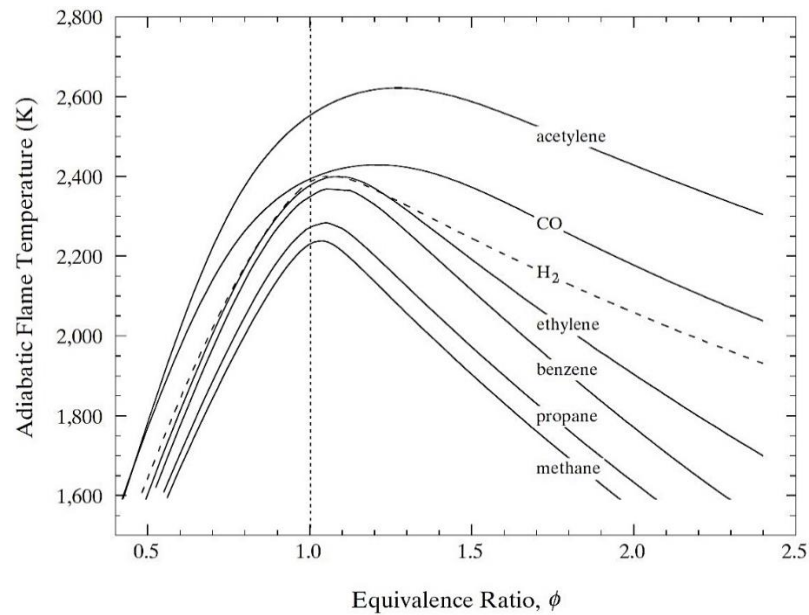


Figure 2.3: Adiabatic flame temperature vs. equivalence ratio for some air-fuel mixtures at standard inlet temperature and pressure [32].

Table 2.1: Difference between non-premixed and lean premixed flames.

Flame Type	Attributes	Advantages	Disadvantages
Non-Premixed	Fuel and oxidizer supplied separately into the combustion zone	• Broader stability limits • Higher turndown ratio*	• Excessive NOx emissions
Lean Premixed	Fuel and oxidizer are premixed before entering the combustor. Equivalence ratio is kept lean.	• Significantly lower NOx emissions	• Narrower stability limits (between blowout and flashback limit) • Lower turndown ratio*

*Turndown ratio refers to the operation range of the burner, which is the ratio between maximum and minimum loads of the burner.

2.1.2 Flame instabilities in LPM combustion

Despite lower NOx emission attributes, LPM flames are prone to combustion instabilities [33,34], in terms of dynamic (acoustic) instabilities as well as static instabilities (flashback and LBO). The positive feedback between the acoustic and heat-release pressure fields within the combustor can result in excessive pressure fluctuations at certain resonant frequencies. Such combustion instabilities can adversely affect the engine operation and eventually lead to hardware failure.

LPM GTs operate at temperatures near the LBO limit. Hence, at low loads and during load transition, a fuel-rich pilot flame is introduced to stabilize the primary LPM one and prevent its blow-off [26]. This is because LPM flames are affected by improper anchoring at fuel-lean condition that can lead to flame blow-off which is known as lean flammability [35,36]. Alternatively, if the velocity of the incoming combustible mixture is lower than the burning velocity of the flame, flashback occurs into the premix ducts [37,38], which is another form of static instability. Reduction of air velocity, due to compressor surge, can thus be a reason for flashback. Premature auto-ignition is another form of flashback. The flow residence time within the premixing region needs to be less than the ignition delay time of the developed combustible mixture, in order to avoid premature auto-ignition inside the premixing region itself [39].

In general, combustion instabilities are considered the greatest challenge of LPM combustors [40,41], and they have been investigated in numerous past studies. Yoon et al. [42] investigated combustion instabilities in a model LPM GT combustor at different inlet mixture velocities. They attributed the onset of unstable flame at lower inlet velocities to both structure and frequency of fluid dynamical vortex. The influence of Reynolds number (range: 3000-35000) on the turbulent flame speed has been examined by Bollinger and Williams [43], who showed that the turbulent flame speed in the burner tube is a function of Reynolds number. Liu et al. [44] examined higher combustor pressures and determined the turbulent burning velocity at different constant Reynolds numbers (range: 6700-14200). They observed that as the pressure increases, the turbulent burning velocity decreases in a negative exponential manner.

2.2 Existing burner technologies in LPM gas turbines

There are various methods for the reduction of NO_x emissions. One of the preliminary methods was the wet low NO_x technique [45]. By injecting water or steam into the combustor, the flame temperature can be reduced, and NO_x emissions can be controlled. At the same time, the power output of the turbine can be improved as well, because of the increased flow rate. This additional water/steam needed to be demineralized first, before being used in the combustion zone; demineralizing the water was not feasible or suitable for many combustion applications. To overcome this issue, the Original Equipment Manufacturers (OEMs) developed the dry LPM combustion concept that requires no steam or water for NO_x abatement. This section surveys the different existing burner technologies developed to operate according to the dry LPM combustion concept.

2.2.1 Dry Low NO_x (DLN) burners

Dry Low NO_x (DLN) LPM GT combustion systems, aka Dry Low Emissions (DLE), have been developed by the OEMs to lower the flame temperature and limit the formation of NO_x through lean operation. **Figure 2.4** shows a two-staged premixed DLN combustor. NG is the primary fuel, yet this combustor can operate well with liquid fuel as well. With NG as fuel, NO_x emission can be reduced down to 15-25 ppmvd (parts per million by volume, dry) using these commercially available systems [26]. DLN systems operate on the principle of LPM combustion, i.e., premixing the fuel and oxidizer before going into the combustor, thus preventing the creation of high-temperature stoichiometric zones and the consequent formation of thermal NO_x. This leads to much lower flame temperatures even at full load [46]. However, the control of CO emissions can be difficult and the

potential for flame blowout increases. DLN systems have primary (premixed) and secondary (non-premixed) fuel circuits. About 3% only of the fuel is injected in the non-premixed mode to produce a pilot flame. The primary circuit takes the remaining 97% of the fuel, which is premixed upstream with air and fed into the swirler [47]. The first generation of DLN systems (DLN-1) ran in four different modes, as illustrated in **Figure 2.5**, namely: (i) primary mode, (ii) lean-lean mode, (iii) secondary mode, and (iv) premix mode.[26] Description of these four modes is listed in **Table 2.2**.

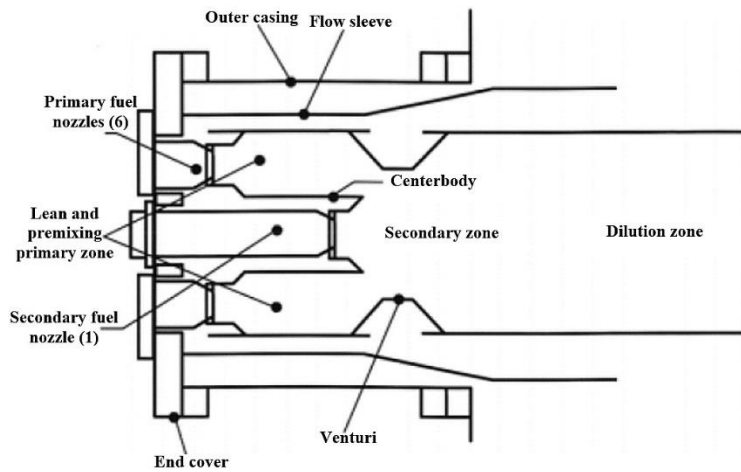


Figure 2.4: Schematic of DLN burner [48].

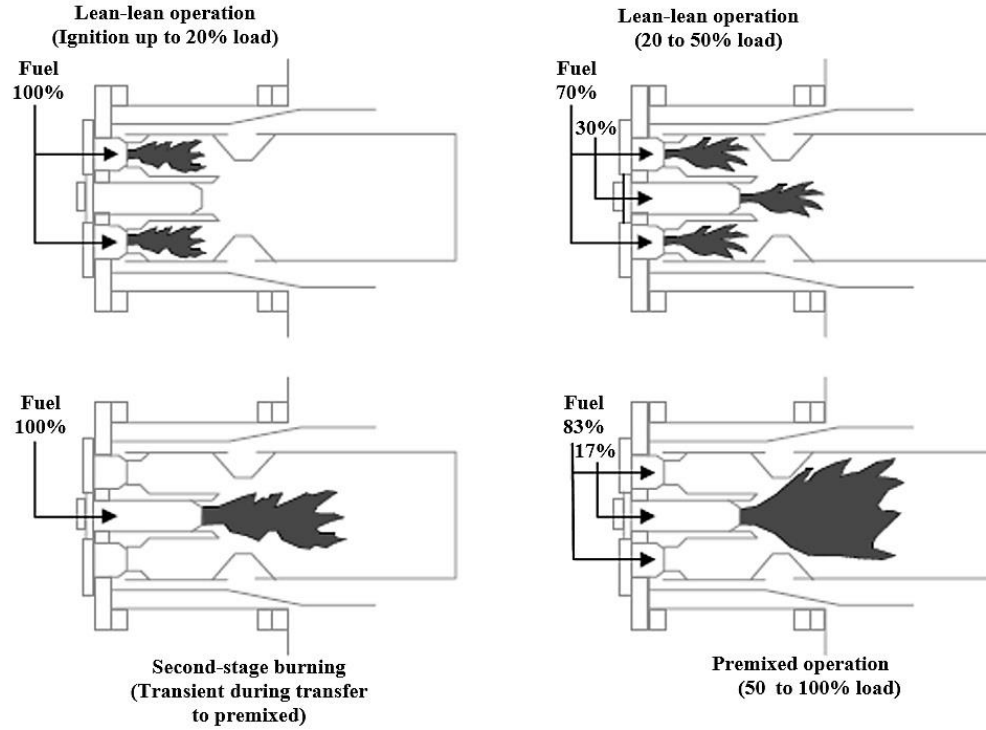


Figure 2.5: Different operating modes of DLN-1 combustor [48].

Table 2.2: Features and applications of different modes of DLN-1 combustor.

Mode	Features	Applications
Primary mode	- All fuel is supplied through the primary nozzles only - Flame remains in the primary stage only	- Ignition up to 20% load - Acceleration and operation are limited to a predefined reference combustion temperature

Lean-Lean mode	- Fuel is injected through both primary and secondary nozzles - Flames produced in both the primary and secondary stages	- To operate in transitional loads (20 – 50% load)
Secondary mode	- All fuel is supplied through the secondary nozzle only - Flame in the secondary stage	- For transition from Lean-Lean mode to Premix mode - For extinguishing the primary-zone flame prior to resupplying the fuel - To create a primary premixing zone
Premix mode	- Fuel is injected through both primary and secondary nozzles - Flame is contained only in the secondary stage	- To operate at medium to full loads (50 to 100% load) - Ensures minimum emissions in the premixed mode

In the second generation of DLN systems (DLN-2), the protruding centerbody and the venturi of the DLN-1 system have been removed from the combustor. This eliminated the need for cooling air for these two parts. DLN-2, as per **Figure 2.6**, refers to the dual-mode,

single-staged combustion system with five fuel nozzles. In addition to gaseous fuels, DLN-2 can operate on liquid fuels as well. When using gaseous fuel, the combustor runs in the non-premixed mode for loads less than 50%, followed by the premixed mode for 50 – 100% loads. When running on liquid fuel, on the other hand, the combustor operates in the non-premixed mode at all loads. DLN-2.6 has been developed after that, with the addition of one more fuel nozzle at the center of the five fuel nozzles of the DLN-2 system. Unlike DLN-2, the DLN-2.6 system has no non-premixed mode and has additional strategies for loading and unloading [48]. Another DLN system has been introduced by General Electric, namely the H-system, also known as DLN-2.5. This system has three modes of operation, non-premixed mode, piloted premix mode, and full premix mode [49].

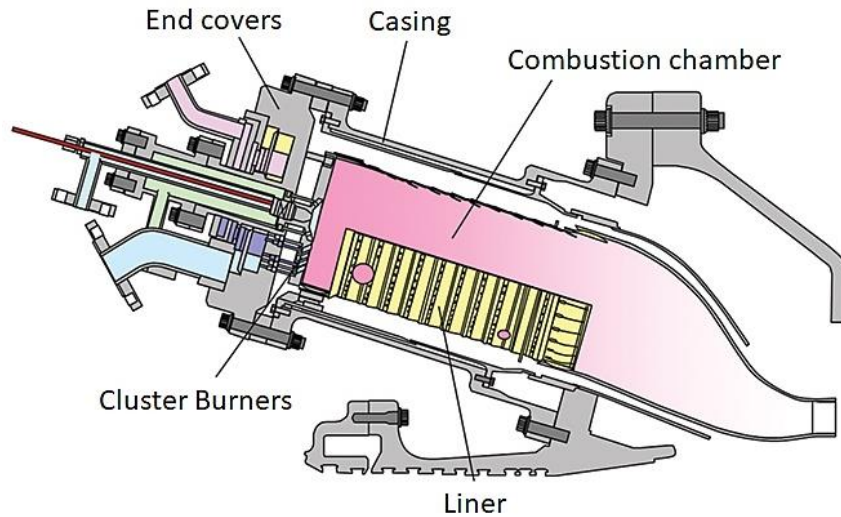


Figure 2.6: DLN-2 combustion system [50].

To achieve stable combustion in these systems during all operating conditions, the fuel and air splits must be precisely controlled. Fuel flexibility, ambient temperature, fuel

calorific/heating values, operating conditions, interaction of turbulent chemistry, and flow rates can considerably affect the combustion stability [51]. Non-premixed flames have a wider stability range; however, NO_x formation is significantly increased at greater splits of non-premixed fuel [52].

There are some issues with the DLN systems operation like combustion instabilities, flashback, and lean blow-off (LBO) [47]. These issues can result in engine shutdown and power losses. Precautionary measures should be taken to prevent the flame extinction in the lean premixed condition of the DLN burners [53]. Without these precautions, LBO can take place as the fuel-air mixture becomes leaner. To avoid this issue, a pilot flame is introduced, where a small quantity of fuel is injected in the non-premixed mode, while the remaining fuel is premixed and burned inside the combustor. If the velocity of the combustible mixture is lower than the local flame speed, flashback occurs into the premix ducts [54]. Reduction of air velocity, due to compressor surge, can also be a reason for flashback. Fast-response fuel control valves should be installed in the combustor to reduce the effect of flashback. Premature auto-ignition is another form of flashback. The flow residence time within the premixing region needs to be less than the ignition delay time of the developed combustible mixture, in order to avoid premature auto-ignition inside the premixing region itself [39]. The challenge thus arises that fuel must be thoroughly premixed with air in a short residence time. Increasing the content of highly reactive fuel constituents (e.g. H₂), increasing the air temperature at combustor inlet, operating at higher equivalence ratios (higher flame temperatures), and/or miscalculating the residence time in the premixing region can all be reasons behind premature auto-ignition. This issue can

damage the premixer modules in DLN systems. In some cases, frequent switch-off of the engine is required because of this auto-ignition issue.

2.2.2 Enhanced Vortex (EV/SEV/AEV) burners

The limited freedom in DLN system operability (limited fuel flexibility and limited range of flame temperature) led to the development of the second generation of premixing burners, known as Enhanced Vortex or EnVironmental (EV) burners, as shown in **Figure 2.7**. This type of burners stabilizes the flame by creating a strong inner recirculation zone through vortex breakdown of an intense flow [55], rather than using swirlers or center bodies. The cross-sectional view of EV burner clearly shows the swirl flow configuration in the combustor. Flow is introduced from two inlets in a purely tangential direction, and the divergent nature of burner cross-section induces vortex breakdown as the flow becomes axial at the burner exit. Hence, flashback is avoided by accelerating the flow prior to the breakdown point and the formation of a strong inner circulation zone that stabilizes the generated flame. Moreover, because of the aerodynamic fixation of the vortex breakdown, the flame is anchored properly, eliminating the chances for blowout. All these are the key attributes of the EV burner flow configuration.

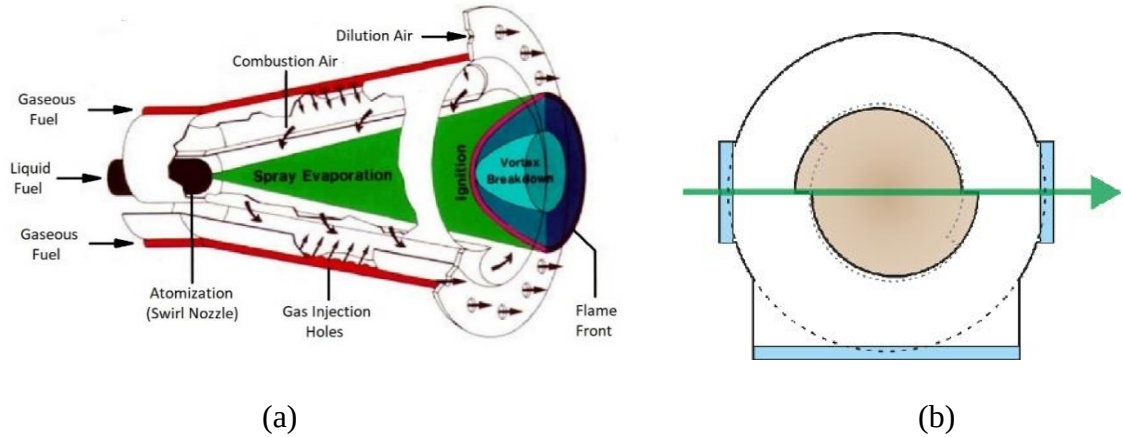


Figure 2.7: Schematic of EV Burner: (a) components[56] and (b) cross-sectional view [57].

Sequential EV (SEV) burners have been developed to improve the existing EV combustion systems further, yielding better efficiency. The principle of SEV systems is to burn the fuel sequentially over two stages, first in the annular combustion chamber using EV burners and then in the second chamber that hosts SEV burners [58], as illustrated in **Figure 2.8** [59]. In the first stage, fuel is burned to preheat the compressed air. The products of the first stage are then expanded in a high-pressure (HP) turbine, where the pressure drops by a factor of two. Then in the second combustor, in the presence of additional cooling air, the remaining fuel is burned, and the products of the combustion expand in a four-stage low-pressure turbine. Some variants also include the DLN and SEV technologies in a single unit, resulting in high power density of the GT [60]. In SEV systems, the compressor can deliver the compressed air at almost twice the pressure ratio of conventional GT compressors. In addition, the superior flame stability of the EV-burner technology, as

described above, enables the SEV burners to operate flashback-free despite the elevated temperature after the HP turbine [61].

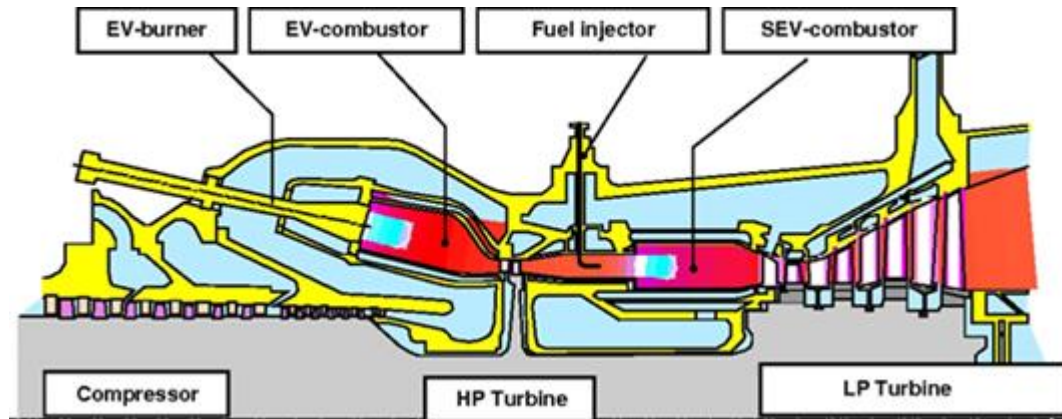


Figure 2.8: Gas-turbine system utilizing SEV burner [59].

The Advanced EV (AEV) burners, illustrated in **Figure 2.9**, are designed for use in combustion systems burning liquid fuels. A central lance hosts a nozzle for spraying the liquid fuel inside the burner cone. AEV burners incorporate four tangential inlet slots (instead of two like EV burners) to establish a strong tangential flow protecting the cone walls from the impingement of fuel droplets. The cone is affixed with a straight mixing tube to facilitate longer evaporation time along with better mixing of fuel and air in the gas phase. As the tangential inlet flow converts to axial inside the cone, the centerline velocity near cone exit becomes double the bulk velocity value. This high axial velocity is kept the same across the mixing tube, to prevent flame flashback. In addition, excess air is used to increase the local axial velocity close to the wall of mixing tube, in order to reduce the possibility of flame flashback there [45].

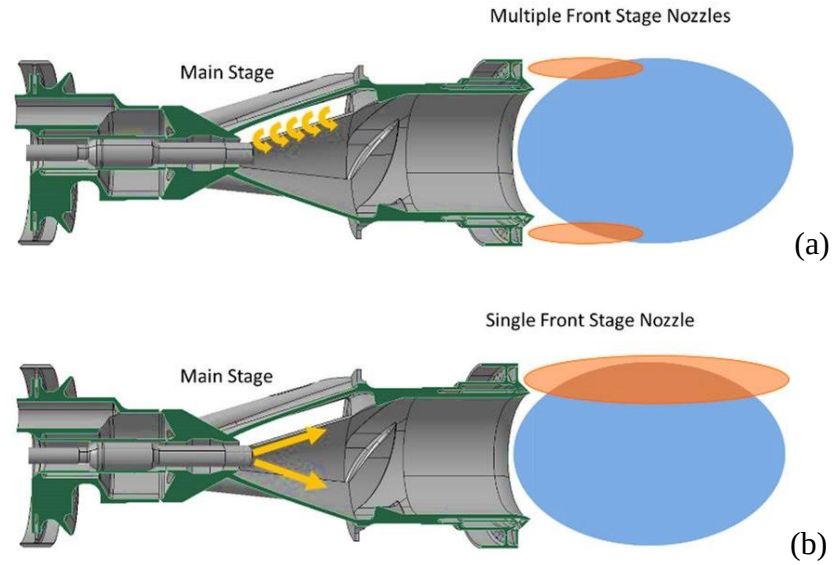


Figure 2.9: Advanced EV (AEV) burner cross-section with: (a) gaseous fuel and (b) liquid fuel [62].

2.2.3 Perforated-plate burners (PPB)

Perforated-plate burners (PPB) are widely used in households and industrial applications. As the name implies, a PPB comprises a plate with an array of holes that divide the incoming combustible mixture into multiple jets. Each jet burns in a small conical flame (sometimes also called ‘flamelet’), as shown in **Figure 2.10** [63], wherein combustor stability depends on diameter and spacing of the burner holes/jets, as well as on the heat transfer to the burner faceplate.

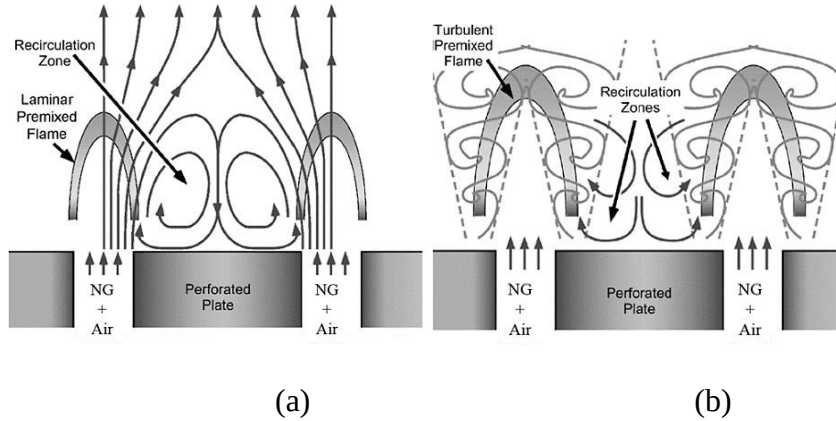


Figure 2.10: Flow fields in perforated-plate burner of: (a) laminar flames and (b) turbulent flames [63].

Using a matrix of PPBs with both propane and CH_4 flames, Rodrigues et al. [64] have observed that flame stability depends on hole spacing but independent of hole diameter. They have reported stable flames with smaller hole spacing. Veetil et al. [65] have investigated numerically syngas-air combustion on a PPB holding laminar flames. They have reported higher flame lift-off as well as strong recirculation for larger hole spacing. Considering laminar air combustion on a PPB, Jithin et al. [66] have discovered that the flame stand-off distance increases with larger hole spacing. Hindasageri et al. [67] have carried out experiments and numerical investigations of the distribution of heat flux from a multi-hole burner holding CH_4 -air flames, considering different hole arrangements at low Reynolds number (Re). They have concluded that the hole arrangement has an insignificant effect on heat flux distribution. Nonetheless, higher heat flux at a steady mass flowrate has been achieved with burners of greater hole pitch. However, the maximum pitch is restricted by the criterion of LBO stability. Kuntikana et al. [68] have examined the thermal characteristics of PPBs in terms of the distance between the burner and an opposing

impingement plate. They have used staggered and inline hole configurations for their burners. Higher thermal efficiency has been achieved with the increase of Reynolds number (Re) of the combustible mixture. With higher Re, the heat flux to the opposing plate distributes more evenly. At stoichiometric conditions, maximum heat transfer has been achieved because of the highest flame temperature. The heat flux has remained unchanged while the thermal efficiency has decreased under fuel-rich operation. Furthermore, the thermal efficiency in their study has reduced at greater distance between the burner and the opposing plate, because of the entrainment of ambient air. Lee and Hwang [69] have reported that temperature and thermal efficiency of a porous baffle plate burner have been found to increase with increasing the main hole diameter. Moghaddam et al. [70] have found that increasing the diameter of the main hole of a multi-hole burner makes the temperature higher, consequently increasing the combustor thermal efficiency. Kedia et al. [71] have examined numerically the reasons behind blowout and stability of LPM CH₄-air flames anchored on a conductive PPB. They have reported that blowout is influenced by both flame stretching and heat transfer to the plate. Timmermans et al. [72] have performed thermo-acoustic instability analysis on a PPB using particle image velocimetry and hot-wire anemometry. Their findings show that low-frequency instabilities occur in the transition regions between laminar and turbulent flow near the wake.

Habib et al. [5] have investigated experimentally and numerically the effect of CO₂ dilution on flame stability under oxy-fuel combustion conditions in a porous plate burner over ranges of equivalence ratio and oxidizer oxygen fraction. They have reported that the combustion temperature decreases with the increase of CO₂ dilution, while the fluctuations in the flame

increase. Flame stability has improved at high equivalence ratio, whereas the flame length has increased at lower equivalence ratio with the flame moving towards the combustor centerline. Rashwan et al. [73] have investigated the effect of the degree of reactant premixing on flammability limits. It is found that the zone of stable operation widens at lower degrees of premixing and becomes narrow at higher premixing ratio. The flammability limits of oxy-fuel flames are more restrictive compared to those of air-fuel flames, as presented in **Figure 2.11**. In a similar study, Rashwan et al. [74] have found that for partially premixed oxy-fuel flames stabilized over a PPB, the combustor can be operated only at oxygen fractions above 29% (by vol.) and that the oxygen fraction should be above 36% for stable combustion. Habib et al. [75] have investigated the LBO limit for non-premixed oxy-CH₄ combustion over a PPB. They have found that the LBO limit increases with the increase of equivalence ratio at fixed firing rate. The relevance of the PPB in the field of GTs has been studied thoroughly by Rodrigues et al. [76] They have observed excellent performance of this type of burners with gaseous fuel, in terms of emissions and combustion efficiency.

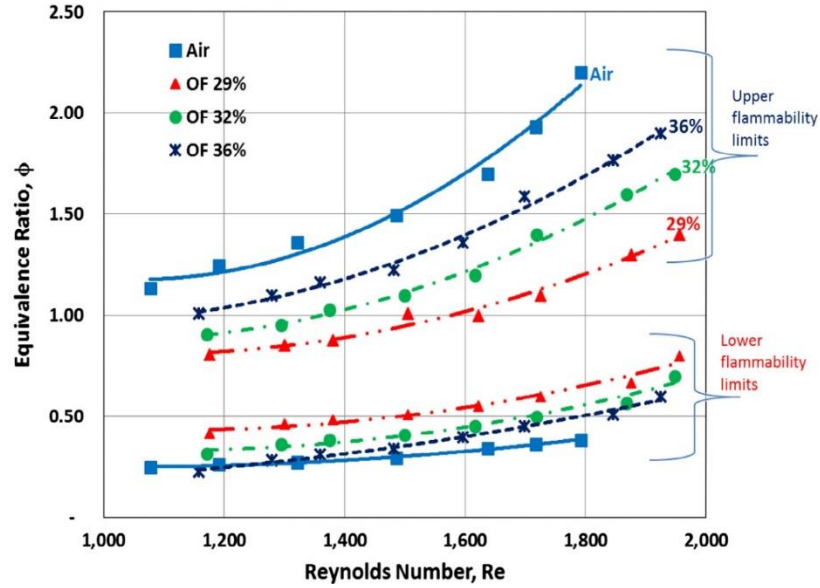


Figure 2.11: Flammability limits of air-fuel vs. oxy-fuel flames stabilized over a perforated-plate burner [73].

2.2.4 Micromixer (MM) burners

Micromixer (MM) burners are the type of burners where the fuel and oxidizer are mixed on a micro-scale. In a typical MM burner, a space or plenum is created by arranging multiple millimeter-scale straight tubes in between front and back faceplates, as illustrated schematically in **Figure 2.12**. The oxidizer is supplied through the straight tubes, and the plenum between the tubes contains gaseous fuel. Each tube has miniature holes through which fuel is injected into the oxidizer flow inside each tube in a jet-like cross flow configuration. These holes are positioned in such a way so that each tube functions as a fuel-oxidizer premixer and delivers a nearly premixed fully developed jet at the front faceplate. Besides, the position of fuel holes can also influence the length required for premixing. Moreover, the mixing length is usually expressed in terms of hole diameter,

where the ratio of hole diameter and mixing length ranges from 1 to 10 [77]. A uniform distribution of fuel through the micromixer holes is ensured by using flow conditioners/baffles inside the plenum. The number of premixed jets (i.e., number of straight tubes/inlet holes) and the spacing between these jets on the faceplate play an important role in defining the combustion and emissions characteristics. The equivalence ratio and oxidizer-flow pressure drop (Δp) within the MM should be selected precisely to prevent flame flashback into the tubes. MM burners can adapt well with scalability and staging and can tolerate fuel dilution [17]. One of the most significant, inherent features of these burners is their fuel flexibility. All these characteristics make MM burners more suitable to work under wider ranges of operating conditions.

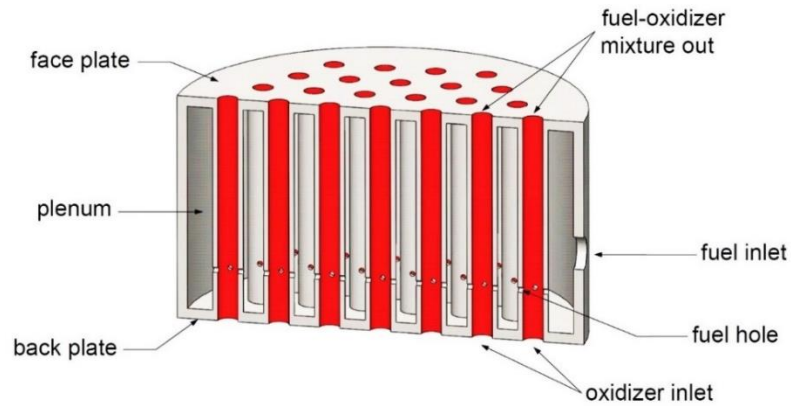


Figure 2.12: Schematic diagram of a micromixer burner.

The lean direct injection (LDI) approach is a precursor to MM burners. In LDI, fuel is injected into the oxidizer through numerous locations to obtain rapid mixing. MM burners thus incorporate the LDI technique but with a small premixing zone. Similar operability like LDI can be attained in MM burners with careful design. LDI has been used in H_2

combustion to eliminate the risks associated with flashback [78,79]. The utilized configurations incorporated: swirl-based mixing in small cups with radial and axial inflow [80], coflow mixing [81], and jet-like cross-flow mixing [82].

York et al. [77] have performed a durability test of a MM burner at firing conditions like those of General Electric's F-class GT at full load, and the test endured for almost 100 hours. Air-fuel combustion has been used with different fuel blends of NG, nitrogen, and H₂. In the study, they have achieved ultralow NO_x emission (single-digit ppm) with a H₂/nitrogen fuel blend containing more than 90% (by vol.) H₂. Funke et al. [83] have investigated the effect of momentum-flux ratio on flame anchoring and NO_x emissions in a MM burner. Using air-H₂ combustion, they have reported a strong correlation between the flamelet anchoring mechanism and the formation of NO_x. Dodo et al. [84] have tested the MM of an integrated gasification combined cycle (IGCC) using H₂-rich syngas-air combustion at medium pressure of 0.6 MPa. They have used fuels that contained CH₄, H₂, and nitrogen, with three carbon-capture rates (0%, 30%, and 50%). Stable combustion has been reported for all three rates, with single-digit NO_x emissions for each case.

A small auxiliary power unit (APU) GTCP36-300, implementing the MM principal, is presented in **Figure 2.13**. It consists of 1600 miniature injectors and takes around 1600 kW of H₂ firing to generate 335 kW of shaft power (21% efficiency) by producing pneumatic and electrical power. In the experiment, a MM burner has been integrated inside an annular reverse-flow combustion chamber [85,86]. Another study has showed that this MM combustor is capable of running on both H₂-rich syngas and pure H₂, while maintaining low NO_x emissions in both cases [87]. Funke et al. [88] have tested the GTCP36-300 APU with an injector diameter of 0.84 mm. They have experimented with H₂ fuel and have

compared their results with the findings from the 0.3 mm baseline case of Ref. [85,86]. Approximately 390% increase in power output in each nozzle has been reported with the use of 0.84 mm nozzles. NO_x emissions are less than 4.0 ppm under all operating conditions, as shown in **Figure 2.14**.

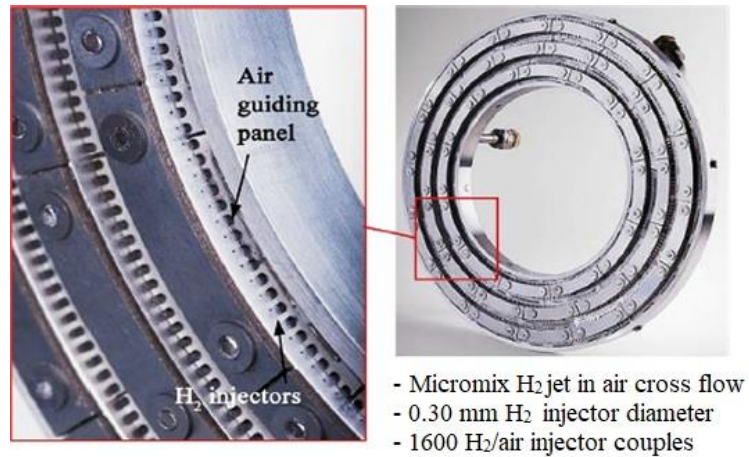


Figure 2.13: Micromixer combustor for the GTCP36-300 APU [86].

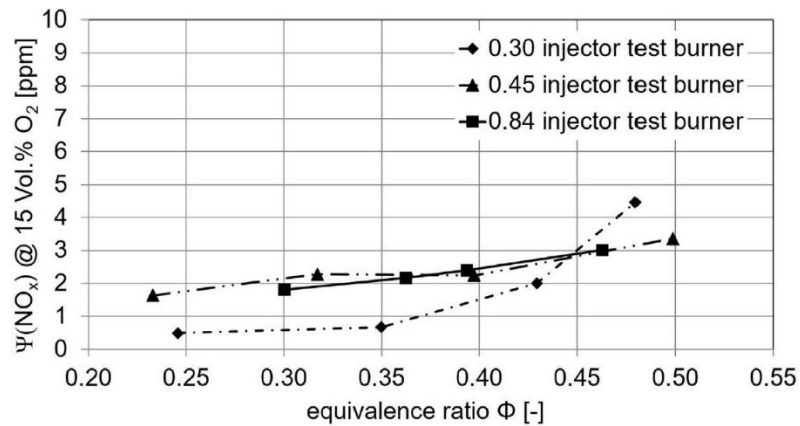


Figure 2.14: NO_x emission at different loads using injectors of different diameters in the GTCP36-300 APU [88].

Ayed et al. [89] have investigated a low-energy-density burner configuration to observe the effects of burner design and combustion modelling on flame structure, flow field, and temperature distribution, where the diameter of the burner fuel injector is 0.3 mm. They observed the potential of reducing NO_x emissions for a specific geometric parameter through regulating the cooling air flow around the flame [90]. Their findings have been implemented in designing a high-energy-density burner with 1.0 mm injector diameter. This resulted in rise of the heat rate by more than 11 times per injector. Funke et al. [91] have studied a similar burner numerically and experimentally and have reported lower NO_x emissions at the higher energy density. MM burners are continuously being developed, in terms of NO_x formation, flame structure, and geometric parameters. Badra et al. [92] have proposed a combustor design based on the MM concept but for non-premixed flames, which can preheat the fuel and oxidizer using the heat from the combustion products. Aliyu et al. [93] have performed one of the first studies of oxy-fuel combustion using a MM-like burner. They have reported that the main parameter controlling flame stability and structure is the adiabatic flame temperature (T_{ad}), as observed in **Figure 2.15**. The flame shape has been found to remain unchanged while operating at constant T_{ad} . **Table 2.3** summarizes the different GT burner technologies discussed in this section.

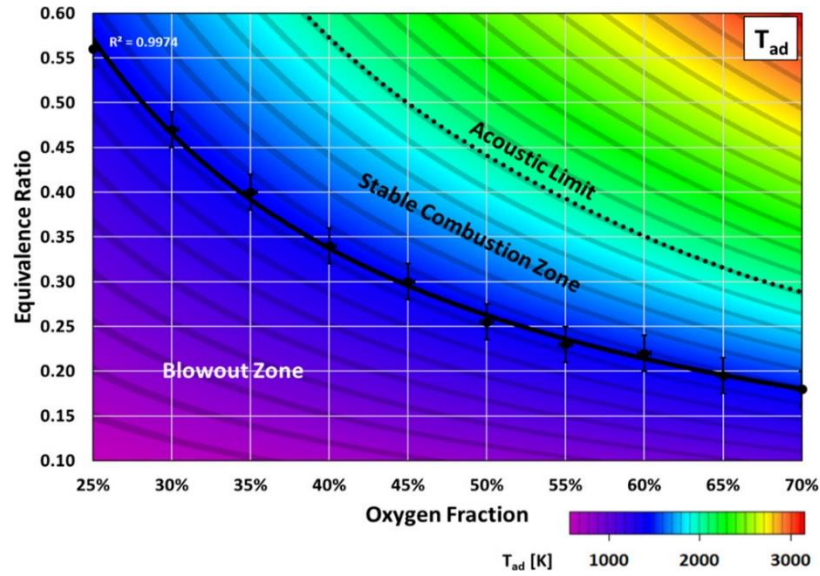


Figure 2.15: Stability map of a MM-like oxy-fuel combustor operating at fixed jet velocity, plotted against the contours of constant adiabatic flame temperature [93].

Table 2.3: Comparison of different burner technologies for gas-turbine combustion applications [19].

Burner type	Characteristics	Advantages	Disadvantages
Dry Low NOx (DLN)	First implementation of LPM combustion	Low CO and NOx emissions; advanced DLN burners can achieve NOx emissions < 10 ppm as well	Extended premix tube required for producing air-fuel mixture upstream of burner, i.e., less compact

		• Swirler/centerbody needs to be used for flame stability • Sensitive to premature auto-ignition and flashback • Flame instabilities at low loads • Non-premixed pilot flame is needed in different stages (high NO_x)	
Enhanced Vortex (EV, SEV, AEV)	Flame stabilization by vortex breakdown	• Lower NO_x emissions • No centerbody/swirler is required for flame stabilization • Less flashback due to accelerated core flow • Non-premixed pilot flame is not required	• Turbulent burning rate variations • Unsteady fluctuation in flame surface and anchor point

		• Dual-fuel (gaseous/liquid) capability (AEV only) • Good performance predicted under oxy-fuel combustion conditions	
Perforated plate (PPB)	Fuel/oxidizer mixture supplied through small holes into the combustor	• Design simplicity • Used in both industrial and household applications • Flame symmetry	• Vulnerable to different combustion instabilities (e.g., flame quenching, blow-off, and flashback)
Micromixer (MM)	Fuel and oxidizer are premixed inside numerous small tubes then supplied to the combustion zone	• NO_x emission can be less than 10 ppm • Can tolerate variations in fuel composition, i.e., superior fuel flexibility • Scalability and staging flexibility	• Equivalence ratios and ΔPs across the burner should be considered carefully to prevent flashback • Dynamic combustion instabilities near

• Good performance	stoichiometric
predicted under oxy-	condition
fuel combustion	• Development ongoing
conditions	for use in GTs

2.3 Oxidizer-flexible combustion

Most of current combustion systems uses air as oxidizer, which has a fixed composition of about 79% N₂ and 21% O₂ by volume. Some systems use O₂-enriched air for improved flame characteristics, higher heat-transfer efficiency, higher processing rates, and enhanced product quality. O₂-enrichment also facilitates additional flexibility or an extra degree of freedom in the combustion system, namely the ability to vary and control the oxygen fraction beyond the fixed 21% of air. Oxy-fuel combustion is another example of oxidizer-flexible combustion, where the oxidizer is CO₂-diluted oxygen, as will be discussed next.

2.3.1 Oxy-fuel combustion technology

Unlike the pre- and post-combustion options of carbon capture, oxy-fuel combustion utilizes oxygen as oxidizer, rather than air, to generate an exhaust stream that consists primarily of CO₂ and H₂O, in order to facilitate cost-effective carbon capture by simple H₂O condensation [47]. The diagrams in **Figure 2.16** illustrate simple oxy-combustion systems. Using pure oxygen, however, produces extreme flame temperatures [94,95]. Recirculation of CO₂ from the exhaust stream to dilute the fuel-oxidizer mixture is a way of controlling the combustor temperature in oxy-fuel combustion [96], as illustrated in

Figure 18. Replacing N_2 with CO_2 as diluent, however, results in high CO_2 concentrations in the flame, and CO_2 is far less inert than N_2 , i.e., CO_2 has a significant effect on the reaction mechanism and kinetics. The emission of CO increases at higher CO_2 concentrations in the O_2/CO_2 oxidizer mixture [97], see **Figure 2.17**. Nonetheless, in the absence of air-based nitrogen, oxy-fuel combustion is almost NO_x -free [98,99], provided that fuels with low nitrogen content are used [100–102]. Thus, if measures/precautions are taken to prevent CO emissions, oxy-fuel combustion with carbon capture becomes a truly zero-emission technology [103,104].

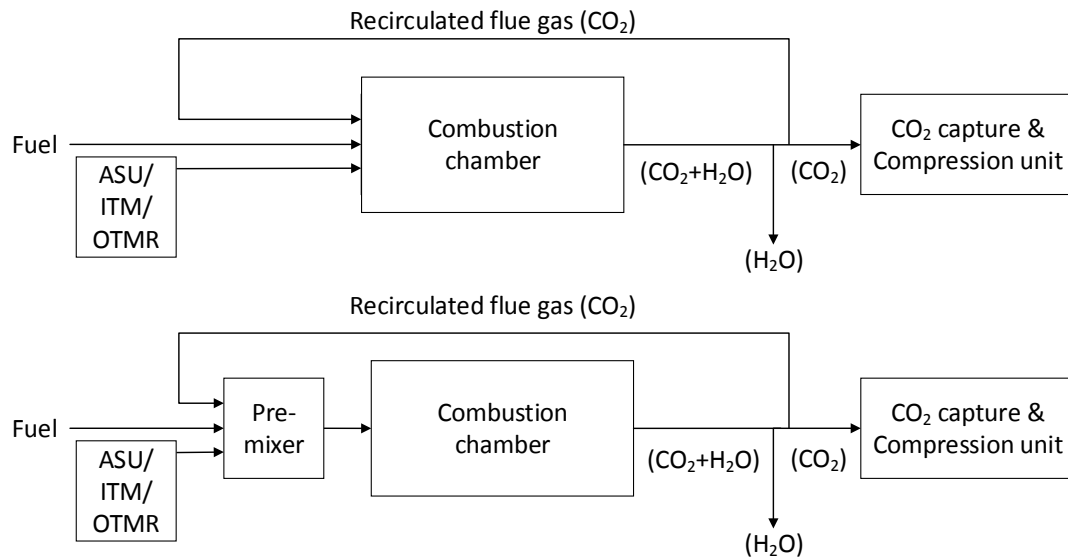


Figure 2.16: Schematics of non-premixed (top) and premixed (bottom) oxy-combustion systems.

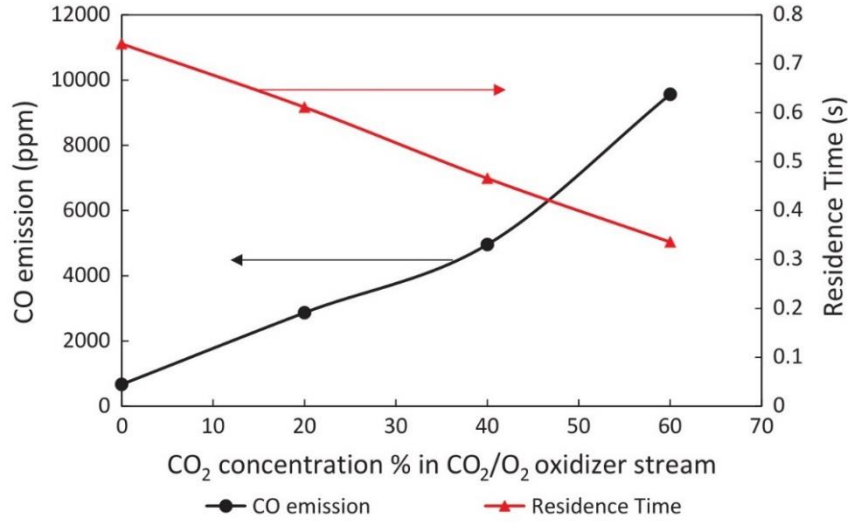


Figure 2.17: Effect of CO₂ concentration in O₂/CO₂ oxidizer on CO emission and residence time [97].

2.3.2 Oxy-combustion in model combustion systems

In addition to reduced emissions in conventional systems, like boilers and GTs, oxy-fuel combustion can decrease the fuel consumption rate as well. In studies on industrial water-tube boilers using oxy-CH₄ combustion, the rates of fuel and oxygen consumption have been found to be lower than those of air-fuel combustion [9,97]. The stability of a non-premixed oxy-CH₄ flame inside a model GT combustor has been investigated by Habib et al. [105]. They reported a minimum oxygen fraction of 21% for stable operation. Unstable flames were observed in their study below 21% OF. Furthermore, T_{ad} has been presented as the main parameter controlling the stability and structure of premixed oxy-CH₄ flames [106]. This has been even found to apply to both oxy-CH₄ (CH₄/O₂/CO₂) and oxygen-enriched air-CH₄ (CH₄/O₂/N₂) flames in a premixed swirl-stabilized model GT combustor,

regardless of oxygen fraction and equivalence ratio [107]. Jourdain et al. [108] have experimented the stability of premixed oxy-CH₄ flames and have compared it with that of air-CH₄ flames under fixed swirl, laminar flow velocity, bulk flow velocity, and adiabatic flame temperature. Similar flame shapes have been observed again for both types of flames. However, the range of operability of oxy-flames has been found smaller than that of air-flames.

The stabilities of partially premixed oxy-CH₄ and air-CH₄ swirl flames have been compared experimentally by Kutne et al. [109] in a model GT combustor. They have found that the oxygen fraction has a substantial influence on flame shape and stability, compared to the equivalence ratio. Oxy-fuel flames showed wider stability at greater oxygen fractions. A similar study [110], targeting the effects of equivalence ratio (ϕ) and adiabatic flame temperature, has showed that at $\phi=0.6$, the air-CH₄ flame disappears from the outer shear layer (OSL), but the oxy-CH₄ flame does not. The dotted regions in **Figure 2.18** show that the air-flame stabilizes in the inner shear layer only, but the oxy-flame persists in both the inner and outer shear layers. The extinction strain rate (resistance to extinction) at $\phi=0.6$ has been found to be higher in the oxy-flame than in the air-flame due to the different transport properties of CO₂ and N₂. This higher extinction strain rate ensures the stability of oxy-flame in the OSL, whereas the air-flame extinguished in the OSL. This behavior of oxy-flames remains similar up to $\phi=0.64$, and any further increase in ϕ beyond that point decreases the extinction strain rate in the oxy-flame and increases it in the air-flame [110].

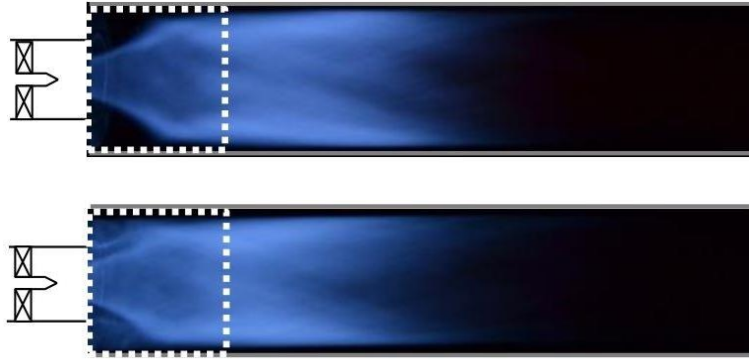


Figure 2.18: Comparison of mean flow configuration in a swirl-stabilized combustor at $\phi=0.6$ for air-CH₄ flame (top) and oxy-CH₄ flame (bottom) [110].

2.3.3 Comparison between air- and oxy-combustion

Air-combustion systems use air as oxidizer, which has a fixed chemical composition (21% O₂ and 79% N₂ by volume). O₂ is the actual oxidizer, while N₂ is mostly a diluent. The inability to change the ratio of N₂ to O₂, coupled with the fact that air is an abundant low-cost resource, makes the control of flame temperature possible only through lean operation, i.e., adding excess air. The associated excess oxygen helps with CO burnout, if the combustion system is operating safely away from its LBO limit. The equivalence ratio is thus the main control knob in air-combustion systems.

The outlook is, however, significantly different in oxy-combustion systems, which use nitrogen-free oxygen as oxidizer. This oxygen is extracted from air in dedicated air-separation units (ASUs), which consume power, thus posing an energy/efficiency penalty in power-generation applications [111]. Unlike air, the extracted oxygen is thus a precious commodity that must be used wisely. Consequently, oxy-combustion systems do not have

the luxury of running lean; they should be operated close to stoichiometry. Thus, fuel must burn in the limited quantity of oxygen available, which is one of the reasons behind the high CO emissions depicted in Figure 8. To control the temperature of oxy-fuel flame, a large portion of the effluent CO₂ is recirculated back into the combustor to dilute the flame, which is termed flue gas recirculation (FGR) or alternatively known as exhaust gas recirculation (EGR) [112]. The oxygen fraction in O₂/CO₂ oxidizer is thus the main control knob in oxy-combustion systems. Note that FGR is compulsory in oxy-combustion systems but optional in air-combustion ones. In conclusion, the combustor designs and operability space/conditions are substantially different between air- and oxy-combustion [19].

In terms of emissions, air-combustion systems generate primarily NO_x and CO emissions, in addition to CO₂, even if pre- or post-combustion carbon capture is implemented, because these processes are less efficient than carbon capture in oxy-combustion systems [113]. Since oxy-combustion is mostly NO_x-free, the primary emission becomes CO only. Furthermore, the absence of nitrogen in the exhaust, in addition to FGR, reduces the exhaust flow rate and, consequently, the size of exhaust-treatment equipment. Significant heat can also be recovered from the exhaust gases through FGR and H₂O condensation [114]. In terms of capital cost, however, oxy-combustion systems require additional units not found typically in conventional air-combustion systems, such as ASU, FGR system, and CO₂ purification unit (CPU) [47], where effluent CO₂ is compressed and purified prior to utilization or storage.

From a combustion perspective, there are also some challenges in the pathway of successful adoption of the oxy-combustion technology. The greater CO₂ concentration

within the combustor (~70% by mass) reduces the chemical kinetics rates, which, in turn, reduces the laminar burning velocity [9,115] as well as the combustion efficiency [19,116], compared to air-combustion. The CO₂-rich oxy-fuel premixed reactant mixture requires more oxygen (above 21%) than the corresponding air-combustion system operating at the same equivalence ratio, in order to get stable flame [117,118]. In a comparative numerical study of a porous combustor, it has been reported that oxy-combustion with oxygen fraction of 30% by volume can yield adiabatic flame temperature similar to that of air-combustion under identical operating conditions [119]. Furthermore, CO₂ is denser than N₂, so CO₂ dilution affects the jet velocity, gas density, and pressure drop [73,120,121]. The heat capacity of CO₂ is also higher than that of N₂. This affects the flame stability by reducing the flame temperature and burning velocity [96,122]. The latter can be influenced by gas transport properties as well [123]. As compared to the air-combustion system, the soot formation has been found lower with the oxy-fuel combustion [124] where the reduction in soot formation can be achieved with the increase in CO₂ percentage in the reactor [125].

The ratio of velocities between fuel and oxidizer, which is known as the critical velocity ratio, has been found to be six times greater in oxy-combustion, compared with air-combustion, using propane as fuel in a swirl-stabilized combustor [123]. Due to this higher critical velocity ratio, the oxy-propane flame goes from ‘attached flame’ to ‘no flame’ regime directly when the operating conditions are moving towards flame blowout. In air-combustion, on the other hand, the flame shifts from ‘attached flame’ to ‘lifted flame’

before transitioning to the ‘no flame’ regime. These different behaviors occur irrespective of the equivalence ratio [126].

2.4 Existing oxy-combustion power-generation systems

Oxy-combustion with carbon capture provides a key pathway to address the urgent global need for affordable, secure, resilient, and reliable sources of clean energy [127]. For example, equipping an existing air-fuel application with post-combustion carbon capture may incur a total capital investment of ~260 million euros with annual operation/maintenance costs of ~43 million euros. Switching the same application from air-combustion to oxy-combustion with carbon capture, on the other hand, requires a total capital investment of ~217 million euros (16% less) with ~37 million euros in annual running costs (14% reduction) [128]. In terms of carbon-capture efficiency, oxy-fuel operation allows for 100% carbon capture, compared to 90% in air-fuel systems with post-combustion carbon capture [113]. The oxy-combustion technology is, however, still in the development phase. Current oxy-fuel facilities are pilot-scale or for demonstration only, i.e., there are no large-scale oxy-fuel power plants yet. Nonetheless, the technology has been demonstrated successfully on a variety of fossil fuels, as will be reviewed next. The fact that the global dependence on fossil fuels is likely to remain strong for decades to come [129] shows the great potential for implementing oxy-combustion with carbon capture in large-scale zero-emission power plants (ZEPPs).

2.4.1 Oxy-combustion of gaseous fuel

The amount of CO₂ emissions per unit power produced by a NG-fired GT plant in a combined cycle is less than half of what a coal-fired equivalent plant produces. The emergence of carbon capture technologies enables further reduction of carbon footprints. The current gaseous-fuel oxy-combustion concepts based on combined cycle can be categorized into the Graz oxy-combustion cycle and the semi-closed oxy-combustion combined cycle (SCOC-CC) [130,131]. The Graz cycle employs the use of steam from steam cycle to cool the combustion chamber and the turbine. A large portion of exhaust gas is recirculated back into the combustion chamber, which contains both steam and CO₂ produced during the combustion [132]. The SCOC-CC, as shown in **Figure 2.19**, differs from the conventional combined cycle in the facts that the gas cycle operates the combustion chamber near stoichiometric conditions and utilizes pure O₂ as oxidizer and CO₂ as coolant instead of air to suppress the excess temperatures. This SCOC-CC has five main sections: topping cycle, bottoming cycle air separation unit, flue gas condenser and CO₂ compression. The topping cycle contains the compressor, combustion chamber and the gas turbine, while the bottoming cycle consists of heat recovery steam generator (HRSG), steam turbine and steam condenser. The flue gas from the gas turbine goes to the HRSG so that the flue gas can cooled down generating steam for steam turbine. Unlike Graz cycle, in the SCOC-CC the steam from the exhaust gas is separated after HRSG. Cooled flue gas is then enters the flue gas condenser where the water vapor is separated from the CO₂. Around 93% of the CO₂ is recirculated back to the compressor and the rest goes to CO₂ compression unit for capturing, storage and transportation [132,133].

oxygen from an ASU and compresses them to 200 bar. They have demonstrated the feasibility of operating at 15–30% oxygen fraction at supercritical pressure in a non-premixed burner, while capturing the remaining flue gas. In a similar fashion, a 20-MW_{th} prototype power plant has been used to investigate performance and operability limits over a wide range of conditions, while operating on NG and other synthetic gases [135]. The burner utilizes two NG-fired combustion chambers; one acts as a gas generator, while the other is a reheat combustor. Successful demonstration of this technology has led to the development of the first-generation ZEPPs.

2.5 Fuel-flexible combustion in gas turbines

The term ‘fuel flexibility’ refers to the ability of a combustion application to deliver acceptable performance when operated with different fuels or fuel compositions. A dual-fuel GT is an example of fuel-flexible systems. A NG-fired GT is also considered fuel-flexible if it can tolerate changes in the composition of NG. The operation of a GT is susceptible to several factors, such as fuel type and composition, oxidizer composition, loading condition, flame type, flame-stabilization mechanism, combustor design, and the acceptable level of emissions. Research is being conducted extensively for developing fuel-flexible combustion systems for GT applications [136–139]. OEMs are investing in developing versatile fuel-flexible GTs that can operate with ranges of fuels, loading conditions, and flame modes. The adaptability of LPM combustion to different fuels, the associated combustion instabilities, and the resulting emissions are also studied numerically and experimentally.

To maintain optimum flame temperature, the fuel type should be selected accordingly. Different fuels can produce different flame temperatures even under similar operating conditions. **Table 2.4** lists the values of adiabatic flame temperature (T_{ad}) for selected fuels at stoichiometric operation [140,141]. GT manufacturers focus specifically on T_{ad} while designing the combustors, because this temperature defines the combustion efficiency along with the cooling requirements of the combustor liner, in addition to correlating with the dynamic flame instabilities [19]. Moreover, T_{ad} characterizes the combustor stability map. It has been confirmed experimentally that stable flames of the same T_{ad} have nearly identical flame macrostructures, even if the equivalence ratio and oxygen fraction are not kept constant [106,107,123].

Table 2.4: Adiabatic flame temperature of some fuels [140,141].

Fuel	Chemical Formula	T_{ad} (K)
Methane	CH_4	2223
Propane	C_3H_8	2261
Hydrogen	H_2	2370
Carbon Monoxide	CO	2381
Syngas	$(CO + H_2)$	2408-2415
(CO/H ₂ [vol%]: 50/50 to 95/5)		

The Wobbe Index (WI) is an important parameter in the characterization of fuel-flexible GTs. It is applicable to gaseous fuels and is defined as the ratio of lower heating value (LHV) per unit mass of the fuel and the square root of fuel specific gravity. The latter can be obtained from the ratio of densities of fuel to air [142].

$$WI = \frac{LHV}{\sqrt{\frac{\rho_{fuel}}{\rho_{air}}}} \quad (2.1)$$

Since WI does not account for the temperature of fuel at combustor inlet, the Modified Wobbe Index (MWI) is introduced as expressed in Equation 2.2 [143].

$$MWI = \frac{LHV}{\sqrt{T_{fuel} \times \frac{\rho_{fuel}}{\rho_{air}}}} \quad (2.2)$$

Figure 2.20 shows the MWI for different industrial fuels. Standard NG (mostly CH₄) is at the center of the MWI map. Increasing the content of higher hydrocarbons (C₂₊) increases the MWI at nearly constant LHV. Liquefied petroleum gas (LPG) is mostly propane and butane; hence, it has a higher MWI. Increasing the H₂ content (i.e., H₂ enrichment), on the other hand, increases the LHV at nearly constant MWI. Both MWI and LHV decrease with the increase of CO and/or inert contents (like H₂O, CO₂, and N₂), e.g., syngas and coke-oven gas (COG). **Table 2.5** shows the ranges of MWI for different industrial fuels, as extracted from **Figure 2.20**. NG itself does not have a unique MWI value, because the composition of NG differs from one geographical location to the other. The WI and MWI

for different gaseous pure-substance fuels are listed in **Table 2.6**. Numerous studies consider the WI or MWI as a validation and justification tool for fuel-flexible operation [144]. GTs can be operated with a variety of low- or high-quality fuels, depending on the availability and application. The MWI provides a numerical characterization of the fuel-flexibility of a GT as well as useful aid in sizing the fuel circuit and injectors at the design stage of the combustor [145,146]. For example, in a wide-Wobbe GT that can be operated with either NG or COG, the fuel system has to account for the fact that significantly larger flow rates of COG are needed to provide the same thermal input energy of NG. Larger fuel passages and injection orifices are thus needed for coke-oven-gas operation. If the orifices are, however, too large to inject NG at reasonable velocity for adequate penetration and mixing into the airflow, then separate systems might be needed for NG and COG.

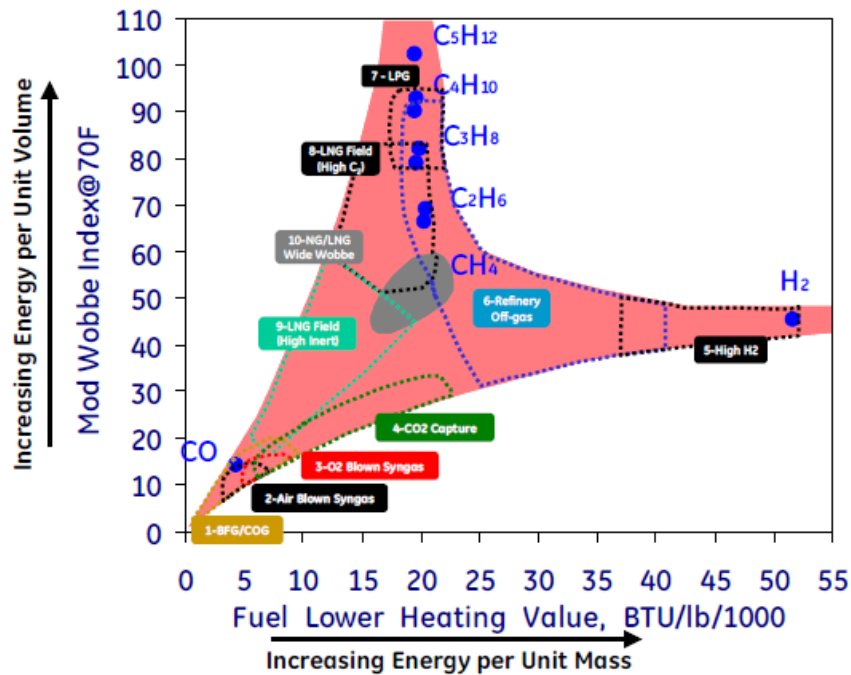


Figure 2.20: Modified Wobble Index (MWI) of different industrial fuels [19].

Table 2.5: Ranges of Modified Wobbe Index (MWI) for some industrial fuels [142].

Fuel Type	Range of MWI
Natural gas ($\sim\text{CH}_4$)	48-53
Syngas	24-29
High- H_2 fuels	40-48
LPG	72-87

Table 2.6: Wobbe Index (WI) and Modified Wobbe Index (MWI) values for different fuels [140,147].

Gaseous Fuel	Wobbe index (WI)	Modified Wobbe index (MWI)
Butylene-1	88.46	82.54
Carbon monoxide	12.80	12.80
Ethane	68.19	62.47
Ethylene	63.82	60.01

Hydrogen	48.23	40.65
Iso-butane	91.96	84.71
Methane	53.28	47.91
n-butane	92.32	85.08
Propane	81.07	74.54
Propylene	77.04	71.88

Research on fuel flexibility of GT combustors is abundant in the literature. A distributed-combustion system with swirl flow has been tested over a range of gaseous and liquid fuels, including propane, CH₄, H₂-enriched CH₄, and diluted CH₄ as gaseous fuels, in addition to ethanol and kerosene as liquid fuels [148–150]. The results have shown almost similar stability and emission characteristics without any modification in the fuel injector and without using any spray device. In a recent study of a swirl-stabilized model GT combustor, premixed oxy-CH₄ flames have been compared with premixed oxy-propane ones in the same combustor [151]. Both fuel types have demonstrated almost identical flame shapes at the same T_{ad} , irrespective of the values of equivalence ratio and oxygen fraction, while the flame speed has been directly influenced by T_{ad} [151]. The following subsections are dedicated to review H₂, syngas, ammonia, and fuel-blended combustion.

2.5.1 Hydrogen and hydrogen-enriched combustion

As mentioned earlier, diluting the oxy-fuel flame with recirculated CO_2 affects the combustion characteristics and flame stability. Moreover, increasing the CO_2 concentration in the combustor affects the reaction kinetics adversely [152]. This causes a reduction in both the combustion efficiency and laminar burning velocity [116,117]. Enriching the hydrocarbon fuels with H_2 can, however, mitigate some of these operational issues associated with oxy-fuel combustion by improving the reaction kinetics and widening the stability limits [153]. In addition to the use of H_2 to enrich commonly used fuels, the utilization of H_2 as a primary fuel is getting more attention in recent years. The LDI H_2 micromix combustion is a well-established technique. H_2 combustion generates clean exhaust without any CO_2 , CO, or unburned hydrocarbons [77]. Lower NO_x emissions have been even observed with pure H_2 combustion [154]. H_2 can also replace the hydrocarbon fuel at low part loads of the GT, in order to increase its turndown and broaden the operability limits [155].

Research shows that enriching hydrocarbon fuels with H_2 reducing the rates of NO_x , CO, and soot formation [156,157]. It has been reported that adding H_2 suppresses the surface growth rate of soot [158,159], in addition to reducing aldehyde emissions because of the reduction in CH_2O and CH_3CHO formation rates [160]. H_2 -enrichment also broadens the flammability limits [94,161]; LBO can be deferred with H_2 addition in GTs [148]. The characteristics, both instantaneous and average, of turbulent premixed flames can be influenced significantly by H_2 -enrichment. This influence can still prevail even with a small amount of H_2 [162].

H₂-enrichment can also increase the unstretched laminar burning velocity [163] and reaction rate [164]. This is attributed to the increase of formation of O, H, and OH radicals in H₂-rich flames and to the higher molecular diffusivity of H₂ [155]. An increase in the mole fraction of OH by 20% is observed with the addition of 20% H₂ to CH₄ [165]. H₂-enrichment of fuel-rich mixtures has no influence on the burning velocity, but it increases with H₂ addition in lean mixtures [166]. The combustion intensity also improves, which is defined as the ratio of turbulent to laminar burning velocities (S_T/S_L), i.e., the rise in S_T is greater than that of S_L [160,167].

The ignition delay time decreases with H₂ addition [168]. This enhancement can be linked to the mole fraction of H₂ in fuel, according to the mixing law suggested by Cheng et al. [169] The reaction-zone temperature elevates at higher hydrogen fraction (HF) because of the greater combustibility of H₂ [106]. However, the overall adiabatic flame temperature decreases with increasing HF, because the hotter reaction zone expands quickly, recirculating relatively cooler products into the reaction zone [153].

Cheng et al. [170] studied premixed swirl-stabilized H₂-air and H₂-N₂-air in an IGCC and reported an optimum swirl number of 0.51. The LBO limit happened at an equivalence ratio of 0.17 and remained constant for different bulk velocities. The Damköhler number (Da) has been found effective in anticipating the LBO limit. For different compositions of H₂/CO/CH₄ fuel blends, the LBO has occurred at a Damköhler number of 0.4 [171]. The authors of the present work, have conducted experimental and numerical investigations [94,172] on the stability of premixed H₂-enriched oxy-CH₄ flames in a model GT combustor. Experimentally captured flame images have been compared with the calculated flame shape based on numerical simulations, as shown in **Figure 2.21**. It has been found

that H₂-enrichment increases the critical strain rate and minimizes the quenching possibilities of the flame. In addition, the Damköhler number increases, and the Karlovitz number decreases with increasing HF. The study has reported that the static stability limits of the combustor are influenced more by the Reynolds number than by the adiabatic flame temperature, as shown in **Figure 2.22**.

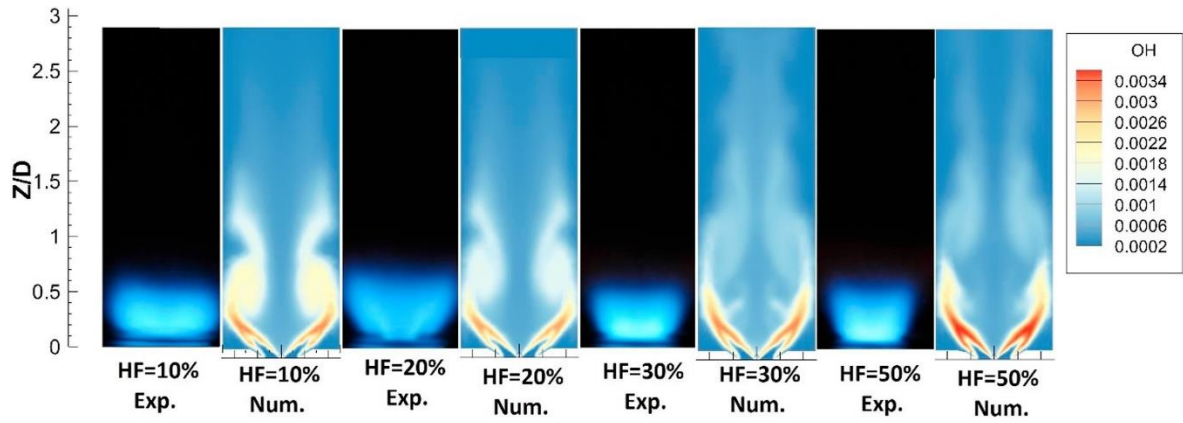


Figure 2.21: Comparisons of experimentally captured and numerically calculated flame shapes at different HF and fixed oxygen fraction of 30% [172].

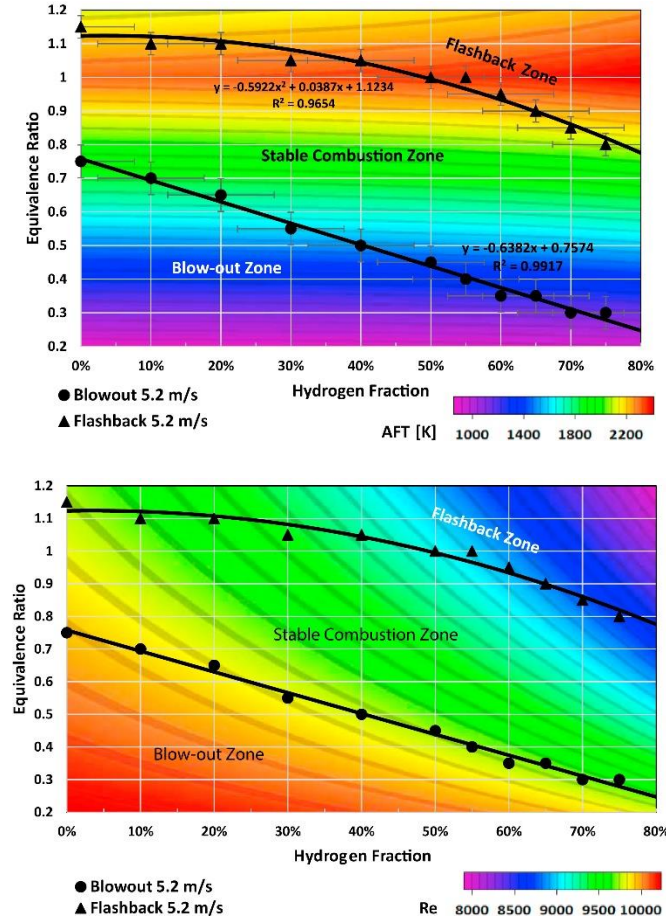


Figure 2.22: Stability map of a model gas-turbine combustor over ranges of hydrogen fraction and equivalence ratio at fixed throat velocity of 5.2 m/s and fixed oxygen fraction of 30%, plotted on the contours of constant adiabatic flame temperature (top) and Reynolds number (bottom) [94].

2.5.2 Syngas combustion

Syngas (or synthetic gas) consists mainly of H_2 and CO , with variable inert content (CO_2 , H_2O , and N_2). Compared to NG (mostly CH_4), syngas has a significantly different combustion behavior. The presence of higher amounts of H_2 in syngas makes it to be more

reactive than NG. Syngas can be produced through partial gasification of fossil fuel, usually coal, in presence of steam and oxygen at given temperature and pressure. Different damaging impurities, like H_2S , NO_x , and sulfur oxides (SO_x) are removed from the syngas after gasification. The pre-combustion carbon-capture option also entails fuel reforming to generate CO_2 -rich syngas, from which CO_2 is removed prior to combustion, resulting in H_2 -rich syngas. Syngas is used in high-efficiency low-emission combined cycles, like the IGCC, which benefits from the associated high combustion temperature. Syngas can also be used to produce pure H_2 using the water gas shift technology [173,174]. Syngas can also be converted to liquid fuels using the Fischer-Tropsch conversion [175,176].

The variable composition of syngas significantly affects its combustion behavior. Syngas-fueled GT combustors thus need to be fuel-flexible. Due to the higher flame temperature of syngas, LPM combustion should be implemented for controlling the temperature and thus reducing the NO_x emissions [177]. Similar to syngas-air combustion, oxy-syngas combustion also produces higher adiabatic flame temperature [178]. The laminar burning velocity of syngas flames have been found to be higher at lower CO content, see **Figure 2.23** [179]. Alzahrani et al. [180] have investigated a set of combustion mechanisms and kinetics in terms of their accuracy for characterizing syngas combustion. They have observed greater laminar flame speeds at higher equivalence ratio, preheat temperature, and H_2 content of the syngas fuel. However, the flame speed has been found to decrease with increasing the operating pressure. The effects of pressure, equivalence ratio, H_2 content, and preheat temperature on NO emission for syngas combustion have been studied by Delattin et al. [156]. **Figure 2.24** shows the variations of NO emission and adiabatic

flame temperature with equivalence ratio, considering different mechanisms for syngas combustion. In all cases, the mole fraction of NO increases with equivalence ratio due to the increasing fuel content in the mixture, which raises the temperature during combustion.

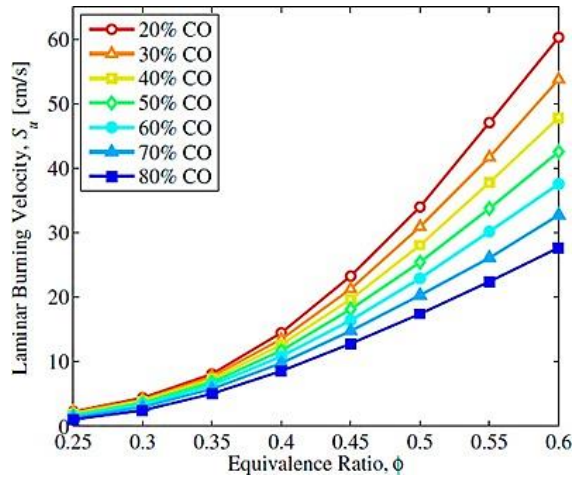


Figure 2.23: Effects of CO content and equivalence ratio on the laminar burning velocity of syngas flames [179].

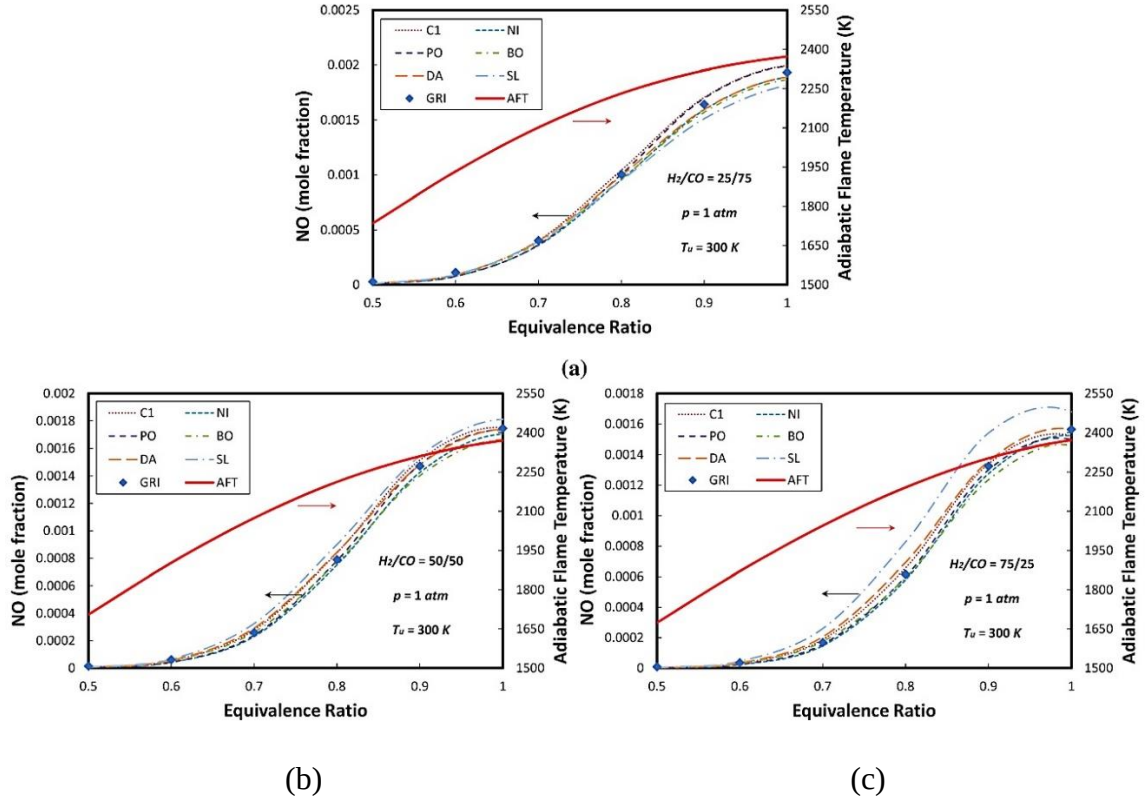


Figure 2.24: Predictions of NO emission and adiabatic flame temperature at different equivalence ratios for H₂/CO syngas compositions of (a) 25/75, (b) 50/50, and (c) 75/25 at operating conditions of 300 K and 1 atm [180].

In a recent study on syngas-fueled oxy-fuel power cycles, the Allam-ZC cycle has been proposed as an alternative for coal-fired power plants, like the IGCC. The net efficiency of this Allam cycle has been reported to be 47.3% at turbine inlet conditions of 25 MPa/1000 °C, condensation temperature of 25 °C, and 0.245 kWh/kg O₂ specific power consumption of the ASU. Emission of NO_x has been found to be almost zero with 100% carbon capture [181].

2.5.3 Ammonia combustion

As seen before, the use of H_2 in combustion offers multiple advantages and satisfies the major emission requirements for power generation. However, storage and long-distance shipping of H_2 pose some challenges. Ammonia (NH_3), on the other hand, has condensation pressure and boiling temperature similar to those of propane, according to the National Institute of Standards and Technology (NIST) database [182], which facilitates easy storage and shipping. Besides, NH_3 can be used as fuel, given that it consists of 17.8% H_2 by mass. NH_3 can be produced from nitrogen, which is separated from air, plus renewable H_2 . As NH_3 is being produced in substantial amount (180 Mt/year) [183] and has been used for a long time as a refrigerant, in the fertilizer industry, or as a raw material, its production, handling, storage procedure and safety regulations are already well established. Despite these advantageous aspects, several issues must be addressed to utilize the full potential of ammonia as an alternative gas turbine fuel. High NO_x emission is one of the biggest drawbacks in ammonia combustion along with several other concerns including health and safety issues, risks of explosion and corrosive nature of ammonia [184,185].

The combustion characteristics of pure ammonia [186,187] and mixture of ammonia with other fuels such as natural gas [186,188–194] and hydrogen [189,195–201] in different fuel compositions have been investigated in recent years for gas turbine applications. Kurata et al. [186] have performed an experimental study on micro-GTs to produce power from NH_3 -based fuels, including NH_3/CH_4 mixtures, NH_3 /kerosene mixtures, and pure NH_3 [186]. The NO_x emission, in this study, has been found acceptable with respect to the emission regulations but is more than that in conventional natural gas-fired gas turbine. It is worth

mentioning that in order to start the gas turbine every time, they have used a specific fuel injection sequence as shown in **Figure 2.25**, where kerosene has to be burned initially to run the turbine after that ammonia can be injected and burned in the combustor. In another work with a swirl-stabilized micro-GT combustor fueled by an NH_3/CH_4 blend, rich-quick-lean combustion has been found better suited for lower emissions, yielding 2 ppmv CO, 49 ppmv NO_x , and almost no emissions of N_2O , HCN, and NH_3 . The combustion efficiency has been reported to be 99.8% with NH_3 fraction less than 30%. The burning velocity of $\text{NH}_3\text{-CH}_4$ -air flames is greater than that of NH_3 -air flames [193], but NO_x emissions are significantly lower in the NH_3 -air flames. In another experiment of $\text{NH}_3\text{-CH}_4$ -air combustion in a laminar premixed burner, NO_x emissions have been seen to be increased with the increase in NH_3 mole fraction. However, after reaching a mole fraction of 0.5, the NO_x emissions started decreasing [194]. The combustion behavior of a horizontal single-burner test furnace, co-fired with pulverized coal and NH_3 has also been tested successfully at the Central Research Institute of Electric Power Industry, Japan [202].

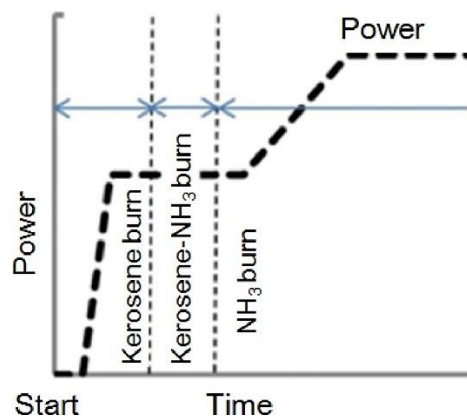


Figure 2.25: Start-up sequence for 50 kW model micro gas turbine with ammonia combustion [186].

Besides natural gas, hydrogen enrichment with ammonia for gas turbine combustion is also being studied for its use in gas turbines. The fraction at which the ammonia and hydrogen is mixed plays a vital role in combustion stability. Valera-Medina et al. [199,201] and Xiao et al. [200] have experimented with different blends and reported unstable combustion at 50:50 ratio while combustion is observed to be stable at 70:30 of $\text{NH}_3\text{:H}_2$ ratio by volume. The NO_x emission with H_2 -enriched ammonia can be reduced by recirculating the exhaust gas which however does not affect the initial H_2 flame [199]. Furthermore, higher NO_x emission can be attributed to the increase in inlet temperatures. High inlet temperature can also result in reduced flame size [201].

2.5.4 Fuel-blended combustion

Fuel blending implies mixing two or more fuels and is used to reduce fuel cost and improve fuel utilization. This technique is especially suitable for industrial and petrochemical plants where there is an abundance of by-product process gas (e.g. hydrogen) available. This process gas can be utilized with the natural gas to enhance the combustion characteristics, achieve higher combustion efficiency and reduce CO_2 and pollutant emissions. Blending also allows for the utilization of less expensive fuels that are commercially available. **Figure 2.26** shows a simple schematic of implementing fuel blending in GT applications, where natural gas is mixed with the available process gas in the blending system and the mixed blended fuel is then fed to the combustion chamber for energy generation. General Electric's 7FA gas turbine with DLN 2.6 technology is an excellent example that can take advantage of the fuel-blended combustion [203].

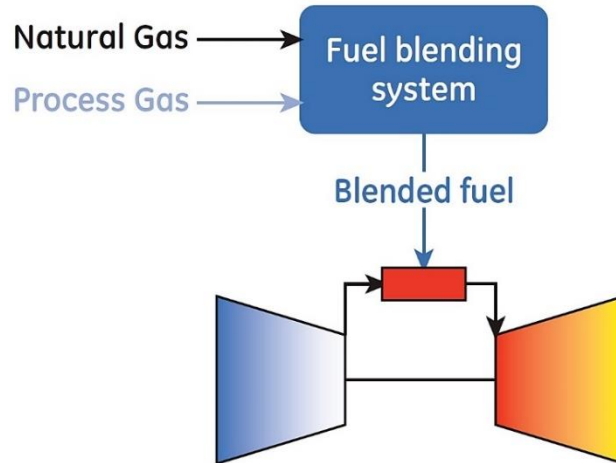


Figure 2.26: Schematic of implementing fuel blending in gas-turbine applications [203].

Numerous researches have been conducted over the years to investigate the fuel blended combustion. The combustion behaviors of alcohol-diesel and kerosene-diesel blends has been investigated in a continuous-combustion system by Asfar and Hamed [204], where increased thermal efficiency and reduced soot concentration in the exhaust are reported. However, NO_x emissions are slightly increased. An experiment has been conducted on the effects of NG-propane blending on the pollutant emissions in a premixed GT combustor [205]. It is observed that the addition of 5 % propane (by vol.) and the variation of equivalence ratio did not have significant effects on NO_x emissions. A performance study of a 25 kW micro-GT engine with biodiesel-bioethanol blends has been performed experimentally [206]. It is found that the engine thermal efficiency improves at a ratio of 80%/20% of biodiesel-bioethanol, compared to the reference case with diesel only; however, the emission levels increases in this case, except for NO_x. The combustion behavior of diesel fuel blended with raw vegetable oils, including jatropha, soybean, and

waste cooking oils, has been studied in a compression-ignition engine [207]. It has been observed that the exhaust-gas temperature recorded with pure diesel is lower than the temperatures recorded with the different diesel/oil blends. The CO emissions of the blends are seen to be low until 80% load but increases rapidly at higher loads.

Based on the above discussion on different GT burners and combustion various gaseous fuel blends, the swirl-stabilized and MM burner are observed to be well performing under oxidizer/fuel flexible approach. **Table 2.7** lists the main findings of different studies conducted with different fuels and oxidizers in swirl-stabilized and MM burners.

Table 2.7: Important studies on fuel-flexible combustion in swirl-stabilized and MM burners.

Burner type	Fuel	Combustion technique	Investigation method	Main findings	Ref.
Swirl-stabilized burner	CH ₄	Premixed oxy-combustion	Experimental	- Stable flames observed at equivalence ratios between 29% and 70% - Reaction kinetic rate is found more useful	[208]

			in deciding the flashback limit than Re • Operability limit broadens with higher Re by moving the limit for blowout to leaner conditions	
CH ₄	Non-premixed oxy-combustion	Experimental	• Stable flame reported at $\phi=0.65$ • Oxygen fraction below 25% drastically impacts flame stability • Combustion found not possible with oxygen fraction below 21%	[105]
CH ₄	Non-premixed	Experimental	• CH₄/O₂/CO₂ flame is found more stable than CH₄/O₂/N₂ flame at higher ϕ	[209]

	oxy- combustion		and fuel flow rate with identical Re and oxygen fraction	
			Both CH₄/O₂/N₂ and CH₄/O₂/CO₂ flames showed similar stability at higher oxygen fractions	
H ₂ - enriched CH ₄	Premixed air- combustion	Experimental	- Mixtures with different fuel compositions showed consistent trend at lower ϕ - Flame shape examined at acoustically uncoupled and coupled condition	[210]
H ₂ - enriched CH ₄	Non- premixed oxy- combustion	Experimental and numerical	- Improved flame stability with H₂-enrichment - H₂-enriched oxy-combustion not	[211, 212]

			possible with $\phi \geq$	
			0.95	
			- Swirlers with 65° or 70° vane angles demonstrated better stability than that with 55° vane angle - Combustion not advised for vane angles beyond 75°	
H ₂ -enriched CH ₄	Premixed oxy-combustion	Experimental and numerical	- Characteristic V-shape flame forms at higher HF - Higher CO emission with higher HF ϕ heavily influences the flame shape and T_{ad}	[94,172]
C ₃ H ₈	Non-premixed air and	Experimental	Critical velocity of oxy-C₃H₈ combustion is six times more than that	[126]

			oxy- combustion	of air-C ₃ H ₈ combustion
				• Critical velocity determines the transition from attached flame to lifted flame • Stable flame observed for oxy-C₃H₈ at swirl number of 1.0 and near stoichiometry
C ₃ H ₈	Premixed	Experimental	oxy- combustion	• LBO limit follows the contour of constant T_{ad} • Flame shapes are identical at same T_{ad} • Blowout and flashback occur at lower Ø in oxy-C₃H₈ flames than that in oxy-CH₄ at

			fixed oxygen fraction	
			Correlation between flame speed and T_{ad} developed for oxy-C_3H_8 flame characterization	
NH ₃ , NH ₃ - CH ₄	Non- premixed air- combustion	Experimental	- Initially kerosene has been utilized to start the gas turbine. - NO_x emission under regulatory limit but higher than conventional combustion system. - Higher air temperature increases the combustion stability - Combustion efficiency ranges from 89-96% in NH₃-air combustion	[186]

-
- Combustion inlet temperature (CIT) maintained within the range of 460 - 580 °C
 - CIT regulates the amount of unburnt NH₃ and NO_x emission and at mid-range CIT both rich and lean NH₃ region co-exists.
 - In NH₃-CH₄-air combustion NO_x emission increased with the increase in NH₃ but after reaching a certain point the NO_x emission reduced with the increase in NH₃
-

NH ₃ - CH ₄	Premixed and non- premixed air- combustion	Experimental and numerical	• Low emission with zero NH₃, N₂O, HCN, 2 ppmv CO, 49 ppmv NO_x has been achieved in fuel rich NH₃-CH₄-air combustion with combustion efficiency of 99.8%. • Rich-lean NH₃-CH₄-air combustion yielded lower NO_x emission than that in NH₃-case	[193]
NH ₃ - CH ₄	Premixed air- combustion	Experimental and numerical	• CO emission has been more than the acceptable level at ϕ from 1.15-1.25 • Fully premixed combustion technique is identified as unsuitable strategy	[213]

			for NH ₃ -CH ₄ fuel injection.	
NH ₃ -H ₂	Premixed air-combustion	Experimental and numerical	• Unstable combustion is observed at NH₃-H₂ ratio of 50:50 (%vol.) • At 50:50 blend, stable flame is reported with ϕ from 0.43-0.52 for 31 W of net thermal power. • Recirculation of flue gas reduced NO_x emission at the same time maintained initial H₂ flame.	[199, 200]
NH ₃ -H ₂	Premixed air-combustion	Experimental and numerical	• Stable flame has been observed at NH₃-H₂ ratio of 70% and 30% (vol.)	[201]

				• With increase in inlet temperature, the flame size reduces while reactivity of OH and NOx increase. • Flame structure with NH₃ in the inner zone and H₂ in the outer zone has demonstrated better stability.	
Micro-mixer burner	H ₂	Premixed air-combustion	Experimental and numerical	• Crossflow mixing of air and H₂ has been done in micromixer • Lower NOx emission is achieved with inherent flashback protection	[89–91]
	CH ₄	Premixed oxy-combustion	Experimental	• T_{ad} seen as a determining parameter for flame	[93]

shape and stability

map

- ϕ has been seen as a determining parameter for distribution of temperature inside the combustor
- Flame shape is influenced by ϕ and oxygen fraction

NH ₃ -	Premixed air-	Experimental	• NO _x increases with	[194]
CH ₄	combustion	and	the increase in NH ₃	
		numerical	fraction in the fuel	
			mixture upto	
			$x_{NH_3}=0.5$	
			• NO _x emission	
			reduces with the	
			decrease in ϕ	

CHAPTER 3

METHODOLOGY

3.1 Combustor description

3.1.1 Experimental setup of the premixed swirl combustor

The characteristics of propane-fueled oxy-combustion are examined in the present study in a swirl-stabilized model gas-turbine combustor (as shown in **Figure 3.1**) adapting the dry low emission (DLE) lean-premixed (LPM) combustion technology. The combustion zone is confined by a 30 cm long quartz tube of 6 mm thickness and 76 mm inner diameter. The incoming fuel-oxidizer mixture is fully premixed with 5.2 m/s bulk throat velocity and whirled using a swirler having 8 vanes at 55° angle. Regulating inlet flow velocity is a common practice gas turbine operation [214], to achieve desired pressure drop across the combustor. Furthermore, this study is based on model gas turbine combustor, hence in order to maintain similar Reynolds number in actual GT combustor with fixed pressure drop, the bulk velocity at the inlet of the combustor is fixed to 5.2 m/s. The swirler has a solid conical centerbody of 9.5 mm outer diameter and 28° cone angle. Swirler in combustion is commonly used for flame stabilization [215,216]. Swirler with sufficient swirl intensity creates recirculation zones, mixing the reactants with products. Swirling effect also enhances the gas entrainment in the combustor and considerably extends the

stability limit [217,218]. The swirl angle is used to express the swirl number (SN) in swirl-stabilized combustor, as evaluated using Equation 3.1 [215,219].

$$SN = \frac{2}{3} \left[\frac{1 - \left(\frac{D_{cb}}{D_{in}} \right)^3}{1 - \left(\frac{D_{cb}}{D_{in}} \right)^2} \right] \tan(\alpha_{sw}) = 0.98 \quad (3.1)$$

Where D_{cb} , D_{in} , and α_{sw} refer to the diameter of swirler centerbody, the inner diameter of mixing plenum, and the swirler blade angle, respectively.

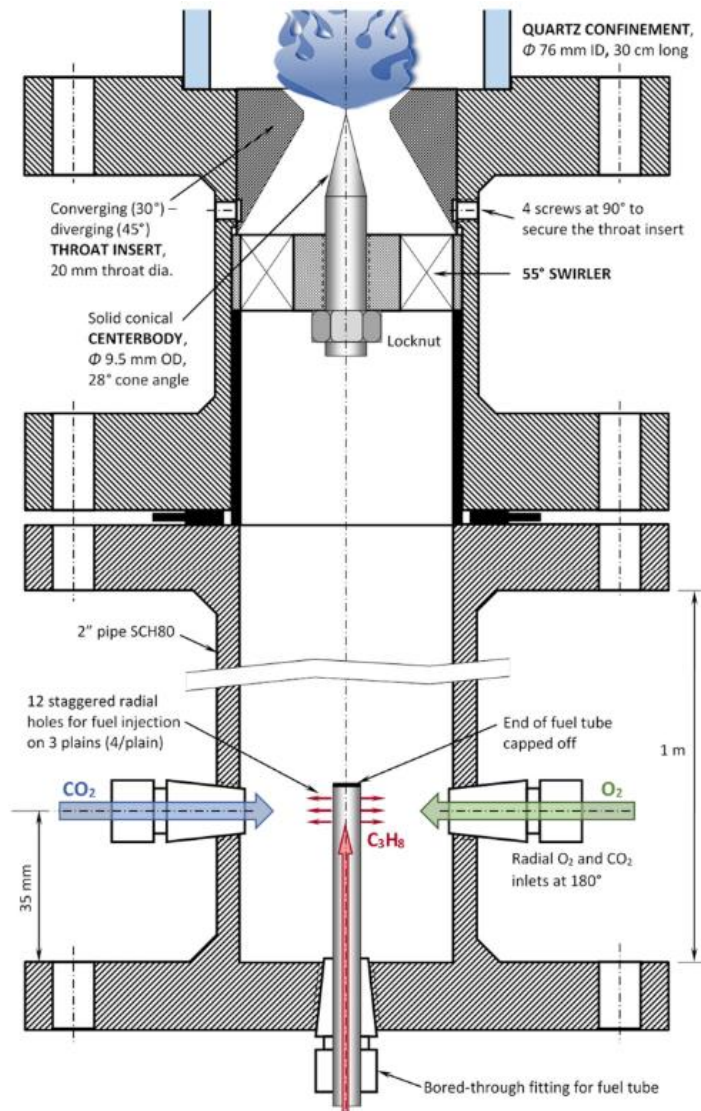


Figure 3.1: Schematic representation (left) and experimental setup (right) of swirl-stabilized model gas turbine combustor.

The gas mixture at the inlet contains C_3H_8 , O_2 , and CO_2 , whereas the exhaust gas mixture consists mainly of CO_2 and H_2O . Carbon dioxide at the inlet simulates the recirculation of the CO_2 from the exhaust stream after H_2O condensation and capture of CO_2 . As shown in **Figure 3.1**, the inlet mixtures are premixed in a 1 m long mixing pipe with a diameter of 2 inches. The fuel is injected through a central tube with 12 radial holes positioned in three

consecutive planes. The oxygen and carbon dioxide gases are injected radially from opposite direction facing towards the central axis of the premising pipe. The premixed gases then fed into the combustion chamber through the swirler followed by a convergent-divergent section.

Mass flow rates of the inlet gases are controlled using mass flow controllers from Aalborg Inc. The mass flow controllers can maintain the desired flow rate with approximately ± 0.5 % full-scale accuracy. This very small variations flow rates result in ± 0.02 and ± 0.4 % uncertainties in equivalence ratio and oxygen fraction, respectively. An additional emergency shut-off valve was used cut off the fuel flow in the event of flashback to prevent any unwanted accident from flashback. All the photographic images of the flame were taken using a 24-MP camera (1/60 shutter speed, 5.6 f-stop, 1600 ISO) in order to compare the experimental flames with the ones predicted from numerical simulations. A R-type thermocouple (PtRh13%-Pt) with 1 mm junction diameter was used to measure the local temperature in the combustion zone. The thermocouple probe was entered into the chamber from the top and moved inside the quartz confinement (both radial and axial directions) using a traverse mechanism. The R-type thermocouple was connected to a data logger and the computer to measure the mean temperature over 1 minute at each location. These experimentally obtained temperatures are used in the validation process of the developed numerical model. To address the correction for radiation to the surroundings, the model by Brohez et al. [220] was implemented for the temperature measurements. Temperature measurements along axial and radial direction (at 10 and 20 cm heights from the throat of the combustor) were performed to evaluate the experimental temperature distribution of the examined flames.

CO₂ is recirculated from the exhaust stream and mixed with O₂ to dilute the fuel-oxidizer mixture to mimic the CO₂-recirculation and regulate combustion temperature. All the three components, (i.e., C₃H₈, O₂ and CO₂) were injected together through one position to simplify the experimental procedure. The mixture then goes through the mixing tube to achieve complete premixed condition. In the experiment, the inlet properties, like bulk velocity, bulk mass flow rate, bulk viscosity and bulk Reynolds number (Re) are considered for the C₃H₈/O₂/CO₂ mixture due to the addition of CO₂ in the inlet. The bulk velocity throughout the experiment was maintained at 5.2 m/s by adjusting of the mass flow rates of the reactant gases. In order to maintain this bulk throat velocity at fixed inlet cross-sectional area, the mass flow rates of individual species were specified in the mass flow controllers in varying ϕ and OFs. The mass flow rate of the mixture was calculated using Equation (3.2), at atmospheric pressure and 300 K reactant temperature.

$$\dot{m}_{mix} = \dot{m}_{C_3H_8} + \dot{m}_{O_2} + \dot{m}_{CO_2} = \rho_{mix} A v_a = \left(\frac{P M_{mix}}{R_u T} \right) A v_u = \left(\frac{P A v_u}{R_u T} \right) M_{mix} \quad (3.2)$$

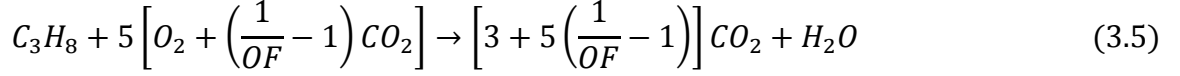
Where M_{mix} can be represented through following Equation (3.3).

$$M_{mix} = 1 / \sum \left(\frac{x_i}{M_i} \right) \quad (3.3)$$

Combining the Equations (2) and (3) provides a simplified form for mass flow rates as expressed in Equation (3.4).

$$\frac{\dot{m}_{C_3H_8}}{44} + \frac{\dot{m}_{O_2}}{32} + \frac{\dot{m}_{CO_2}}{44} = \left(\frac{P A v_u}{R_u T} \right) \quad (3.4)$$

The general stoichiometric reaction for the oxy-propane combustion can be given as



The CO₂ dilution can be determined by the fuel to diluted oxidizer ratio at stoichiometric condition as given in Equation (3.6).

$$(F/O)_{stoichiometric} = \frac{44}{5 \left[32 + \left(\frac{1}{OF} - 1 \right) 44 \right]} = \frac{11}{40 + 55 \left(\frac{1}{OF} - 1 \right)} \quad (3.6)$$

The equivalence ratio for oxy-propane combustion can be evaluated using Equation (3.7).

$$\Phi = \frac{(F/O)_{actual}}{(F/O)_{stoichiometric}} = \left(\frac{\dot{m}_{C_3H_8}}{\dot{m}_{O_2} + \dot{m}_{CO_2}} \right) \left[3.636 + 5 \left(\frac{1}{OF} - 1 \right) \right] \quad (3.7)$$

Furthermore, the expression for diluted oxidizer mixture can be written as a function of OF as provided in Equation (3.8).

$$\frac{\dot{m}_{C_3H_8}}{\dot{m}_{O_2} + \dot{m}_{CO_2}} = \frac{32 OF}{32 OF + 44(1 - OF)} \quad (3.8)$$

Solving Equations (4), (7) and (8) for any given Φ and OF can be used to evaluate the required set points of C₃H₈, O₂ and CO₂ mass flow rate controllers at fixed inlet velocity of 5.2 m/s. Using the equations, a text matrix was developed to examine the flames with a wide range of Φ (range: 0.1-1.0) and OF (range: 15-70%).

The bulk viscosity of the reactant mixture[221] and the bulk density were evaluated using Equations (3.9) and (3.10), respectively.

$$\mu_{mix} = \frac{\sum y_i \mu_i \sqrt{M_i}}{\sum y_i \sqrt{M_i}} \quad (3.9)$$

$$\rho_{mix} = \frac{P \sum \dot{m}_i}{R_u T \sum (\dot{m}_i / M_i)} \quad (3.10)$$

Using the bulk viscosity and bulk density, the Reynolds number for the reactant mixture can be determined by Equation (3.11).

$$Re = \frac{v D \rho_{mix}}{\mu_{mix}} \quad (3.11)$$

Even though the bulk throat velocity was maintained at 5.2 m/s throughout the experiment, the change in Re occurred due to the change in Φ and OF values. The value of Re , for the experiment, ranged from 8865 (for $\Phi=1.0$, OF=70%) to 11,192 (for $\Phi=0.1$, OF=15%). Similarly, the values of T_{ad} were also calculated for the experimental set points. Species dissociation was not considered in the calculation of T_{ad} , since it was observed from the previous studies [220,221] that the is decreased by 100-200 °C only because of the dissociation of CO₂.

Initially a stable combustion zone was identified by evaluating the blowout and flashback in different Φ and OF. Following approaches were practiced for each OF to map the blowout and flashback limit in a safer experimental condition.

(a) The combustor was ignited at a safe stable point, away from both blowout and flashback, which was obtained from initial light off attempts.

(b) The flow rates of the reactant species were adjusted to achieve desired OF and Φ .

For a same OF, leaner Φ was sought if the flame was observed to be near the flashback limit. Higher audible noise is an indicator of flashback tendency and

flame being in the flashback vicinity. Alternatively, higher Φ was sought if the flame was near blowout limit.

- (c) Stable operating Φ was noted after obtaining the desired OF. After that the equivalence ratio was increased gradually to determine the flashback point. Careful transition of Φ was attempted in smaller intervals between the set points as the flame approaches towards the flashback limit. Noise becomes louder at the flashback limit. The flame then swiftly flashes upstream of the burner back followed by the ignition of incoming reactant mixtures and results in a small explosion. The particular value of the Φ is noted as a flashback point for the given OF.
- (d) For blowout limits at a given OF, the Φ is reduced carefully from the safe ignition point. Smaller intervals between the points were attempted as the flame approaches the blowout limit and the flame goes off. The Φ is noted as the blowout limit for the particular OF.
- (e) The overall stability map was then generated by repeating the steps (b) to (d)) for different OFs.

3.1.2 Multi-hole burner setup

Premixed oxy-fuel flames of propane have been examined in the multi-hole gas turbine combustor. The multi-hole combustor houses 61 inlet holes of 3.175 mm (1/8") diameter spaced at 5.5 mm. The burner is surrounded by steel base plate while the combustion zone is enclosed with 6 mm thick quartz tube with 76 mm inner diameter. **Figure 3.2** depicts the

multi-hole combustor setup, where $1/6^{\text{th}}$ of the combustor volume has been considered as a computational domain (shown in **Figure 3.2(b)**) for numerical analysis in order to reduce the computational time. Earlier experimental studies by Aliyu et al. [93] and Hussain et al. [222] reported several advantages of multi-hole burners including flashback prevention and improved stability. This includes the flashback prevention due to lower inlet cross-sectional area; multi-hole burners are relatively more effective in preventing flashbacks than the conventional LPM burners. In addition, the spacings between the inlets in multi-hole combustor act as bluff bodies between the flamelets and aides in flame stabilization [63].

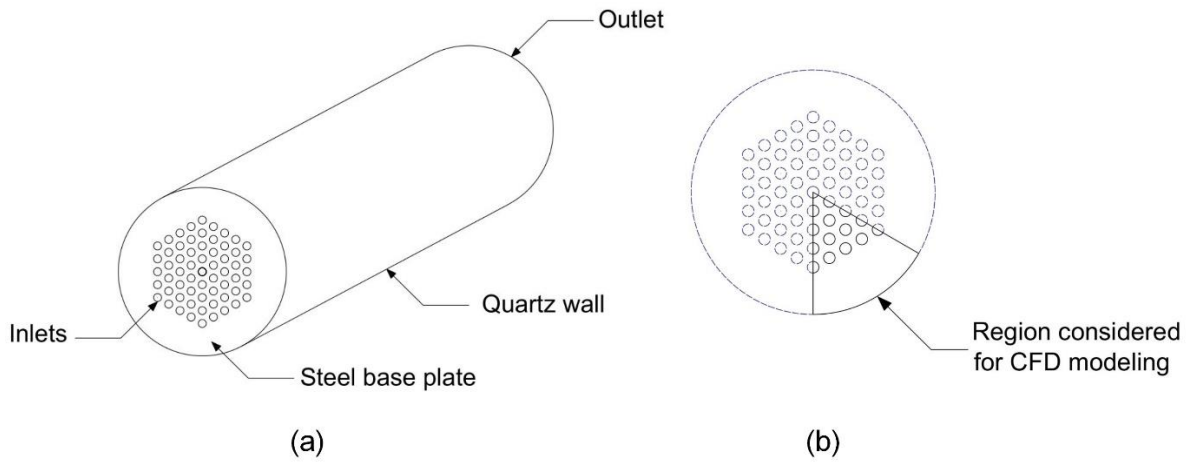


Figure 3.2: (a) Schematic diagram of the combustor area for the micromixer combustion, and (b) base plate with inlets showing the region considered for modeling.

3.2 Numerical modeling

3.2.1 Governing equations

Conservation equations of mass, momentum, and energy along with transport equation for scalar variable in the three-dimensional (3D) computational domain were solved using the Large Eddy Simulation (LES) model for Swirl-stabilized flames in ANSYS Fluent 19R3. In order to examine eddy-formation and its effect of the combustion, LES model was selected for the swirl-stabilized combustor. Heat transfer, flow, and emission characteristics were predicted through solving the equations for 3D domain simultaneously. The general conservation equation for mass, momentum, energy as well as species transport is provided in equation (3.12),[223] where u_j is the velocity component along j direction, Γ_ϕ is the diffusion component, S_ϕ is the source term, while Φ and ϕ correspond to Reynolds averaged and fluctuating components of the dependent variable, respectively.

$$\frac{\partial}{\partial x_j} (\bar{\rho} \bar{U}_j \Phi + \bar{\rho} \bar{u}_j \phi) = \frac{\partial}{\partial x_j} \left[\Gamma_\phi \frac{\partial \Phi}{\partial x_j} \right] + \rho \bar{S}_\phi \quad (3.12)$$

3.2.1.1 Radiation model

Radiative heat transfer was predicted using the discrete ordinate (DO) modeling scheme, which is valid for a wide range of optical thickness and suggested for modeling oxyfuel combustion.[224] The DO model for the current study was implemented in way such that

one radiative iteration is done with every ten energy-iterations. Absorption coefficient of the gaseous mixture, verified over a wide range of operating conditions, was calculated using the weighted sum of gray gas model, namely WSGGM.[225] Equation (3.13) shows the total emissivity (ε) in terms of the weighted sum of gray gases, where $\alpha_{\varepsilon,i}$ refers to the emissivity weighting factor for the grey gas i at temperature T , κ_i indicates the adsorption coefficient, P represents the partial pressure of the absorbing gases, and L represents the gas layer thickness (or path length).

$$\varepsilon = \sum_{i=0}^{i=I} \alpha_{\varepsilon,i}(T) [1 - e^{-\kappa_i PL}] \quad (3.13)$$

3.2.1.2 Turbulence model

Large eddy Simulation (LES) turbulence model

Turbulence in the flow can be divided into two types of eddies, namely large and small eddies. The large eddies refer to the characteristic length of the mean flow, while the small eddies cause dissipation of turbulence kinetic energy. The LES modeling approach was utilized in this study for solving turbulence through filtering-out smaller eddies. Equation (3.14)[172] can be used for the low-pass filtering operation for a quantity φ , where the integration covers the entire domain while G represents the filter function to determine the scale of resolved eddies. Consequently, Equations (3.15) and (3.16) show the expression for continuity and Navier-Stokes equation after incorporating the filtering function.

$$\bar{\varphi}(x, t) = \int G(r, x) \varphi(x - r, t) dr \quad (3.14)$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho \bar{u}_i) = 0 \quad (3.15)$$

$$\frac{\partial}{\partial t} (\rho \bar{u}_i) + \frac{\partial}{\partial x_j} (\rho \bar{u}_i \bar{u}_j) = \frac{\partial}{\partial x_j} \left(\mu \frac{\partial \sigma_{ij}}{\partial x_j} \right) - \frac{\partial \bar{p}}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} \quad (3.16)$$

Here σ_{ij} and τ_{ij} , corresponding to stress tensor from molecular viscosity and subgrid-scale stress, are expressed by Equations (3.17) and (3.18), respectively.

$$\sigma_{ij} \equiv \left[\mu \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \right] - \frac{2}{3} \mu \frac{\partial \bar{u}_i}{\partial x_j} \delta_{ij} \quad (3.17)$$

$$\tau_{ij} \equiv \rho \overline{u_i u_j} - \rho \bar{u}_i \bar{u}_j \quad (3.18)$$

Moreover, the subgrid-stresses resulted from the filtering operation were modeled by merging isotropic part of the subgrid-scale stresses and filtered static pressure terms. The modeling of the deviator part using turbulent viscosity is shown in Equation (3.19)

$$\tau_{ij} = -2\mu_t \bar{S}_{ij} \quad (3.19)$$

Where, μ_t and $\bar{S}_{ij}$ represents the turbulent viscosity and the rate of strain tensor, respectively. Turbulent viscosity (μ_t), was solved in this study using the Smagorinsky-Lilly model as provided in Equation (3.20).

$$\mu_t = \rho L_s^2 |\bar{S}| \quad (3.20)$$

Here, L_s represents the mixing length for subgrid-scale as expressed in Equation (3.21), while the term $|\bar{S}|$ can be evaluated from Equation (3.22). Here, the terms κ , d , C_s , and V

in Equation (3.21) symbolize the Kármán constant, distant to the closest wall, Smagorinsky constant, and volume of the computational cell, respectively.

$$L_s = \min(\kappa d, C_s V^{1/3}), \quad (3.21)$$

$$|\bar{S}| \equiv \sqrt{2\bar{S}_{ij}\bar{S}_{ij}} \quad (3.22)$$

Reynolds-Averaged Navier-Stokes (RANS) turbulence model

Unlike the swirl-stabilized combustor, the total inlet stream is divided into multiple-smaller streams reducing/eliminating the swirl-effect and make the flow with reduced turbulent and more towards laminar regime. Due to this, Reynolds-averaged Navier-stokes (RANS) turbulence model is utilized in this section in-stead of computationally heavier LES model. The standard k- ϵ has been incorporated in simulating the three-dimensional (3D) LPM combustion of oxy-propane using commercial code ANSYS Fluent 19R3, where the kinetic energy (k) and dissipation rate (ϵ) are determined by solving following Equations (3.23) and (3.24), respectively. Here, G_k and G_b represent turbulence kinetic energy generation as result of velocity gradients and buoyancy, while Y_M refers to contribution of fluctuating dilatation in compressible turbulence to overall rate of dissipation. The terms $C_{1\epsilon}$, $C_{2\epsilon}$ and $C_{3\epsilon}$ are the constants, where as σ_k and σ_ϵ correspond to Prandtl numbers for k and ϵ , respectively. Lastly, the turbulent viscosity (μ_t) is evaluated by combining the k and ϵ , as presented in Equation (3.25) [226].

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \varepsilon - Y_M + S_k \quad (3.23)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(\rho \varepsilon u_i) \\ = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{1\varepsilon} \frac{\varepsilon}{k} (G_k + C_{3\varepsilon} G_b) - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} + S_\varepsilon \end{aligned} \quad (3.24)$$

$$\mu_t = \rho C_p \frac{k^2}{\varepsilon} \quad (3.25)$$

3.2.1.3 Reaction model

Modeling of CO₂-diluted oxy-propane combustion was done using the partially premixed combustion model that was modified to accommodate fully-premixed combustion, by specifying the inlet mean mixture fraction. Moreover, the inlet mixture fraction variance is set to 0 (zero) to maintain a constant Φ at the inlet. Partially premixed model in ANSYS FLUENT, being a combination of premixed and diffusion combustion model, possesses the advantages of both the predecessor models, at the same time allowing more control over the species and reactions as compared to the premixed combustion model [226]. Transport equations for mean reaction progress variable ($\bar{c}$), mean mixture fraction ($\bar{f}$), and mixture fraction variance ($\bar{f'}^2$) were solved to acquire other scalar variables like density weighted average scalars. Here, the reaction progress variable corresponds to the mass fraction of a suitable species, for which the value of mass fraction is zero in the unburnt mixture and 1.0 in the completely burnt mixture. Mixture fraction can be evaluated

from Equation (3.26), where s and Y are oxygen to fuel ratio and mass fraction, respectively. The term Y_{ox} represents the mass fraction of oxygen, Y_{fu} represents the mass fraction of fuel, whereas the subscripts 0 and 1 refer to the inlet stream of oxidizer and fuel.

$$f = \frac{sY_{fu} - Y_{ox} + Y_{ox,0}}{sY_{fu,1} + Y_{ox,0}} \quad (3.26)$$

Temperature and species fractions, i.e. density-weighted average scalars, can be evaluated from the probability density function (PDF) and progress variable using Equation (3.27). Subscripts, u and b , in this expression correspond to unburnt and burnt mixtures, respectively.

$$\bar{\phi} = \bar{c} \int_0^1 \phi_b(f) p(f) df + (1 - \bar{c}) \int_0^1 \phi_u(f) p(f) df \quad (3.27)$$

The progress variable, on the other hand, can be expressed in terms of species mass fraction and calculated using Equation (3.28), where Y_i and $Y_{i,ad}$ are mass fraction of product species and mass fraction of species after complete combustion. The values of the progress variables range from 0 to 1, 0 is assigned for the unburnt mixture while 1 is assigned for the burnt mixture.

$$c = \left(\frac{\sum_{i=1}^n Y_i}{\sum_{i=1}^n Y_{i,ad}} \right) \quad (3.28)$$

The product formation of refers to the rate of the formation of products (or product formation rate, i.e., PFR) corresponds to the rate at which the product formation occurs and can be expressed by Equation (3.29).

$$PFR = \frac{\Delta[Products]}{\Delta t} \quad (3.29)$$

Flame thickness (δ) can be calculated from the correlation between unburnt thermal conductivity (λ_u), density (ρ_u), specific heat capacity (c_p), and laminar flame speed (S_L), as indicated in Equation (3.30).

$$\delta = \frac{\lambda_u}{\rho_u c_p S_L} \quad (3.30)$$

The laminar flame speed (S_L) for premixed reactants can be evaluated through an approximation method in CHEMKIN using Equation (3.31), where T^0 , T_b , T_u , and $Y_{f,u}^m$ represent layer temperature, burned temperature, unburned temperature and mass fraction of the unburned fuel.[227,228] Further details of the expression can be obtained from the study by Göttgens et al.[227]

$$S_L = AT^0 Y_{f,u}^m \frac{T_u}{T^0} \left(\frac{T_b - T^0}{T_b - T_u} \right)^2 \quad (3.31)$$

The Damköhler number (Da), evaluated from equation (3.32), refers to the ratio of reaction rate to diffusion rate. The terms l_t and u' indicate the integral length scale and root mean square (RMS) of velocity fluctuation.

$$Da = \frac{l_t / u'}{\delta / S_L} \quad (3.32)$$

Power density can be calculated from Equation (3.33). Here, $\dot{m}_{fuel}$ and CV_{fuel} are the mass flow rate and calorific value of fuel, whereas $V_{combustor}$ and $P_{combustor}$ are the volume and pressure of the combustor [222,229]. Calorific values of the CH₄, CO, H₂, and C₃H₈ are 55.5, 10.1, 141.8, and 50.3 MJ/kg, respectively [230].

$$PD = \frac{\dot{m}_{fuel} \times CV_{fuel}}{V_{combustor} \times P_{combustor}} \quad (3.33)$$

Pattern factor (PF) as provided in Equation (3.34) corresponds to the temperature uniformity at the combustor outlet, where $T_{maximum}$ and $T_{average}$ are the maximum and average temperatures at the outlet of the combustor, respectively [231].

$$Pattern\ factor = \frac{T_{maximum} - T_{average}}{T_{average} - T_{inlet}} \quad (3.34)$$

Thermal power (TP) is the power of the exhaust gases as expressed in Equation (3.34), where $\dot{m}_{air\ or\ oxidizer}$ and $\dot{m}_{fuel}$ refer to the mass flow rates of oxidizer and fuel, respectively. The term C_p is the mean heat capacity of the oxidizing mixture [232].

Thermal power

$$= (\dot{m}_{air\ or\ oxidizer} + \dot{m}_{fuel}) \times C_p \times (T_{average,outlet} - T_{inlet}) \quad (3.34)$$

3.2.2 Boundary conditions and meshing

3.2.2.1 Swirl-stabilized burner

Since the swirl-stabilized model gas turbine combustor was enclosed with a cylindrical quartz tube, an a quarter of the tubular combustor volume, as shown in **Figure 3.3**, was considered as the computational domain. Tetrahedral type meshing is adopted in the model along with the bias factor along the axial direction. Grid test was performed in different mesh sizes (element quantity: ~28K, ~33K and ~36K) in terms of the combustor axial temperatures as shown in **Figure 3.4**. Finally, a mesh of about ~29K cells, with fine meshes near combustor inlet and relatively coarser mesh near the outlet zone, was selected for the numerical investigation. Details of the grid independence test for the combustor model can be found in a previous numerical study by the Authors of the present study on the same combustor [233].

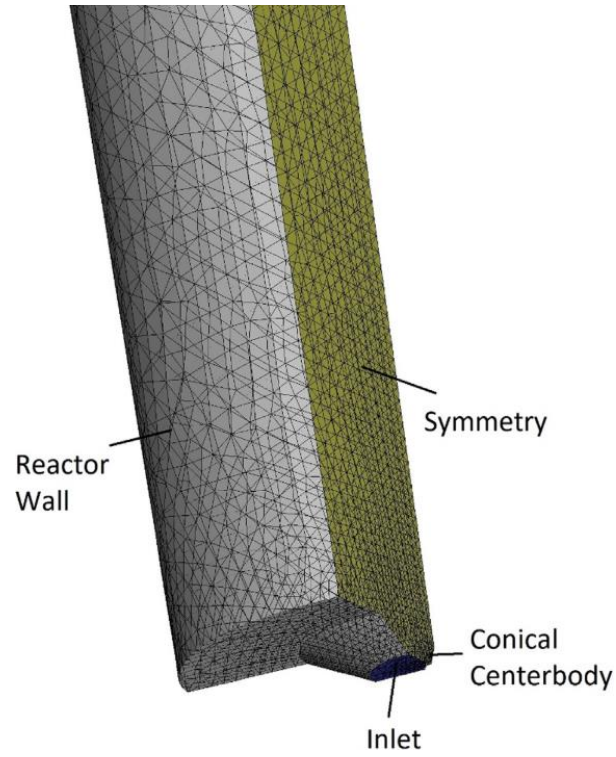


Figure 3.3: Combustor mesh and boundary conditions adopted in the developed numerical model for swirl-stabilized combustor.

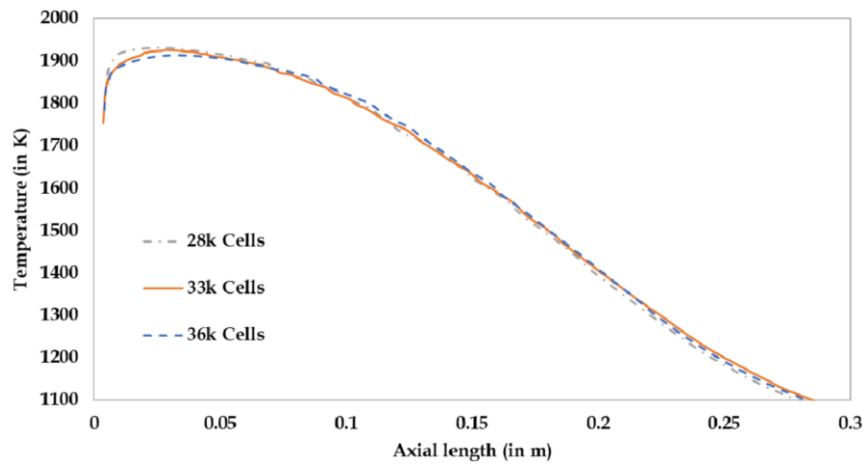


Figure 3.4: Mesh sensitivity analysis for swirl-stabilized combustor model [233].

A set of numerical simulation cases were performed considering different sets of fuel-oxidizer compositions at constant bulk throat velocity of 5.2 m/s injected into the combustion zone through the combustor headend. The axial and tangential components of the reactant mixture were set in the inlet boundary condition to achieve a swirl flow of $SN=0.98$. Partially premixed combustion was incorporated for species modeling, while the vortex method algorithm was utilized in solving for the fluctuating velocity. Mean mixture fraction was calculated for different inlet compositions of the reactants, whereas the corresponding laminar flame speeds were obtained from ANSYS CHEMKIN using the GRI-Mech 3.0 mechanism [234]. The velocity of the inlet flow, equivalence ratio, inlet reactant components and their mole fractions were specified to evaluate respective laminar flame speed. There for the first step, the inlet conditions of the reaction such as, inlet flow velocity, equivalence ratio, reactants, and their mole fractions. For the intermediate step, where freely propagating flame speed was considered and the data files for the gas phase kinetics, reactions thermodynamics, and gas transport was selected. Using the input values and the data files, the laminar flame speed was evaluated in the final step.

The combustor wall was set as a stationary wall with no-slip shear condition. Mixed type thermal boundary condition was considered, employing both and external-radiation heat transfer. Convective heat transfer coefficient for the wall was defined as $20 \text{ W/m}^2\text{K}$ with unity external emissivity, meanwhile temperatures for the external-radiation and free-stream were 300 K and 290 K, respectively. A range of convective heat transfer coefficients was tested, among which the one with $20 \text{ W/m}^2\text{K}$ demonstrated temperatures more comparable to the experimental temperatures. In addition, wall thickness of 6 mm was considered for the quartz wall with semi-transparent type boundary. Density, specific heat

and thermal conductivity of the quartz combustor wall were set to 2200 kg/m^3 , 671 J/kg.K and 1.3 W/m.K , whereas the refractive index was considered constant at 1.3. To accurately calculate for the tangential component of the swirling flow, the symmetry faces of the quadrant are regarded as periodic boundary condition.

3.2.2.2 Multi-hole burner

Steady state condition with gravitational effect is considered in the modeling using commercial CFD Software ANSYS Fluent 20R2. Standard k- ϵ model is employed to evaluate the turbulent flow inside the combustion chamber. Discrete ordinate (DO) model is selected to determine the radiation, where one iteration is performed per every ten energy iterations. Partial premixed combustion model is incorporated in the model for species modeling and modified for complete premixing of the inlet gases. The laminar flame speed is defined in each case which is obtained from ANSYS CHEMKIN using GRI-Mech 3.0 reaction mechanism [234]. SIMPLE algorithm is considered to couple the pressure and velocity. Least square cell based gradient is selected with second order discretization for the governing equations. The residuals for all equations are set at 10^{-6} to achieve more precise solution.

One sixth of the cylindrical combustion chamber is considered here to minimize the computational time. Since the inlet holes are distributed in a hexagonal manner in on the base-plate, thus $1/6^{\text{th}}$ of the volume is considered, as depicted in **Figure 3.2(b)** above. Velocity inlet boundary condition is employed in the inlets in such a way that all the inlet

holes supply identical fuel oxidizer mixture at a bulk velocity of 5.2 m/s. The inlet composition is defined by specifying the mean mixture fractions for each case. The base steel plate is considered as a no-slip wall with adiabatic thermal condition. Periodic symmetry is considered for the two cut-surfaces of the computational domain. No-slip wall with a fixed ambient temperature is considered for the quartz tube. Semi-transparent condition with external-radiation and convection is imposed to allow radiation and heat transfer through the quartz tube. The temperatures for external-radiation and free-stream are set at 300 and 290 K, respectively, whereas the convection heat transfer coefficient is specified at 20 W/m²K. The selected boundary conditions for different surfaces of the geometry are illustrated in **Figure 3.5**.

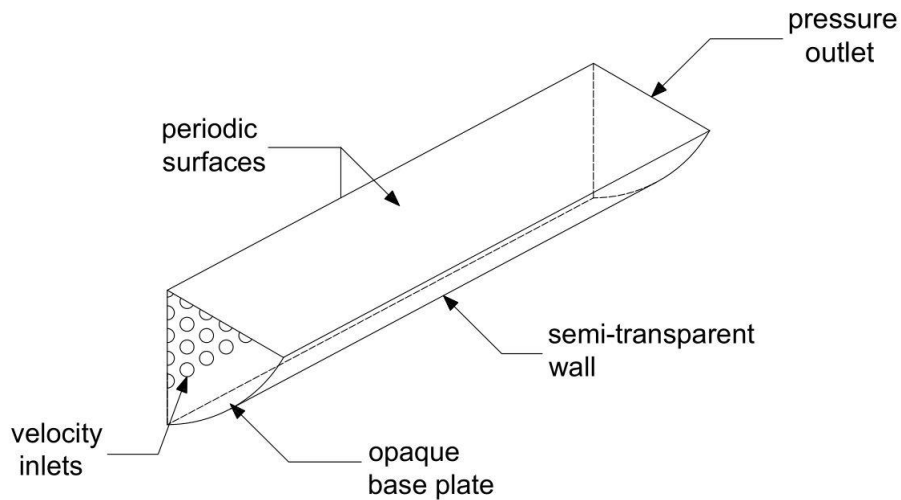


Figure 3.5: Boundary conditions for the computational domain of multi-hole combustor.

Hex-dominant element type has been incorporated in the meshing, as illustrated in **Figure 3.6**. Mesh bias has been employed to achieve finer meshing in the near burner region and coarser meshing in the near outlet zone of the combustor. This allows more mesh elements

to be congregated near inlet, resulting in more detailed calculation in the region where highest product formation from unburnt to burnt mixture takes place. Four different mesh sizes, i.e. 106k, 124k, 164k and 207k, have been examined prior to the investigation in different fuel-oxidizer composition. This grid independence test is carries out to eliminate the dependency of numerical results on mesh size.

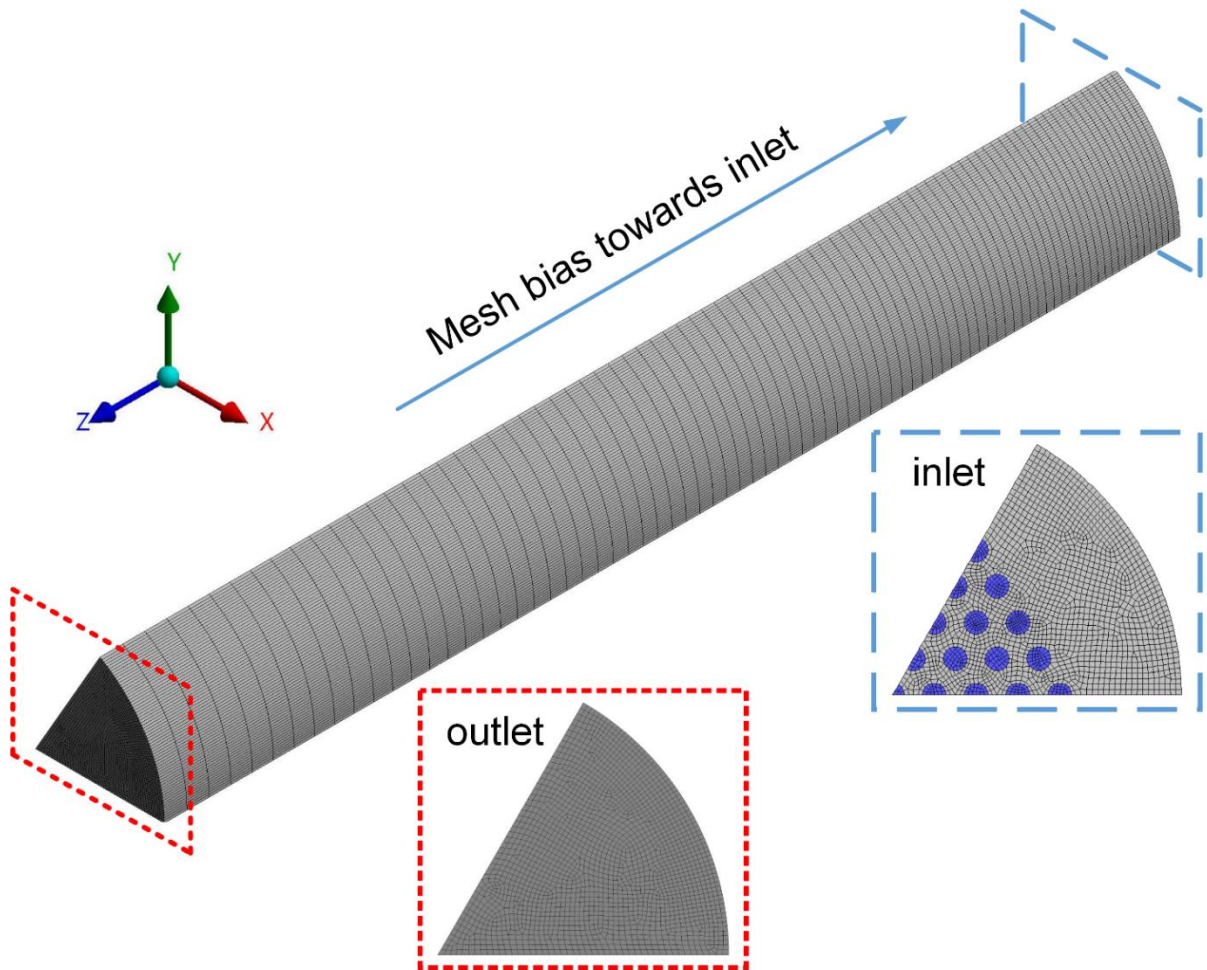


Figure 3.6: Meshing type used in the 3-D standard k- ϵ turbulence model.

Table 3.1 presents the variation in combustor temperatures and CO mole fractions at combustor outlet. Average overall combustor temperatures, axial temperature, outlet temperatures show less than 0.5% difference among the tested mesh sizes. The mole fractions of CO at combustor outlet, on the other hand, demonstrated a maximum of 3.55% variation with different mesh sizes. The meshes are further examined in terms of their axial (centerline axis of the combustor) temperature distributions, as depicted in **Figure 3.7**, where the mean difference of less than 1% (~0.07%) from the previous mesh was observed from mesh size of 164k. Thus, considering the variation in the studied parameters, the mesh configuration with 164k elements have been selected for the numerical investigation presented here. It is worth mentioning that the selected mesh has slightly over predicted CO emission compared to 124k elements and under predicted in contrast with 207k mesh elements.

Table 3.1: Combustor temperatures and CO emission in different meshing sizes for multi-hole burner.

Mesh size	1,06,141 (106k)	1,23,845 (124k)	1,63,778 (164k)	2,06,645 (207k)
Average combustor temperature (K)	1522.99	1523.03	1521.505	1520.58
Percentage difference from previous mesh size (%)	-	0.002823	0.10023	0.060832

Average combustor outlet temperature (K)	1372.73	1372.32	1368.56	1365.94
Percentage difference from previous mesh size (%)	-	0.030459	0.274156	0.191736
Average axial temperature (K)	1690.77	1689.92	1682.02	1684.56
Percentage difference from previous mesh size (%)		0.050594	0.469674	0.15089
Avg. outlet CO mole fraction at combustor exhaust	1.92×10^{-6}	1.88×10^{-6}	1.84×10^{-6}	1.78×10^{-6}
Percentage difference from previous mesh size (%)	-	1.945920	2.037669	3.552813

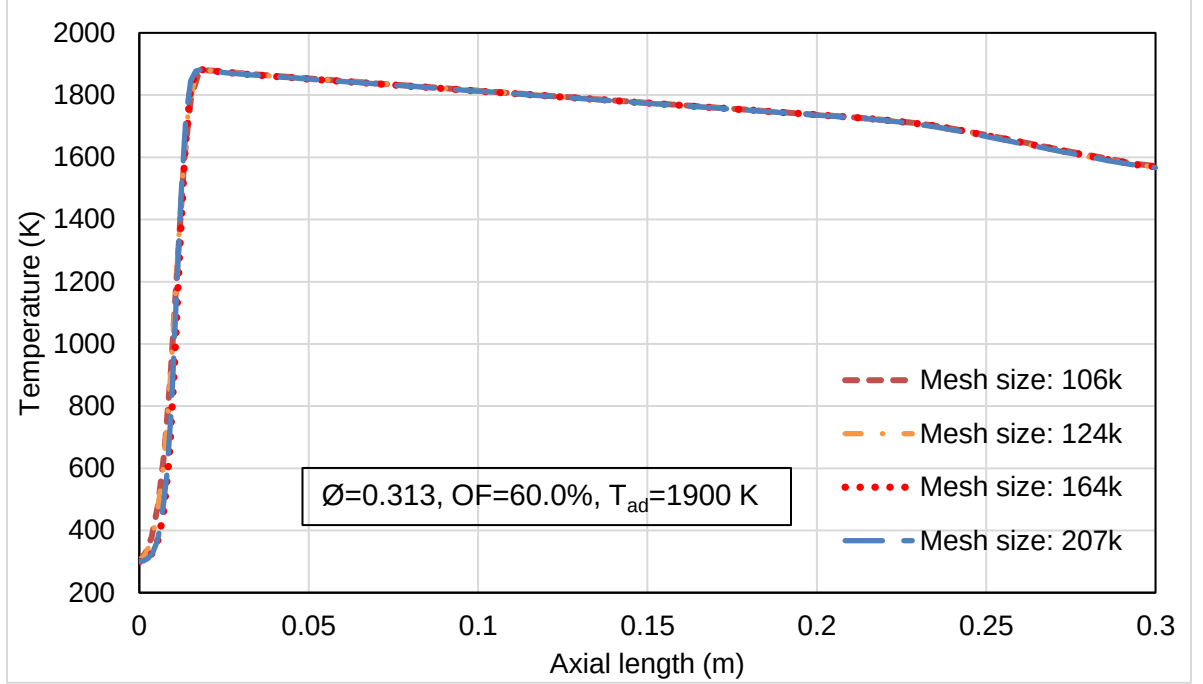


Figure 3.7: Axial temperature profiles in different meshes.

3.3 Validation of the developed model

The numerical model developed for the swirl-stabilized combustion in this study was validated using recorded experimental data in a previous study by the authors on oxy-propane combustion [151]. The case used for validation has $OF=0.30$ and $\Phi=89\%$. The calculated axial (at combustor centerline) and radial (at $z=10$ cm) temperature distributions using the present numerical model have been contrasted with the experimentally measured temperatures, as presented in **Figure 3.8**. The distributions show acceptable agreement between the calculated and the recorded data. A slight difference between the experimental and numerical temperatures is observed towards the combustor axis. This can be attributed to the high flame core temperature and error in temperature measurement with the

thermocouple. Simulation errors can also play an important factor in this temperature difference. On the other hand, the difference in temperatures becomes marginal towards the combustor wall. This is because the quartz combustor wall parameters are well validated against the physical setup. Moreover, The probability density function (PDF) model and LES turbulence model adopted in the numerical simulations in this study are widely used and validated in the open literature for the premixed turbulent flames [235–237]. Further comparisons of the numerical results and experimental data, in terms of flame macrostructure, are provided in the following section, and the comparisons show good levels of agreements as well. Further validation work has also been conducted for the oxy-methane and hydrogen-enriched oxy-methane flames. The details of the validation process can be obtained from numerical study on the same combustor on oxy-methane combustion for $\text{CH}_4/\text{O}_2/\text{CO}_2$ [172], $\text{CH}_4/\text{H}_2/\text{O}_2/\text{CO}_2$ [172,238] flames.

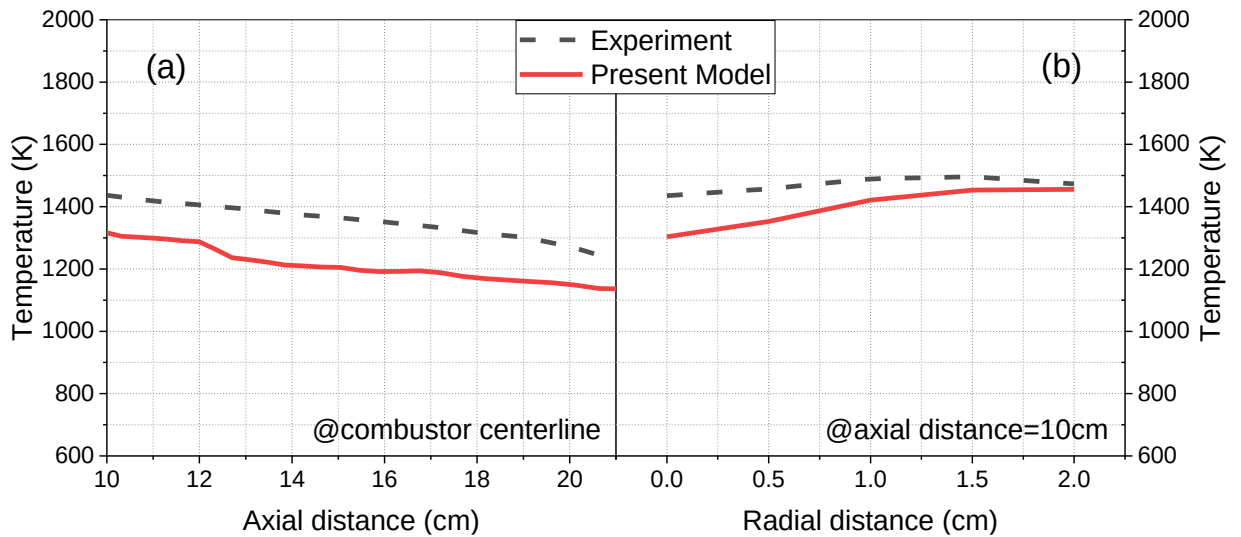


Figure 3.8: Numerical versus experimental temperature profiles along (a) axial direction and, (b) radial direction at an axial location of $z=10$ cm, $\text{OF}=0.30$, and $\Phi=89\%$.

Experimental data from Ref [151].

The Reynolds-Averaged Navier-Stokes (RANS) model used in the multi-hole combustor model (i.e. standard $k-\epsilon$ turbulence model) is used and validated in a wide variety of combustion simulations [239–242]. In order to evaluate the similarity between the simulation and the theoretical adiabatic flame temperatures, the maximum temperatures obtained from the model are contrasted with the corresponding theoretical adiabatic flame temperature for each case. **Figure 3.9** presents the simulated maximum temperature and theoretical T_{ad} for the studied cases, where the difference ranges from 1.01-4.61% marking the validity of the present numerical temperature data. The lower values of maximum temperature than respective T_{ads} are due to the heat loss through convection and radiation heat transfer considered in the model.

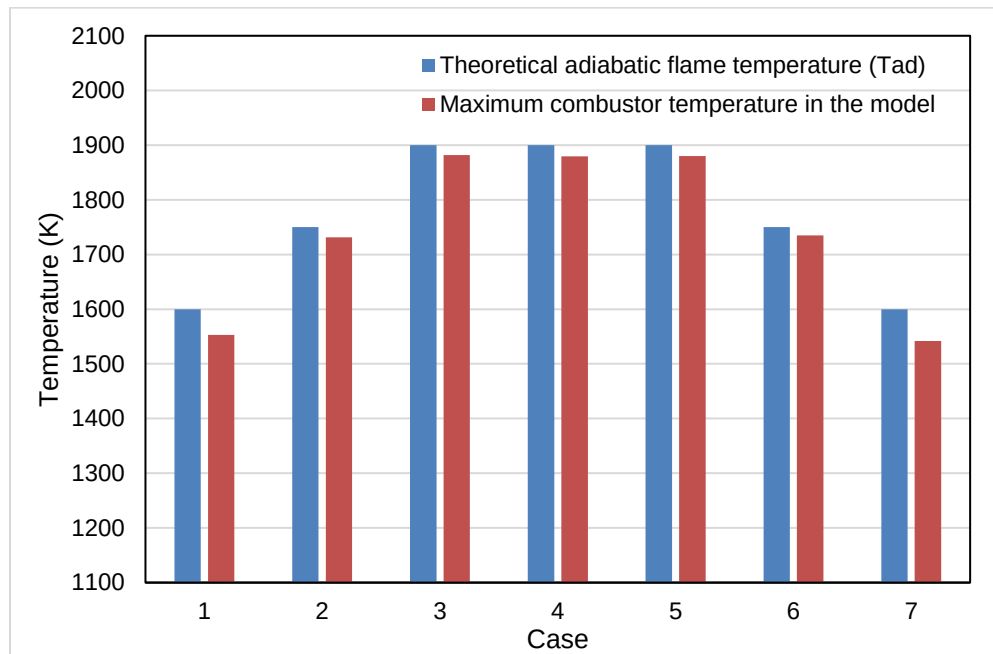


Figure 3.9: Comparison between model results and theoretical adiabatic flame temperatures in multi-hole burner.

CHAPTER 4

RESULTS AND DISCUSSION

Oxy-fuel flames are examined and assessed in terms of several combustion and emission characteristics. The investigation of oxy-combustion flames has been divided into four sections, (a) swirl-stabilized premixed oxy-propane flames in different feed composition, (b) effect of adiabatic flame temperature in oxy-methane flames in swirl-stabilized burner, (c) comparison of propane with methane and syngas under oxy-combustion in a swirl-stabilized combustor, and (c) premixed oxy-propane flames in a multi-hole gas turbine combustor.

4.1 Swirl-stabilized premixed $C_3H_8/O_2/CO_2$ flames in various fuel-oxidizer compositions

Premixed oxy-propane ($C_3H_8/O_2/CO_2$) flames have been investigated numerically different inlet mixture condition. A set of points within the stable combustion region was selected to present the change in flame shapes in different OF and ϕ within the stable combustion zone (**Figure 4.1**) presented in experimental study by Ali et al. [243]. The selected flames of different OF and Φ , are listed in **Table 4.1**. Here, cases 1-3 are at fixed OF (60%) and cases 6-7 are in constant Φ (0.50). Furthermore, since experimental results from Ali et al. [243] showed a strong influence of T_{ad} on lean flammability limit and this study studies oxy-fuel flames in the LPM condition, thus two cases (cases 4 & 5) are also examined in fixed T_{ad} (2302 K). Adiabatic flame temperature is defined as the maximum temperature of the combustion reactants that can be achieved under no heat loss to the surroundings. Adiabatic flame temperature is a function of Φ and OF, and is determined through iterative calculation using mixture composition, reaction enthalpy and enthalpies of formation. After modeling the selected cases, numerically obtained flames were compared in terms of flame shape, temperature distribution, velocity streamlines, vorticity, in addition to combustion and emissions characteristics. The results are presented here in a dimensionless manner independently of the combustor dimensions, where the axial and radial locations are expressed in relevance to the combustor length and diameter as Z/D and R/D , respectively.

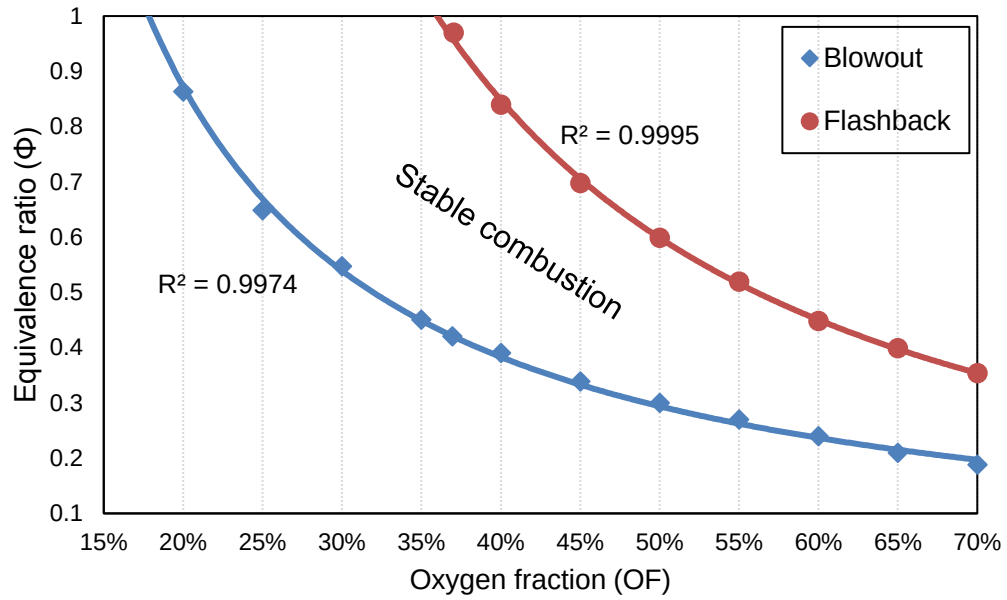


Figure 4.1: Static stability map, in terms of flame blowout and flashback limits, of the model gas turbine combustor holding $C_3H_8/O_2/CO_2$ flames at fixed bulk inlet velocity of 5.2 m/s [243].

Table 4.1: Conditions of oxy-propane flames considered in the present numerical study for swirl-stabilized combustor.

Case number	Equivalence ratio (Φ)	Oxygen fraction (OF)	Adiabatic flame temperature (T_{ad}), K	Remark
1	0.260	60%	1681	Fixed OF
2	0.340	60%	2006	
3	0.420	60%	2303	
4	0.597	45%	2302	

5	0.800	35%	2302	Fixed T_{ad}
6	0.500	48%	2156	
7	0.500	39%	1837	Fixed Φ
8	0.500	35%	1694	

4.1.1 Flame Macrostructure of $C_3H_8/O_2/CO_2$ flames

Flame visualization is a vital step towards comprehending combustion behavior and can provide insights into the flame extinction mechanisms. The experimental [151] and numerical flame shapes of the aforementioned cases are compared side by side in **Figure 4.2**. The experimental flame shapes were captured using a medium speed camera, while the numerical ones are expressed through the contours of OH radicals at the center-plane of the combustor. Flame shapes are vital in predicting combustion behavior and instability. Particle image velocimetry (PIV) is among the most used techniques for flame visualization where OH^* chemiluminescence is employed for evaluating the flame structure, reaction characteristics, heat release rates, etc. [244,245]. Thus, here the numerical flame shapes are also represented by the contours of OH radicals. It is to be noted that the quenching effect of the cold combustor bottom wall was not addressed in all simulation cases, which has resulted in slight deviations of the calculated flame shapes from the experimentally captured ones, as presented in **Figure 4.2**. The presence of dark regions at the combustor wall and ORZ (near burner headend) can be attributed to low

reactions rates due to this quenching effect of the cold combustor base wall. In contrast, the computational flames are visibly spread-out to the burner wall.

In **Figure 4.2**, the flame shapes for cases 1-3 represent the effect of varying Φ at fixed OF. For smaller Φ , case 1, the generated flame is tall and weak and has a spread-out shape. As Φ increases, T_{ad} also increases, making the flame stronger with heightened flame speed. The increase in flame speed (FS) can be seen from **Figure 4.3**. Due to this increase of T_{ad} and FS, the flames become relatively shorter and compact in case 2, and even more compact in case 3. Shortened flame length indicates the enhanced reactivity of the combustible mixture, which concurrently increases the concentrations of OH radicals within the combustor as the numerical flame shapes indicate in **Figure 4.2**. Increasing Φ , from case 1 to case 3, resulted in rise of OH concentrations. As Φ increases from cases 1-3, the presence of H atoms increases in the mixture which reacts with oxygen and results in increased Oh concentration. The flame shapes obtained in cases 4 and 5 from both experiments and simulations are almost identical in shape. This can be attributed to the fact that these two flames have the same T_{ad} , which aligns with the findings from the experiment [151]. Similar conclusions were reported in previous studies [93,106,107,151,208,229]. Despite being of different Φ , the flame lengths of these two cases are alike because of the different OF values for the two flames to have the same T_{ad} . Furthermore, $C_3H_8/O_2/CO_2$ flames in swirl-stabilized combustors acquire the characteristic V-shape at higher T_{ad} . The V-shape is clearly visible in the numerical contours, since the shapes are presented by the center-plane contours of OH radicals. Meanwhile, for the experimental setup utilizes a medium speed DSLR camera which is incapable of capturing the center-place radical distribution in the flame. This makes it difficult to identify the V-shape from the

experimentally captured flame images. The influence of varying OF at constant Φ can be observed by comparing the flame shapes for the cases 6-8. Here, the flame in case 6 is short and strong, the flame in case 7 is relatively weaker and taller, and the flame in case 8 is the tallest and weakest among these three flames. Since reactivity is enhanced in oxygen-rich environments with the accelerated combustion chemistry and, consequently, improved flame speed (see **Figure 4.3**), the flame becomes weaker when going from case 6 to case 8 due to the scarcity of oxygen within the combustor. The reduced chemistry also affects the OH concentration, which can be clearly seen from the numerical representation of these three flames. The computational flame structures also indicate the spread-out nature of the flame at lower OF. Among all these cases, the discrepancy between the experimental and numerical flames in cases- 1, 3, 6 and 8 can be attributed to several factors. The use of medium speed camera to capture photographic images of the flames acts as a contributing factor for the difference in experimental and numerical flame visualization, since it is inapt in capturing the OH* radicals utilizing the OH* chemiluminescence like some ultra-violet cameras. Furthermore, the current model is limited only to the anchored flame. This inability of generating a lifted flame in the developed model also plays a vital role in the variation between in experimental and numerical flame images.

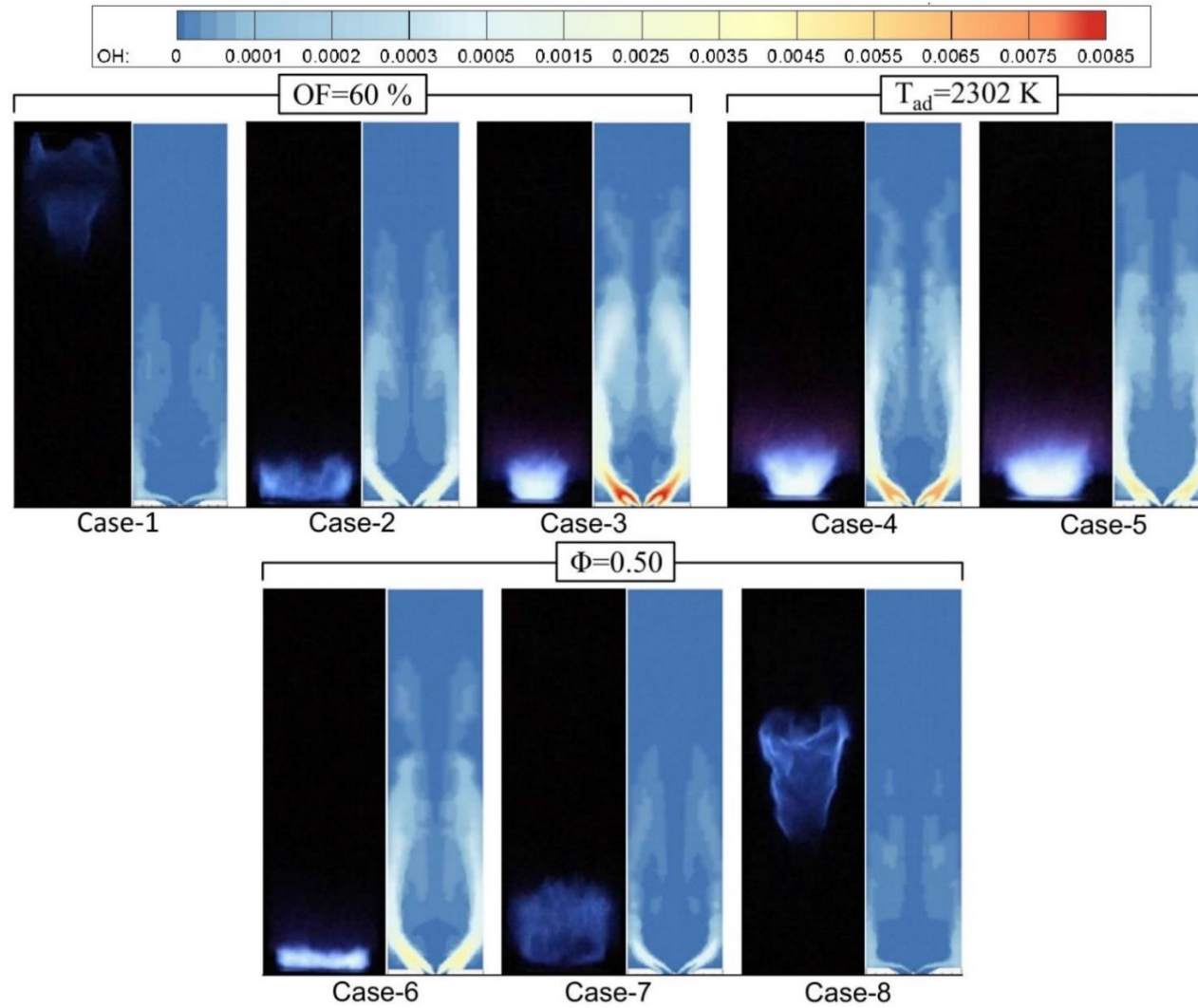


Figure 4.2: Comparison of experimental (captured using a medium-speed camera) and numerical (based on OH contours) flame shapes for the cases 1-8 under different operating conditions.

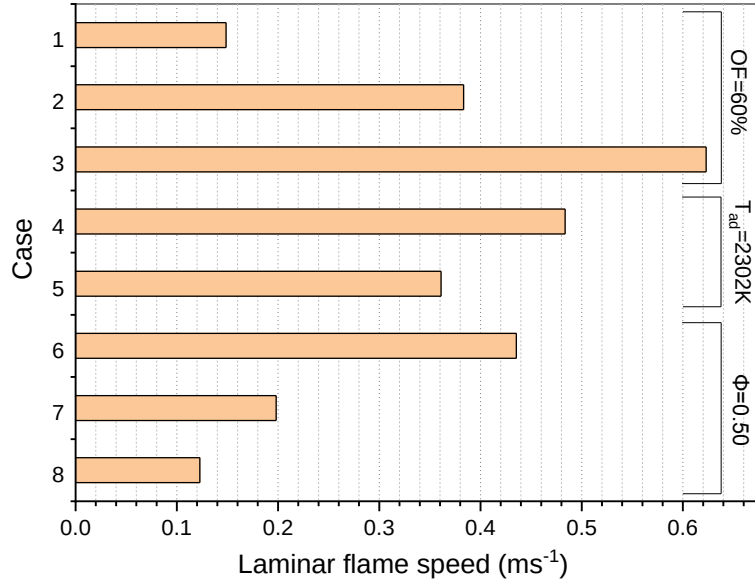


Figure 4.3: Laminar flame speed of the different cases under investigation of different operating parameters.

4.1.2 Flow-field structure of C₃H₈/O₂/CO₂ flames

The above analysis of flame shape and macrostructure are complemented here with a deep dive into the flowfield structure, which is useful for understanding how the flame is stabilized and why it assumes a certain shape within the combustor. The flowfields of the eight examined cases are investigated in terms of the calculated velocity streamlines and contours of vorticity magnitude, along with their corresponding temperature distributions. The creation of recirculation zones, primarily the outer recirculation zone (ORZ) near the combustor wall and the inner recirculation zone (IRZ) near the combustor centerline, play vital roles in flame stability, as are discussed in succeeding section. In experimental conditions, these zones can be identified from the formation of eddies using particle image

velocimetry (PIV) formation. In the simulations both these zones can be distinguished and comprehended from the velocity streamlines inside the combustion zone. Vorticity, on the other hand, shows the tendency for rotation in the flowfield and is important in the formation of turbulent eddies. Combustion temperature is one of the most important parameters for the design and manufacturing of any combustion system; temperature is thus examined here in a detailed manner.

Figure 4.4 illustrates the velocity streamlines over center-plane contours of combustion temperature. The IRZ and ORZ are identifiable by eddies in the flowfield. In all cases, the presence of two IRZs is evident, one near the inlet and another near the outlet of the combustor, whereas the ORZ is seen only in stable flames (cases 2-7). The flame, i.e., primary reaction zone, is recognizable by the high-temperature region between the IRZ and ORZ, which explains why both play vital roles in flame stability.

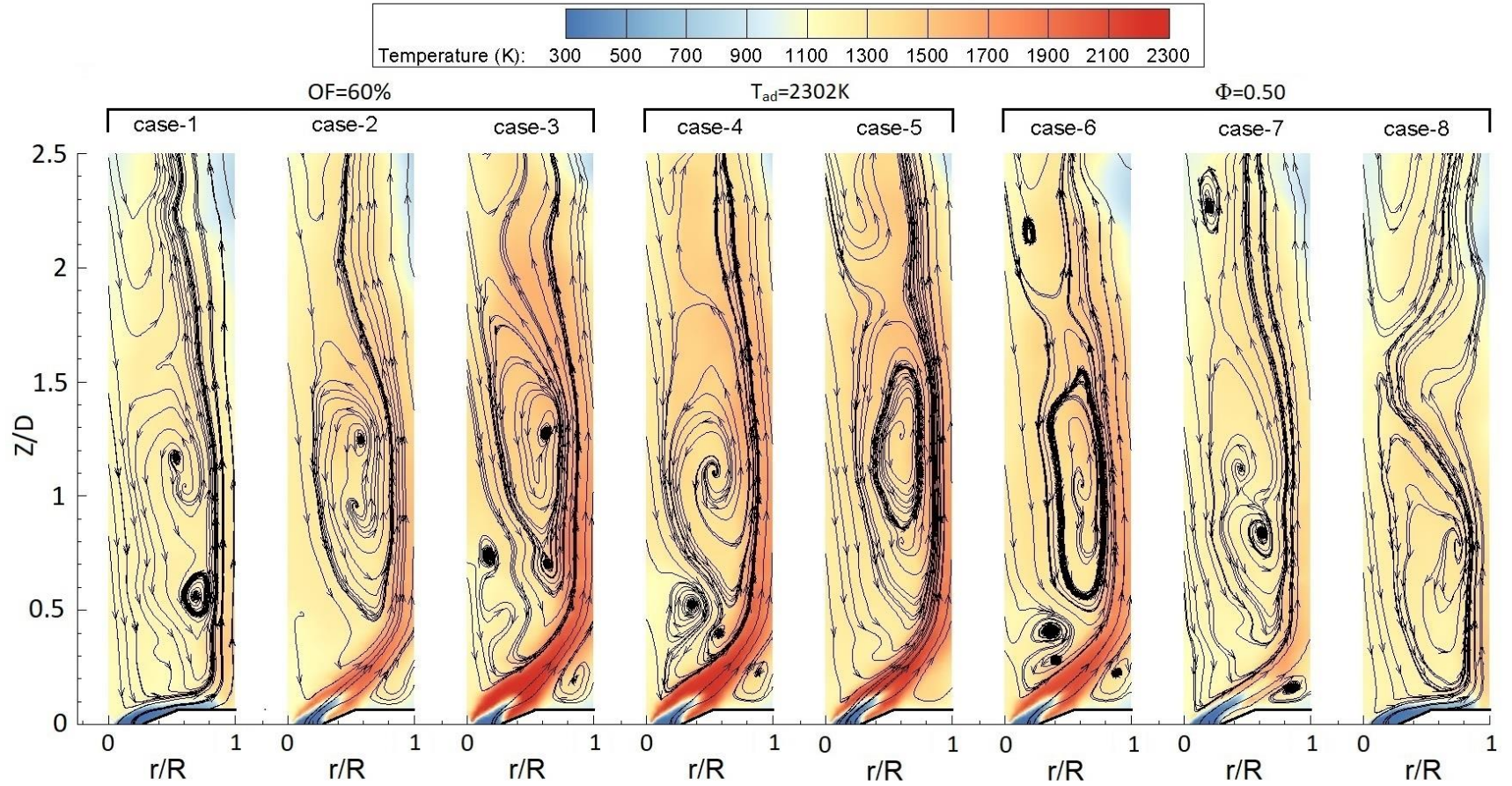


Figure 4.4: Velocity streamlines mapped over the contours of combustor temperature for the different flame cases.

The effect of increasing Φ at fixed OF=60% can be observed from cases 1-3. At lower equivalence ratio ($\Phi=0.24$, case 1), the flame is weaker and spread-out, compared to the flames at $\Phi=0.34$ (case 2) and $\Phi=0.42$ (case 3). The spread-out flame eliminated the formation of an ORZ in case 1. As Φ increases, the ORZ starts to appear in form of a small clockwise eddy, and at $\Phi=0.42$, the spinning of the eddy becomes stronger. At higher Φ , the FS is greater, resulting in the formation of a more intense ORZ after the sudden expansion of the reacting mixture into the larger combustor volume. Therefore, the eddy in ORZ can be regulated by controlling the value of operating Φ , similar to what was concluded in a study of air-propane combustion in a backward-facing step combustor [246]. The intense eddy formation aides in improvement turbulent mixing of the species, as a result the reaction rate also improves leading to thicker and stronger reaction zone [247]. Furthermore, the probability density function (PDF) approach, incorporated in the simulations, plays a vital role in modeling the interaction between the turbulence and chemistry of the reacting flow [226].

Increasing Φ also affects the turbulent eddies within the IRZ. Two eddies, spinning counterclockwise, can be seen from the combustor inlet to an axial location of $Z/D=1.5$ in case 1. Increasing Φ to 0.34 in case 2 causes these eddies to merge into one larger eddy of two epicenters that is shifted downstream. At $\Phi=0.42$ (case 3), the merged counterclockwise-spinning eddy becomes stronger and moves further downstream, to be located within the range $0.5 \leq Z/D \leq 2$. Nevertheless, with this shift of the larger primary eddy, a smaller clockwise-spinning one appears within $0.5 \leq Z/D \leq 1$ in case 3. The formation of the smaller secondary eddy indicates turbulence-reactions interaction within the flame. The shifting of the eddies away from the combustor inlet can be attributed to the increased

flame speed at elevated Φ (**Figure 4.3**), exhibiting firm anchoring of the flame to the burner inlet. This phenomenon was also reported in a recent work by the authors on hydrogen-enriched oxy-methane combustion [172], where the formation of secondary eddy and the downstream shifting of the eddies were observed with increased hydrogen addition. In the present case of oxy-propane combustion, the hydrogen content in the flame increases with the increase of Φ , which affects the IRZ in a manner analogous to that of hydrogen-enriched oxy-methane combustion.

The velocity streamlines in cases 4 and 5 of common $T_{ad}=2302$ K show that each flame has a large counterclockwise-spinning primary eddy located within the range $0.5 \leq Z/D \leq 2$. However, in case 4, two additional secondary eddies, spinning opposite to each other, appear in the IRZ near the combustor inlet. Additionally, the circulation in the ORZ is more visible in case 4, compared to that in case 5. The higher OF in case 4 plays a significant role in improving the combustion chemistry and, subsequently, leads to the creation of these additional eddies.

Aside from these minor differences between cases 4 and 5, it can be seen that they exhibit nearly identical temperature profiles. **Figure 4.5** sheds more light on this similarity by showing the radial temperature contours at different axial locations in these two cases. It can be seen that the temperature distributions for both cases are almost identical, despite having different OF and Φ . These comparable temperature profiles can be attributed to the identical T_{ad} for both cases. Similar findings were also reported from the earlier experimental work [151]. At $Z/D=0.5$, two temperature zones are distinguishable: a high-temperature (1600-1900 K) zone near combustor wall and a relatively lower temperature zone (case 4: 1200-1500 K, case 5: 1300-1500 K) at the center region. Due to the swirl

effect the reaction zone is pushed towards the wall of the combustor, this causes the creation of high-temperature at zone near wall and low-temperature at combustor axis. Temperature profiles at $Z/D=1.5$ show that the temperature is almost evenly distributed along the radius, and the temperature ranges from 1300 K to 1500 K for case 4 and from 1200 K to 1500 K for case 5. At $Z/D=2.5$, three temperature zones are observed for the two cases: inner and outer zones of relatively low temperature, in addition to a third zone of higher temperature located in-between the inner and outer zones. The outer and inner zones have almost similar temperature ranges, namely (1200-1300 K) and (800-1200 K) for cases 4 and 5, respectively, while the temperature in the third middle zone ranges from 1300 to 1400 K. The temperature profiles at $Z/D=3.5$ show similar trends to those obtained at $Z/D=2.5$. At $Z/D=3.5$, the temperatures in the inner, outer, and middle zones are about 1100 K, (900-1100 K), and 1200 K, respectively for both cases 4 and 5. From $Z/D=0.5$ to 3.5, sharp radial temperature gradient reduces as an effect of the inner-recirculation zone. IRZ circulates high-temperature species from the combustor wall towards center and causes temperature distribution more uniform as the flow progresses downstream.

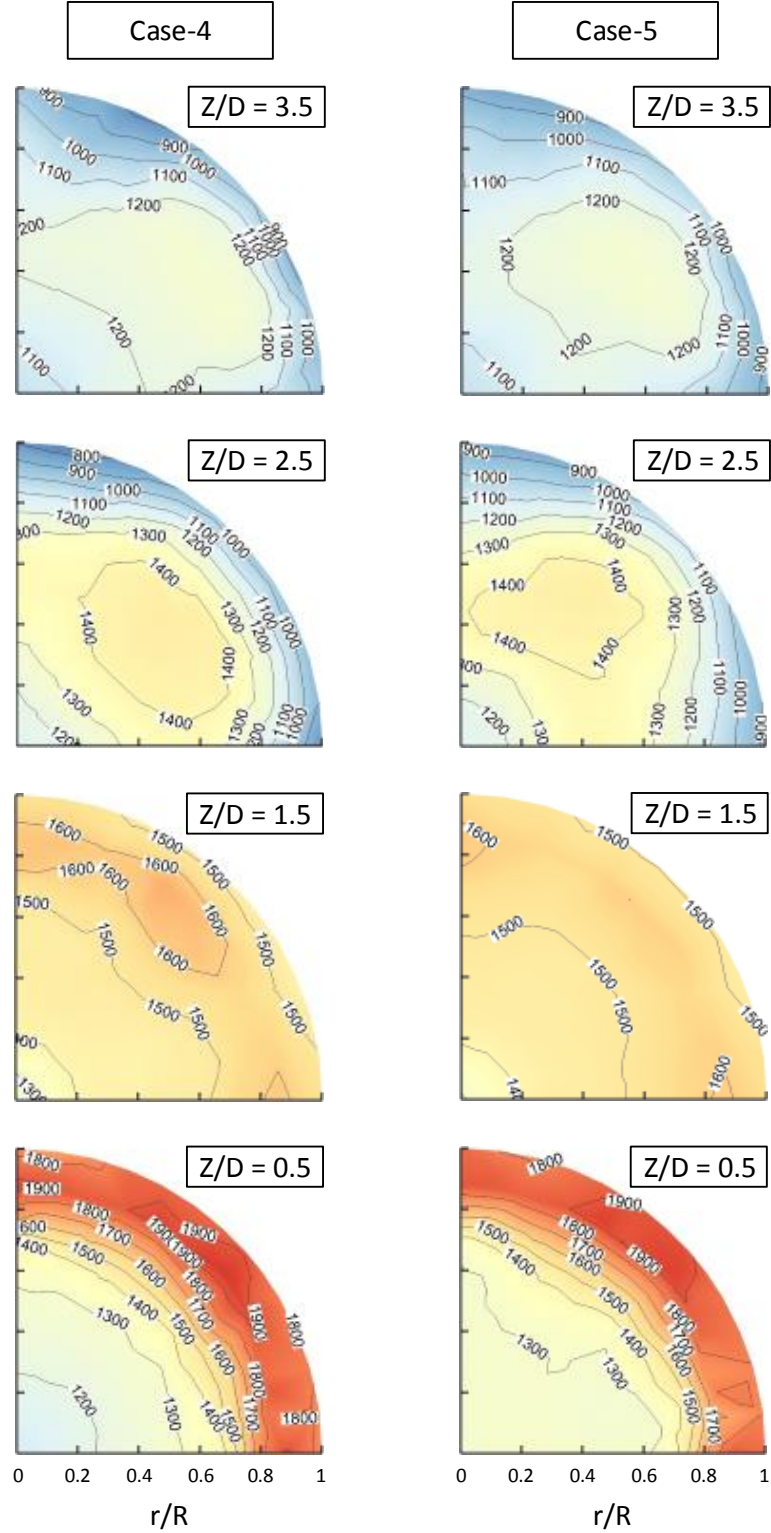


Figure 4.5: Temperature (K) contour plots for flame cases 4 and 5 of the same adiabatic flame temperature of 2302 K at different axial location of $Z/D = 0.5, 1.5, 2.5$ and 3.5 .

The effect of OF on the formation of eddies is evident in cases 6-8 at fixed $\Phi=0.5$ in **Figure 4.4** above. At higher OF=48% (case 6), a primary eddy forms and rotates counterclockwise within the zone $0.5 \leq Z/D \leq 1.5$, while two secondary eddies (spinning opposite to each other) are visible between the combustor inlet and $Z/D=0.5$ within the IRZ. At OF=39% (case 7), the secondary eddies disappear, whereas the primary eddy becomes larger and shifts upstream. At the lowest OF=35% (case 8), the primary eddy in the IRZ becomes weaker and moves towards the combustor inlet even more. The ORZ is also strongly affected by OF; strong rotation can be seen in the ORZ at higher OFs. The ORZ weakens and reduces in size as the OF decreases and the flame spreads out. At OF=35% (case 8), the flame is fully spread-out, eliminating the ORZ and making the flame more unstable.

Figure 4.6 depicts the velocity streamline over temperature contours on radial planes at $Z/D=0.5$ and 1.5 to demonstrate the change in flowfield in radial directions. In all the cases the majority of the streamlines are near the combustor wall at $Z/D=0.5$. This can be attributed to the shifting of the reaction zone (between the inner and outer shear layers) towards the wall due to the swirling effect as shown in **Figure 4.4**. The swirling effect induced by the swirler vanes mainly contribute to the shifting of this reaction area near the wall. On the other hand, the radial velocity streamlines at axial position of $Z/D=1.5$ are observed to be converging towards the center line axis of the combustor. Recall Figure 8, where the primary IRZs for the flames ends near (of right after) $Z/D=1.5$ which allows the species stream to move from the combustor walls. Moreover, as the flow progress downstream, the swirling effect on the flame also decrease.

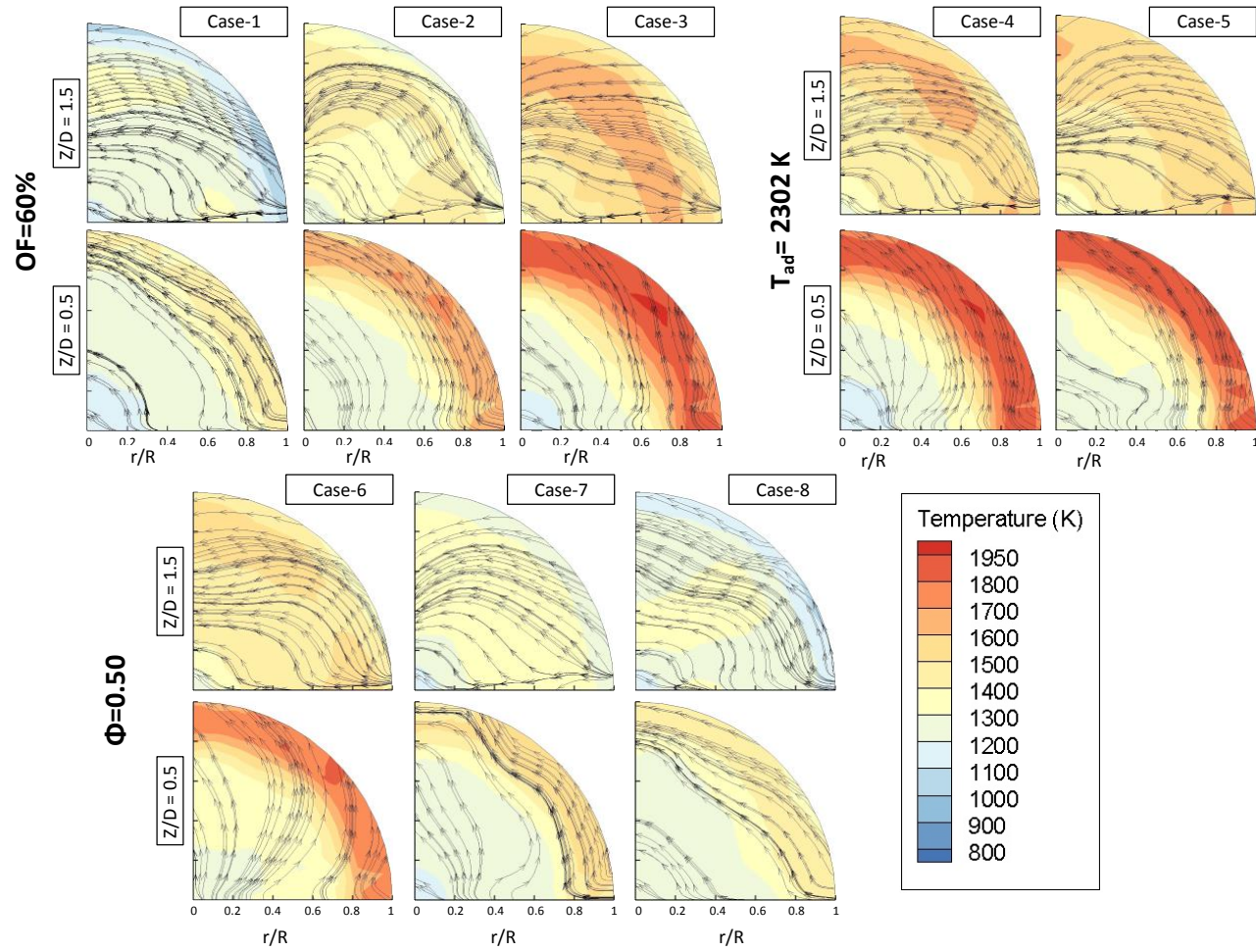


Figure 4.6: Velocity streamlines mapped over the contours of combustor temperature for the different flame cases at $Z/D=0.5$ and 1.5 .

Figure 4.7 depicts the distributions of vorticity magnitude, along with their corresponding temperature contours, for the eight examined cases. The regions of high vorticity indicate the inner shear layer (ISL) between the IRZ and flame, as well as the outer shear layer (OSL) between the flame and ORZ. This confirms that the flame (highest temperature) is stabilized between the two shear layers and two recirculation zones, as explained earlier. As Φ increases at fixed OF (cases 1-3), the ISL thickness increases slightly, which can be attributed to the elevated vorticity level near the central axis. Furthermore, the reaction zone between ISL and OSL becomes thicker and reaches higher temperature, which increases the buoyant forces, shifts the IRZ eddies downstream, and, consequently, increases the vorticity. This explains why the IRZ has been observed to shift downstream at higher Φ in **Figure 4.4**. The vorticity levels are somewhat identical for cases 4 and 5 of constant T_{ad} ; however, vorticity is marginally higher in case 4 due to its higher OF. As the OF reduces from 48% (case 6) to 35% (case 8), the vorticity reduces alongside the thickness and length of OSL, which eliminates the ORZ and, consequently, makes the flame weaker.

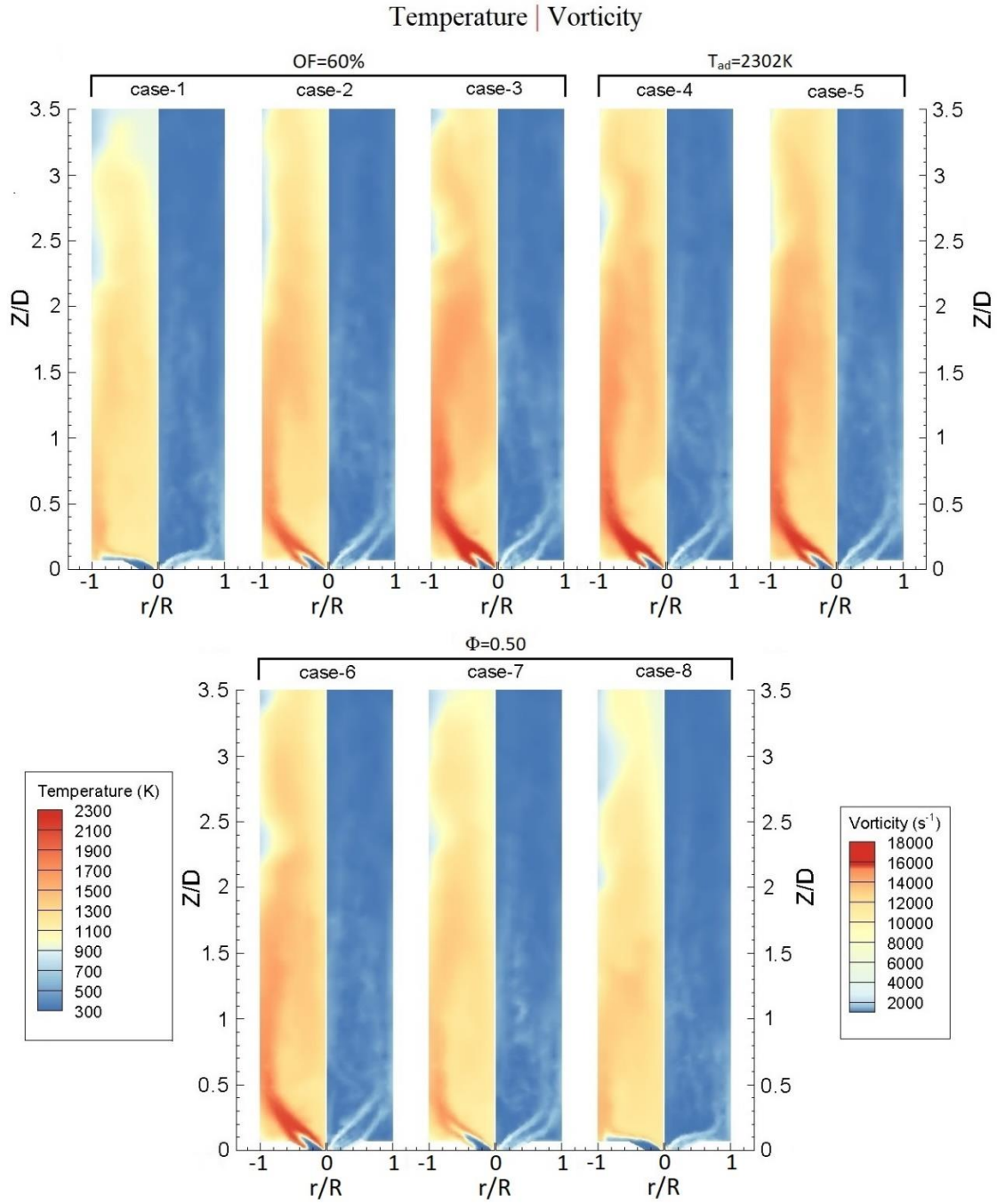


Figure 4.7: Contours of temperature (left) and vorticity (right) for the different flame cases.

4.1.3 Combustion characteristics of $C_3H_8/O_2/CO_2$ flames

Some combustion characteristics of the present $C_3H_8/O_2/CO_2$ flames are discussed in this section in terms of product formation rate (PFR), progress variable, flame thickness (δ), and Damköhler number (Da). As the name implies, PFR refers to the rate at which the products are formed, while the progress variable represents the transition from unburnt mixture to fully burnt mixture. δ refers to the thickness within which the unburnt mixture is heated to the ignition temperature by the reaction zone. Da represents the ratio between the reaction rate and the diffusion rate. High Da number indicate faster forward reaction rates while low values indicate that the reactions are kinetically controlled [248].

Figure 4.8 exhibits the center-plane contours of PFR (left side) and progress variable (right side) near the combustor inlet (up to $Z/D=1.5$). At lower Φ , case 1, the PFR can be seen only in the ISL, whereas the OSL is not visible due to the spread-out nature of this weak unstable flame. Increasing Φ from case 1 to case 3, the PFR rises in both ISL and OSL, and its spatial distribution becomes more compact, indicating shorter and stronger flame. The progress variable also follows a similar trend, and the transition region from unburnt mixture to completely burnt products also becomes shorter. It is worth mentioning that, although the numerical code is inept of capturing the transition from the ORZ to the IRZ stabilization modes,[249] the switch can still be realized through the PFR trends. For cases 4 and 5 of identical T_{ad} (2302 K), the PFR is stronger in case 4 with a smaller region of unburnt mixture. This can be attributed to lower Φ and higher OF (less fuel, more O_2 , less diluent) in case 4, which helps the fuel-oxidizer mixture burn faster and achieve a more compact flame than that in case 5, since the chemical aspect of flame dominates the rate of

combustion.[238] In cases 6-8, the effect of reducing OF is analogous to that of reducing Φ from case 3 to case 1; as OF decreases, the flame length increases up to case 8, where the PFR can be seen only in the ISL, while the OSL is not visible due to the spread-out nature of this weak unstable flame.

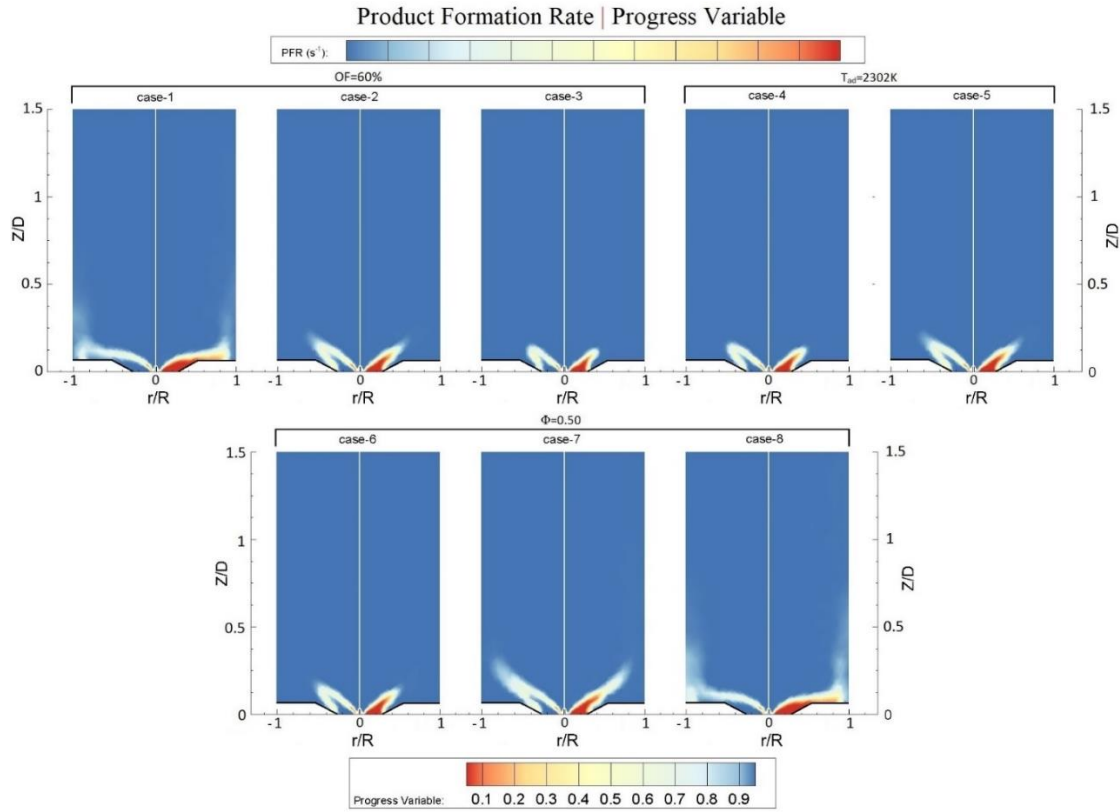


Figure 4.8: Contours of product formation rate (left) and progress variable (right) for $C_3H_8/O_2/CO_2$ flames at different flow conditions.

Figure 4.9 presents the flame thickness and Damköhler number for the different flame cases. It can be seen that δ reduces with the increase in Φ at fixed OF because of the more compact flame size observed at higher Φ . Moreover, the compact structure refers to a

stronger flame with significantly higher Da, as observed in **Figure 4.9(b)**. Higher Da value here is due to faster reaction rates as compared to the turbulent mixing rates. Since the flame is more compact in case 4 compared to case 5, as concluded from Figure 12, the flame thickness is lower ($64.7 \mu\text{m}$) with greater Da (45.1) in case 4, compared to $\delta=84.7 \mu\text{m}$ and Da=26.3 in case 5. Lastly, the flame thickness increases and Da decreases with the reduction in OF at fixed Φ for cases 6-8. This confirms that the effect of reducing OF is analogous to that of reducing Φ , as discussed in **Figure 4.8**.

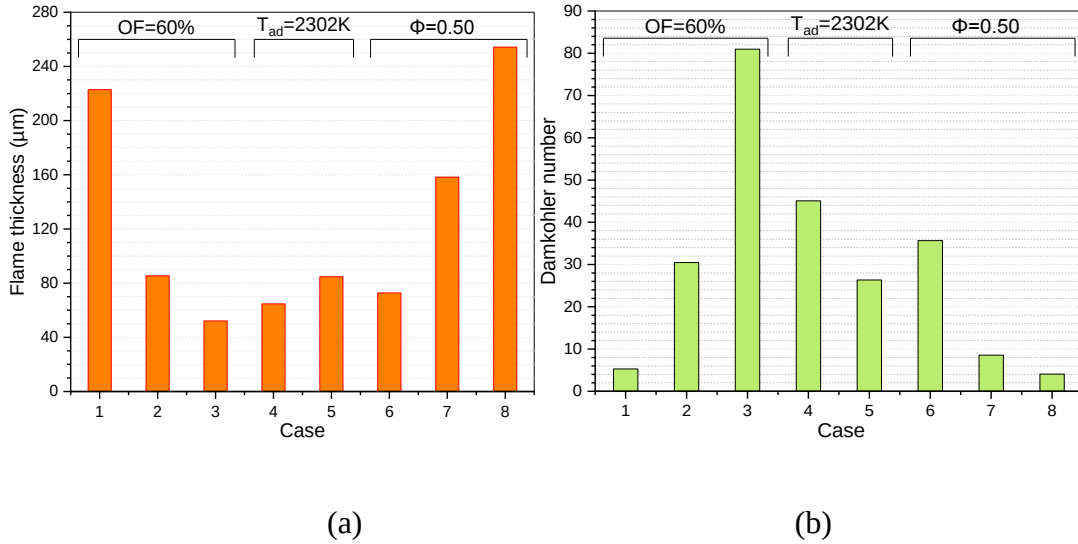


Figure 4.9: Effect of mixture composition on (a) flame thickness and (b) Damköhler number.

4.1.4 Emission attributes of $\text{C}_3\text{H}_8/\text{O}_2/\text{CO}_2$ flames

The distributions of the mole fractions of C_3H_8 , O_2 , CO , and CO_2 within the combustor can provide deeper insight into flame structure, reaction progression, and emission characteristics. **Figure 4.10** depicts the distributions of C_3H_8 and CO mole fractions. Propane is more spread-out towards the corner of the combustor and the presence of CO is marginal in case 1. At a lower Φ ($\text{OF}=60\%$), the supply of oxidizer is adequate for both C and H atoms in the fuel. As Φ increases, the concentration of C_3H_8 reduces, and CO concentration increases. This can be attributed to the higher flame speed (**Figure 4.3**) and reaction rates at higher Φ , resulting in complete burning of C_3H_8 . Moreover, at higher Φ , carbon has to compete with hydrogen for oxygen, which increases the CO concentration, since the H and O atoms tend to react more quickly. This also explains the reduced oxidation of CO to CO_2 , which is another reason for the increased CO in the combustor. Cases 4 and 5 can also be explained using the same mechanism. The concentrations of C_3H_8 and CO are higher in case 5, compared to those in case 4, due to the higher Φ and lower OF of case 5. Among the cases 6-8, the CO mole fraction reduces with the decrease in OF at fixed $\Phi=0.5$. This is attributed to lower flame speed (**Figure 4.3**) and retarded reaction rates that hinder the burning of C_3H_8 , which is an additional proof that the effect of reducing OF is analogous to that of reducing Φ .

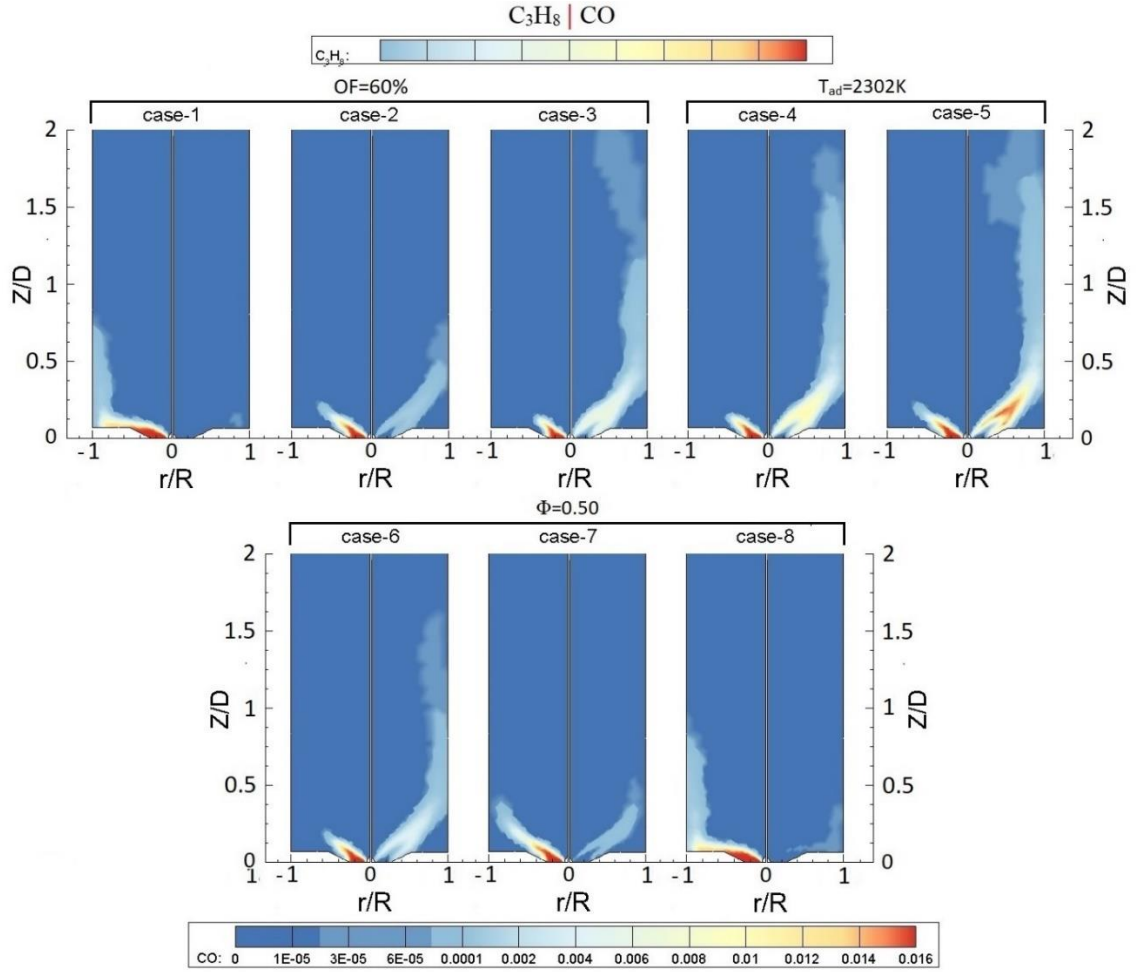


Figure 4.10: Contours of mole fractions of C_3H_8 (left) and CO (right) for the different flame cases.

The concentrations of CO in parts per million (ppm) along the combustor centerline are presented in **Figure 4.11** for all examined cases, while **Figure 4.12** plots the average C_3H_8 and CO concentrations at combustor exit to quantify incomplete combustion. As shown in **Figure 4.11**, the majority of CO emission is produced within the axial range $0 \leq Z/D \leq 2.5$. This can be attributed to the effect of IRZ existing within the same axial range. As the flow progresses towards the exit, some of the CO reacts with the available oxygen and converts to CO_2 . Accordingly, the CO emission at combustor outlet is much lower than the

maximum value of its axial distribution. Among the different mixture compositions, case 5 ($\Phi=0.8$ and $OF=35\%$) demonstrated the highest CO emission both in the axial direction within the combustor and at combustor exit. As previously discussed in **Figure 4.10**, case 5 contains relatively more fuel and less oxygen than all the other cases due to its higher Φ and lower OF . Because of such relatively fuel-rich condition, the fuel does not get enough oxygen to react with, thus cannot convert completely to CO_2 and, subsequently, results in higher CO emission than the other cases.

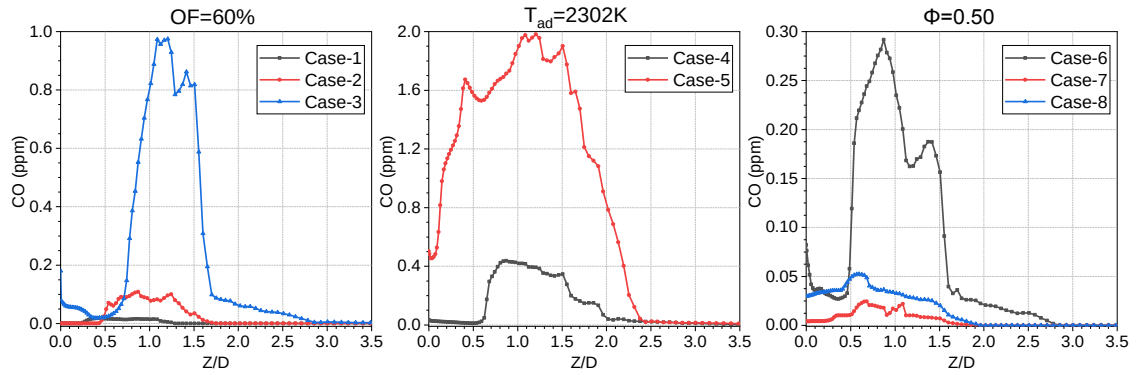


Figure 4.11: CO concentrations along the combustor centerline for the different flame cases.

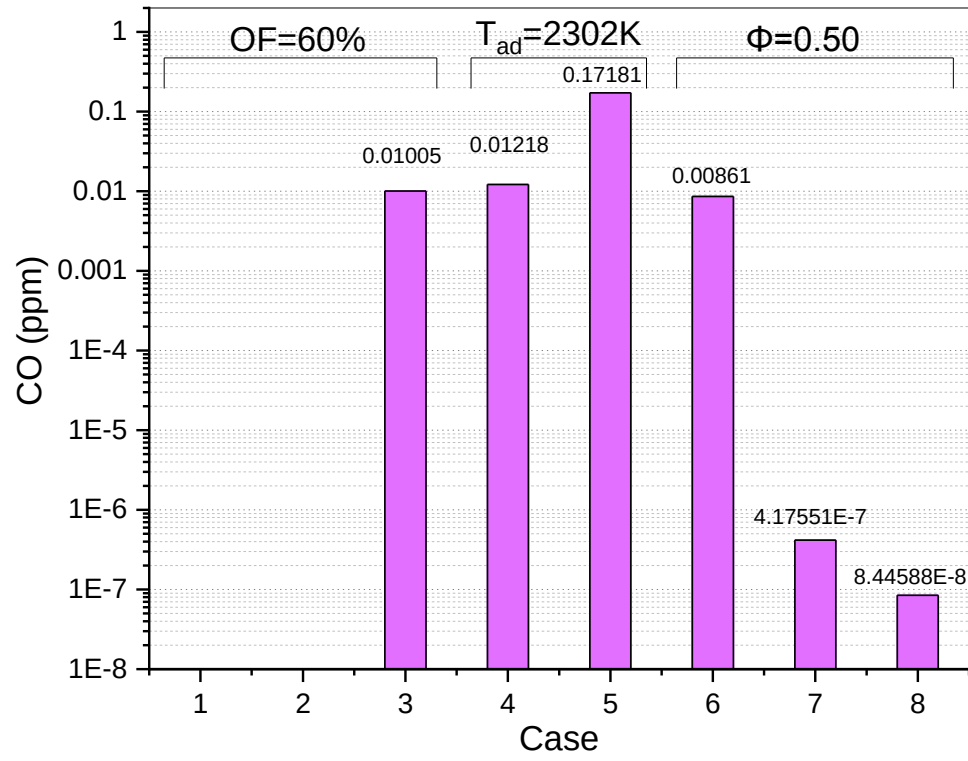


Figure 4.12: Average CO concentrations at combustor outlet for the different oxy-propane flame cases.

4.2 Effect of adiabatic flame temperature in oxy-methane flames in swirl-stabilized burner

Oxy-fuel flames of methane are investigated in this section to determine wide variety of characteristics in terms of, temperature and flow fields, vorticity, product formation rate (PFR), progress variable (PV), and species concentrations. Inlet fuel-oxidizer mixture is diluted with CO₂ and well premixed and swirl, in a swirler of 55° swirl angle, upstream before entering the combustor at inlet bulk flow velocity of 5.2 m/s under atmospheric conditions. The results are presented in a dimensionless manner where the radial and axial directions are expressed as R/D and Z/D, respectively. Here, Z, R and D refer to the length, radius and diameter of the combustor, respectively. Various inlet compositions examined in this section to evaluate the AFT effect are listed in **Table 4.2**. The results are presented in a dimensionless manner where the radial and axial directions are expressed as R/D and Z/D, respectively, where Z, R, and D refer to the length, radius, and diameter of the combustor, respectively.

Table 4.2: Test matrix for different adiabatic flame temperature conditions for CH₄/O₂/CO₂ flames.

Case #	AFT (K)	Oxygen fraction (OF)	Equivalence ratio (Φ)
A1	2500 k	35%	0.954
A2		50%	0.627
A3		65%	0.451
B3	2300 k		0.395
C3	2100 k		0.342

4.2.1 Velocity streamlines over temperature contour of CH₄/O₂/CO₂ flames

Visualization of flame shape is one of the preliminary steps in understanding the flame-flow interactions and can provide perception on flame stability and extinction mechanisms. In order to assess the flow field structure of the oxy-methane flames, **Figure 4.13** and **Figure 4.14** present the velocity streamlines plotted over the temperature contours at OF=65% and over a range of AFT and in different OF at AFT=2500 K, respectively. The formation of inner recirculation zone (IRZ) and outer recirculation zone (ORZ) characterizes the overall features of turbulent reacting flow field. Stronger recirculations in the IRZ can be observed at lower AFT (case A3) than those for the flame at higher AFT (Case C3), as shown in Figure 3a. This may be attributed to the increased flow rates to the

combustor to operate at lower AFT resulting in better flow swirling and interactions between the burned and unburned gases. The IRZ expands in size further towards downstream of the combustor with the decrease in AFT from case A3 (AFT=2500 K) to case B3 (AFT=2300 K), with counterclockwise flow circulation at axial distances of $0 \leq Z/D \leq 1.3$ and $0 \leq Z/D \leq 1.5$, respectively. Then, the IRZ splits into two counter-rotating eddies for case C3 at AFT=2500 K and spans over longer axial distance of $0 \leq Z/D \leq 1.7$. The ORZs, on the other hand, are almost identical for flames of different AFT at fixed OF. The change in OF at same AFT does not result in significant changes in the shape and size of the IRZ as shown in Figure 3b. Almost identical flame shapes are obtained at fixed AFT indicating the dominant role of AFT in controlling flame shape and stability of premixed oxy-methane flames. The ORZ is almost similar, where the recirculation intensity slightly increases with the rise in OF. So, the shape and size of the IRZ dominate the flame shape and flame-flow interactions whatever the operating AFT and OF.

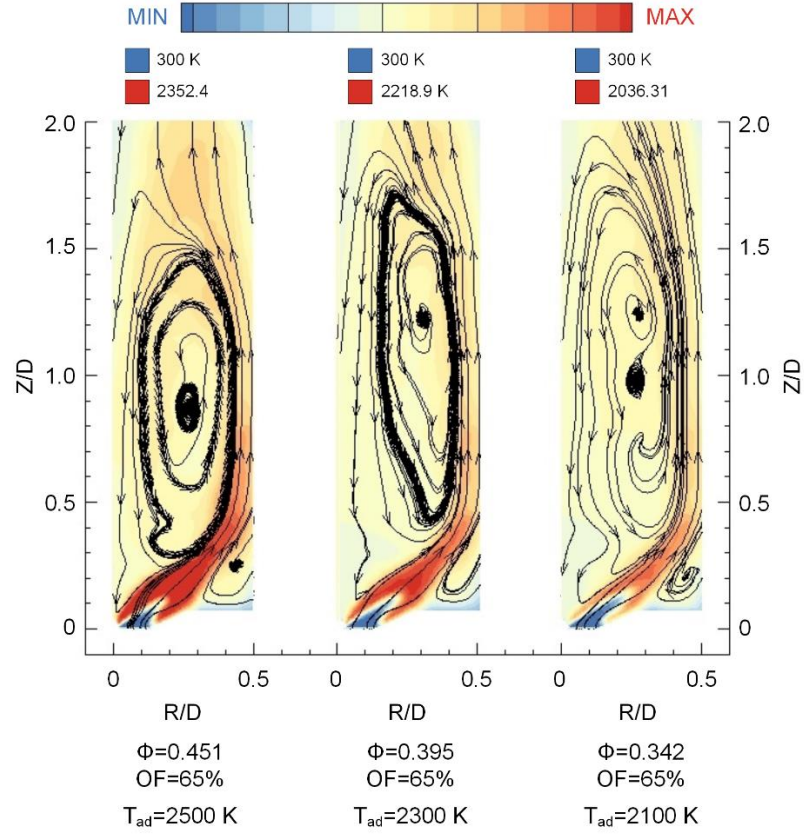


Figure 4.13: Velocity streamlines mapped over temperature contours at fixed OF of 65% and AFTs of 2500K (A3), 2300K (B3), and 2100K (C3) for oxy-methane flames.

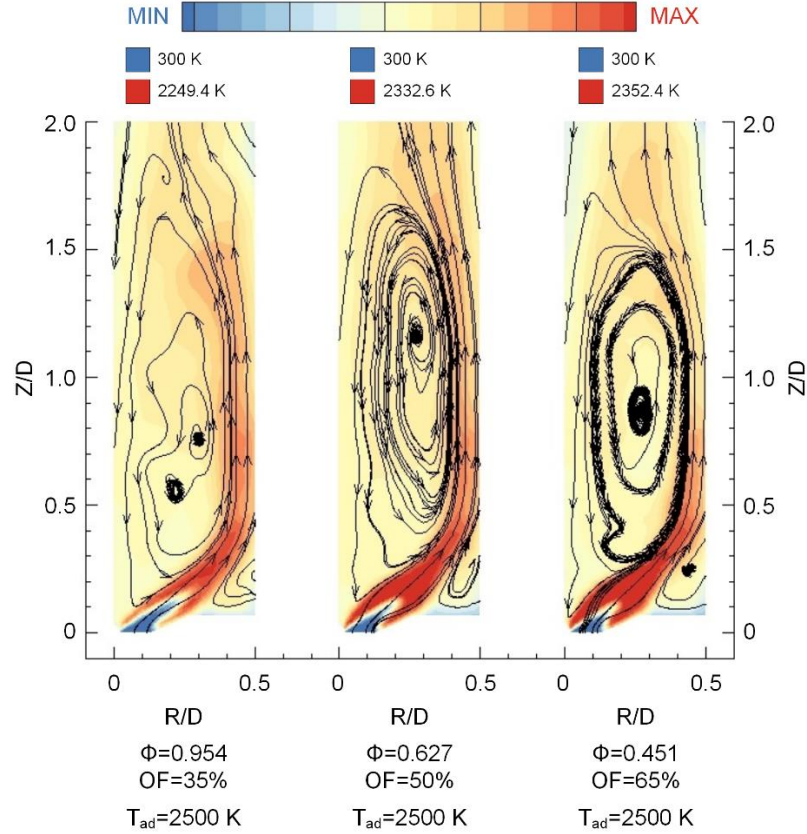


Figure 4.14: Velocity streamlines mapped over temperature contours at fixed AFT of 2500K and OFs of 35% (A1), 50% (A2), and 65% (A3) for oxy-methane flames.

4.2.2 Temperature and vorticity in $\text{CH}_4/\text{O}_2/\text{CO}_2$ flames

The rotation tendency of gas mixture along with the eddy formation inside the combustion chamber is further discussed in this section. **Figure 4.15** and **Figure 4.16** illustrate the temperature and vorticity distributions on the center-plane of the combustor. The temperature in the flame core increases with the adiabatic flame temperature. Majority of the combustion reactions take place in the flame core, which is surrounded by the inner shear layer (ISL) and the outer shear layer (OSL), as illustrated in the vorticity contours.

The length of the ISL decreases with the decrease in AFT at fixed OF. The thickness of the flame core between ISL and OSL also reduces with the reduction in AFT. This can be attributed to the increased vorticity level in higher AFT. High flame temperature increases the buoyant forces in the combustor and increases the vorticity magnitude. Likewise, the vorticity level rises with the increase in OF, making the ISL shorter and thicker, which subsequently results in a compact oxy-methane flame (depicted in **Figure 4.16**).

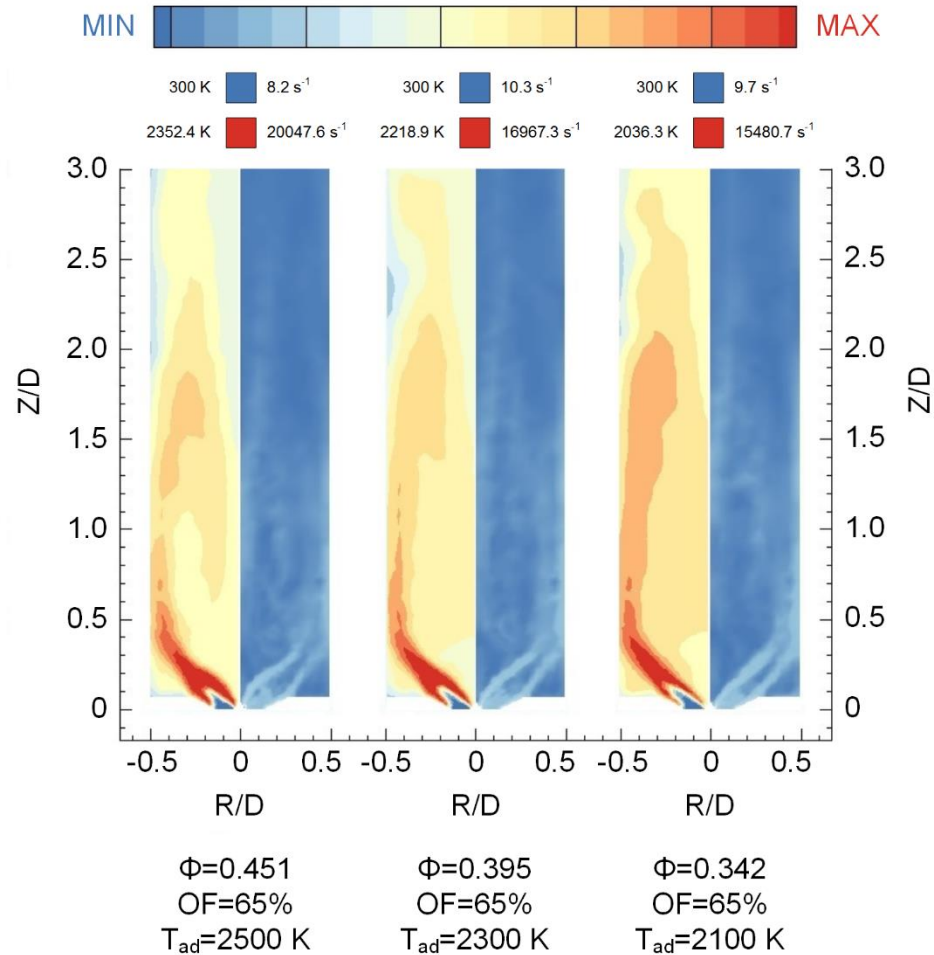


Figure 4.15:Temperature and vorticity contours at fixed OF of 65% and AFTs of 2500K (A3), 2300K (B3), and 2100K (C3).

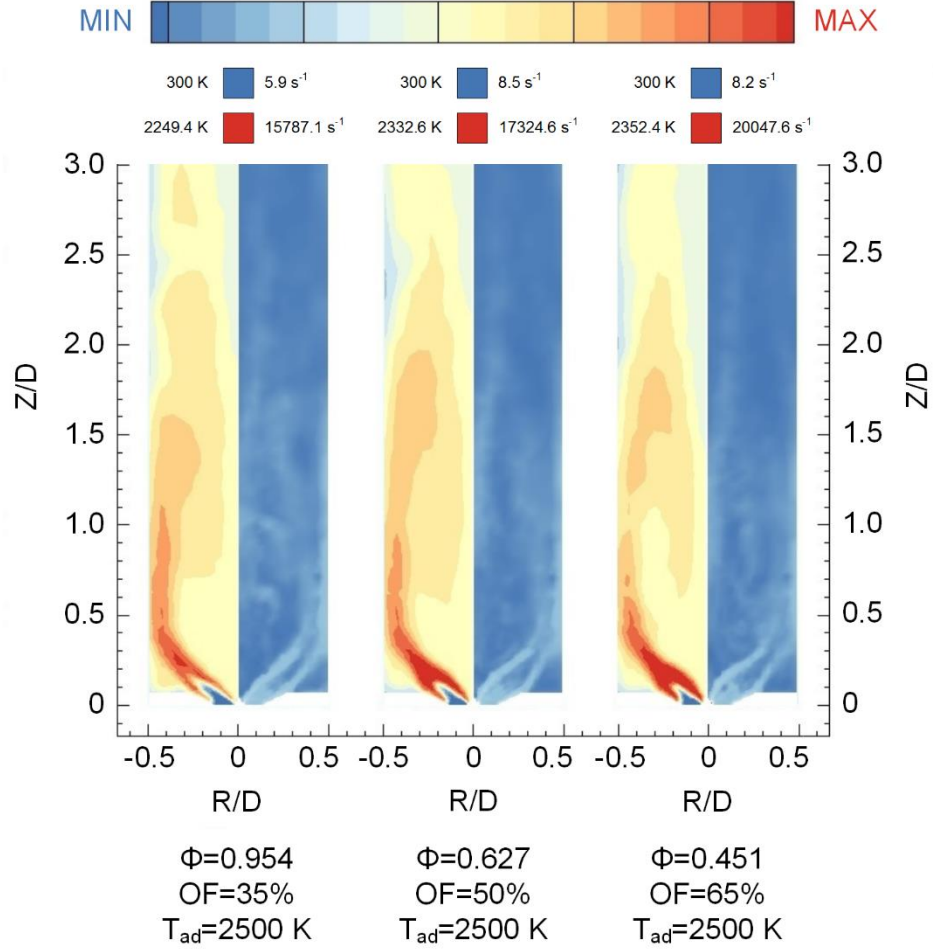


Figure 4.16: Temperature and vorticity contours at fixed AFT of 2500K and OFs of 35% (A1), 50% (A2), and 65% (A3).

Figure 4.17, **Figure 4.18** and **Figure 4.19** illustrate the temperature profiles within the combustor in axial and radial directions, respectively. As shown in **Figure 4.17**, the combustor in axial direction increases from the inlet to $\sim Z/D=0.7$ for AFT=2500 K while the temperature increase can take place upto $\sim Z/D=1.3$ for lower AFTs. This is attributed to the compact nature of the flame in elevated AFT as presented in **Figure 4.15** above. The gradual temperature decrease after this point is due to the creation of eddies in IRZ, which

distributes the convective heat within this zone. For a fixed AFT of 2500 K, the rise in temperature is observed upto $\sim Z/D = 0.7$, 1.1 and 0.7 for 35%, 50% and 65% OF, respectively.

Figure 4.17 and **Figure 4.18** illustrate the axial temperature profiles within the combustor over ranges of AFTs and OFs. At higher AFT, namely at 2500 K, the axial temperature increases rapidly from the inlet temperature until it reaches its maximum at $\sim Z/D=0.7$, then it decreases sharply towards the combustor exit section. Such changes in temperature distributions are more uniform when operating the combustor at low to moderate AFTs. This can be attributed to the compact nature of the flame in elevated AFT as presented in **Figure 4.15** above. As well, the reduction in Φ at lower AFTs allow for more oxidizer flow rate to the combustor resulting in better flow swirl and stronger recirculation zones (see **Figure 4.13**) that causes more uniform temperature profiles. The flames at fixed AFT of 2500 K showed reduced combustion temperature when increasing the OF from 35% to 65%. This can be attributed to the significant reduction Φ , from 0.954 to 0.451, that results in more excess oxidizer flow rate to the combustor, which cools down the flame.

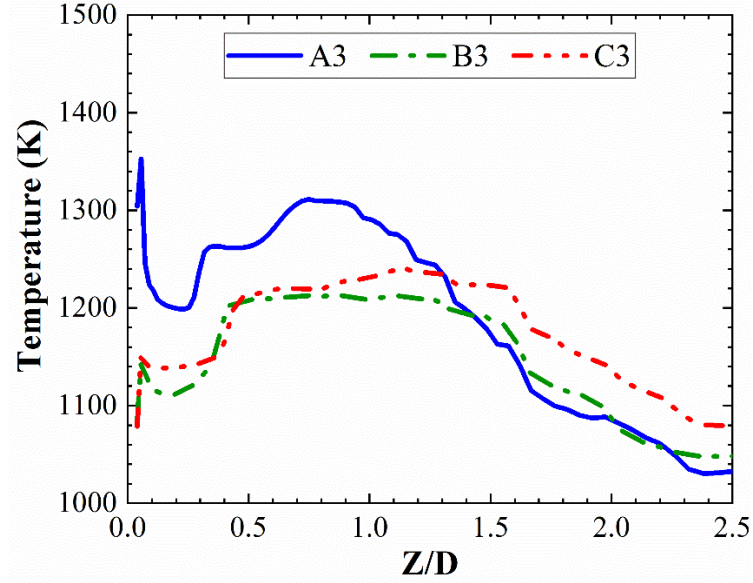


Figure 4.17: Axial temperature distributions at fixed OF of 65% and AFTs of 2500K (A3), 2300K (B3), and 2100K (C3).

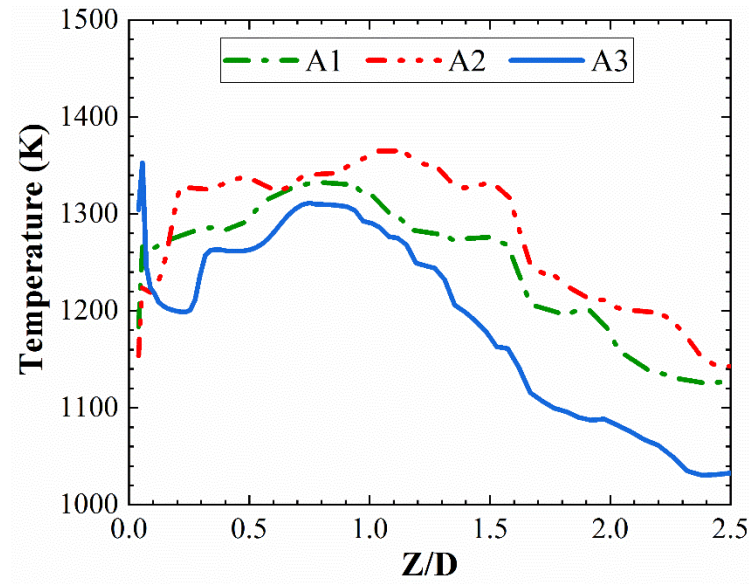


Figure 4.18: Axial temperature distributions at fixed AFT of 2500K and OFs of 35% (A1), 50% (A2), and 65% (A3).

The radial temperature distributions at different axial distances ($Z/D=0.5, 1.5, 2.5$, and 3.5) for the studied cases are provided in **Figure 4.19**. In **Figure 4.19**, the temperature increases almost marginally up to $R/D=0.3$ at $Z/D=0.5$, elevates sharply till $R/D=0.43$, and decreases again due to heat transfer through the combustor wall. At $Z/D=1.5$, temperatures increase till $R/D=0.42$ and then starts decreasing. Temperatures at this axial point range from 1100 K to 1600 K. At $Z/D=2.5$, the temperatures, ranging from 700 K to 1400 K, increase from the Center point to $\sim R/D=0.2$ (up to $R/D=0.28$ for some cases) and then decrease. Lastly, the radial temperatures near exit ($Z/D=3.5$) range from 700 K to 1200 K for all the cases, where temperatures increase until $\sim R/D=0.38$. The changes in the radial temperature profiles are sharper at low to moderate AFTs due to the enhanced flow recirculation and wider IRZ. Fixing the operating AFT does not result in significant changes in radial temperature profiles due to the similarity of shape and size of the IRZ (see **Figure 4.14** above) when fixing the AFT.

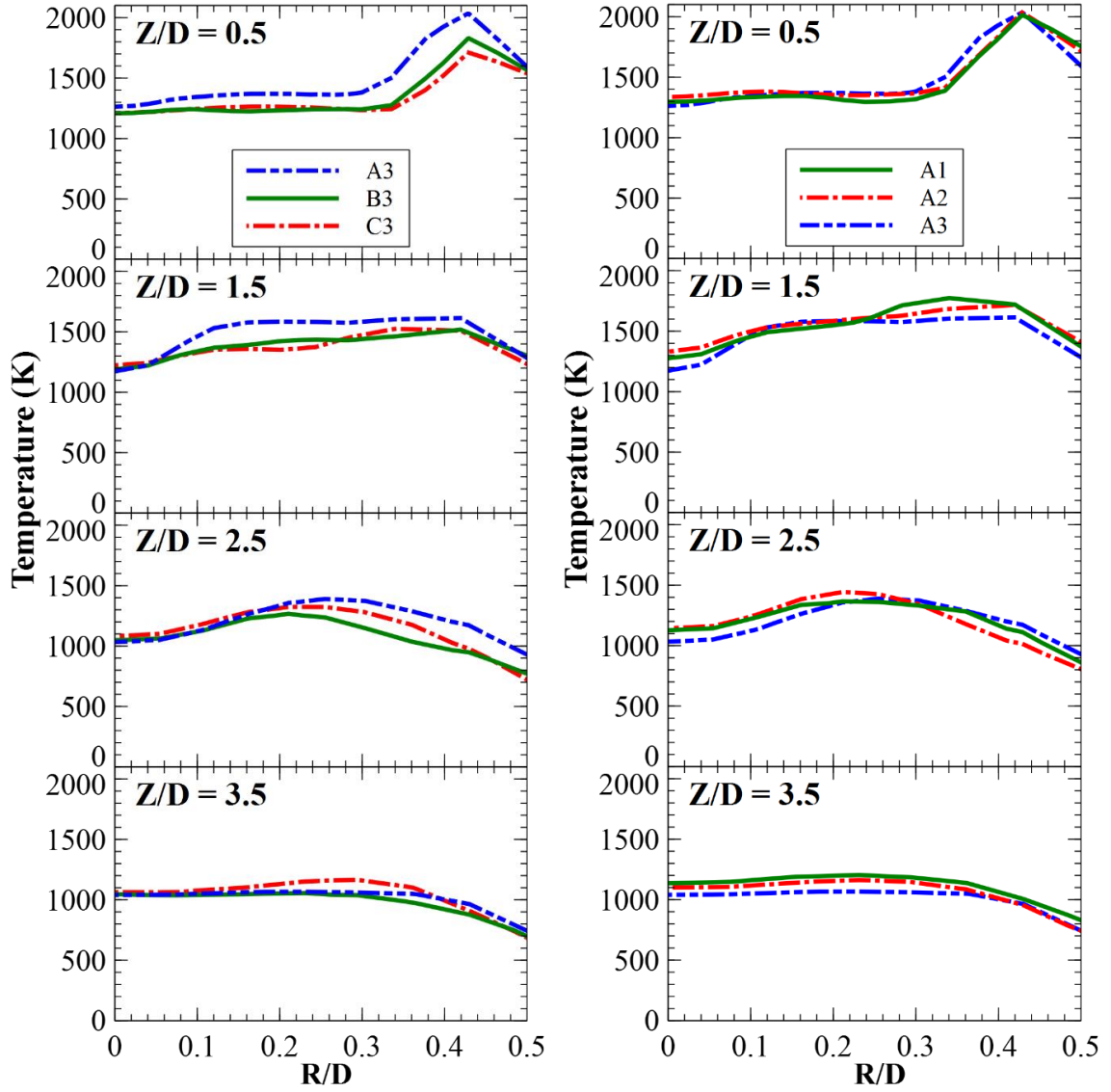


Figure 4.19: Radial temperature distributions at (left) fixed OF of 65% and AFTs of 2500K (A3), 2300K (B3), and 2100K (C3); and (right) fixed AFT of 2500K and OFs of 35% (A1), 50% (A2), and 65% (A3).

4.2.3 Combustion characteristics of CH₄/O₂/CO₂ flames

Combustion behaviors of CH₄/O₂/CO₂ flames are examined in this section in terms of several parameters, including product formation rate (PFR), combustion progress variable (PV), Damköhler number (Da), and species concentrations. **Figure 4.20** and **Figure 4.21** show the PFR (left) and PV (right) for different flames, where PFR refers to the rate at which the products are formed, and PV corresponds to the transition from unburnt to burnt gases. All the flames in Figure 7 are stabilized on both ISL and OSL near the combustor inlet. The PFR is higher in high AFT at fixed OF (in **Figure 4.20**), making the flame more compact in these cases. Alternatively, at lower AFT, the flames are relatively more spread out towards to combustor wall. In addition to the PFR, PV also demonstrates similar trend with increasing AFT. Fixing the AFT while increasing the OF (in **Figure 4.21**), resulted in insignificant changes in both PFR and PV and the flame slightly gets shrinked. Oxy-methane flames can be investigated using the relation between reaction rate and diffusion rate i.e., Damköhler number (Da) as in **Figure 4.22**. At higher AFT (in fixed OF), the flames become more compact and stronger indicating faster reactions at the flame core. Faster reaction rates, consequently, increase the Da as well, which is depicted in **Figure 4.20**. Similarly, in Figure 8b, Da increases with the OF at Fixed AFT due to the increased chances for effective collision reactions in the high OFs.

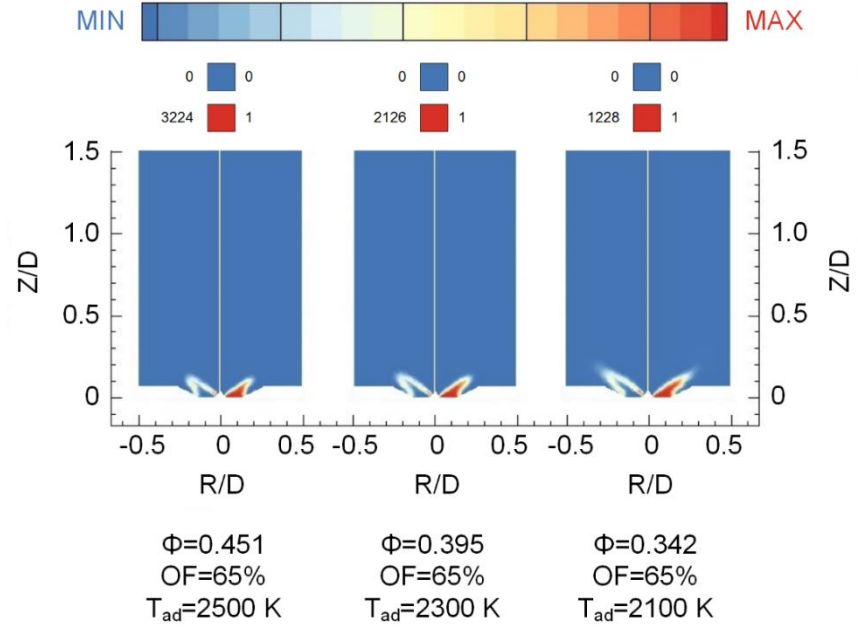


Figure 4.20: Product Formation Rate (PFR) and Progress Variable (PV) contours at fixed OF of 65% and AFTs of 2500K (A3), 2300K (B3), and 2100K (C3).

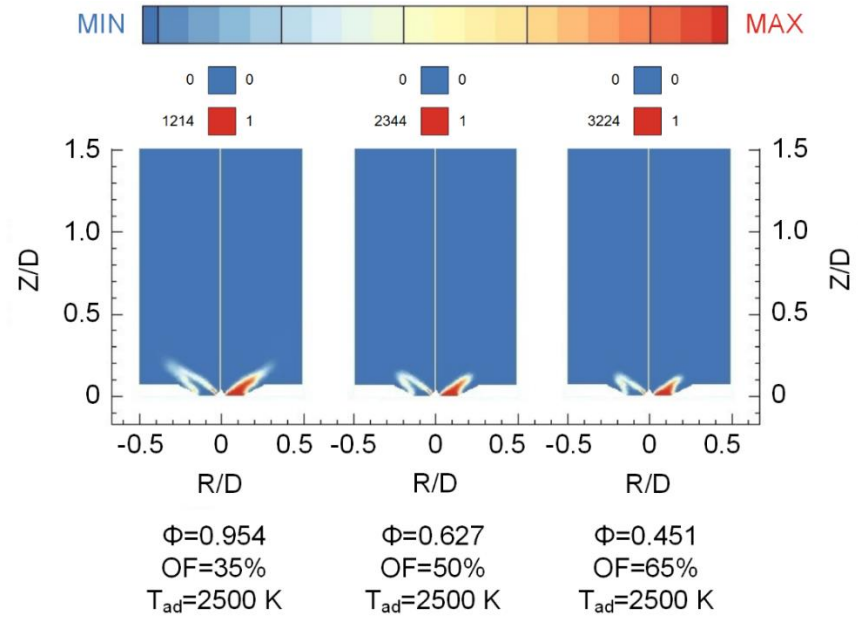


Figure 4.21: PFR and PV contours at fixed AFT of 2500K and OFs of 35% (A1), 50% (A2), and 65% (A3).

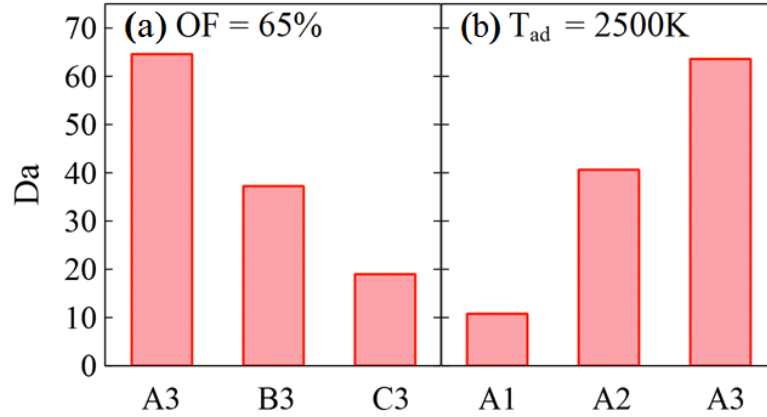


Figure 4.22: Variations of Damköhler numbers with (a) AFTs at fixed OF of 65% and (b) OF at fixed AFT of 2500K.

The distribution of species mole fractions is also essential in comprehending the combustion characteristics. **Figure 4.23** and **Figure 4.24** illustrate the contours of CH₄ mole fractions in the combustion zone. In order to obtain high AFT at fixed OF, higher value of Φ is considered which increased the CH₄ concentration in the inlet mixture as shown in **Figure 4.23**. Similarly, Φ is reduced with increasing OF to achieve identical AFT. As a result, the CH₄ mole fraction reduces as the OF increases from cases A1 to A3 (in **Figure 4.24**). In experimental investigations, the combustion flames are presented typically through the distribution of intermediate CH*, C₂* and OH* radicals. Among these, OH* radicals are used more in case of fuel-lean flames in order to determine the flame shape [250,251]. Thus, the shapes of the different flames in this study are also represented using the contours of OH mole fractions as provided in **Figure 4.25** and **Figure 4.26**. The concentration of OH radicals increases in higher AFT (high Φ) due to relatively higher fuel supply (in **Figure 4.25**). The oxidizer content in A3 is inadequate to eliminate/reduce the intermediate OH radicals. This can be attributed to enhances reactivity

in higher Φ . As the Φ is lowered from case A3 to C3, the fuel-oxidizer ratio reduces, the fuel concentration in the inlet mixture reduces and, subsequently, the levels of OH mole fractions reduce within the flame core. On the other hand, OH contours of flames at fixed AFT assume almost identical shape in **Figure 4.26**, where the OH intensity increases with the OF. Oxygen enrichment accelerates the combustion chemistry and subsequently increase the flame speed. Hence the availability of more O_2 from A1 to A3 flames enhances the chemistry and produces more OH radicals. This effect of O_2 -enhancement was also reported in the study by Maidana et al. [252].

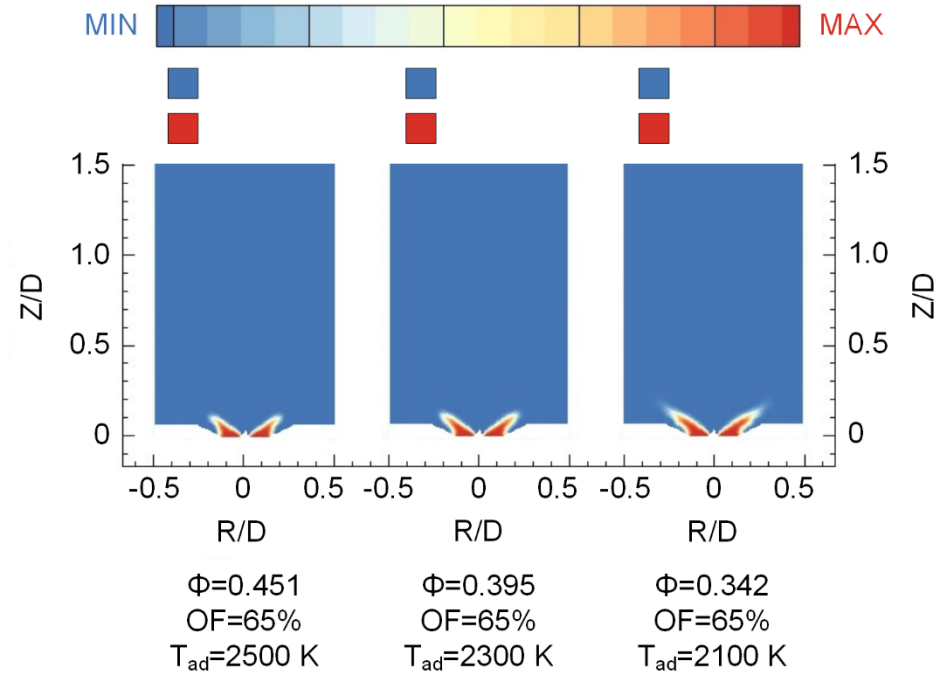


Figure 4.23: Mole fraction contours of CH₄ at fixed OF of 65% and AFTs of 2500K (A3), 2300K (B3), and 2100K (C3).

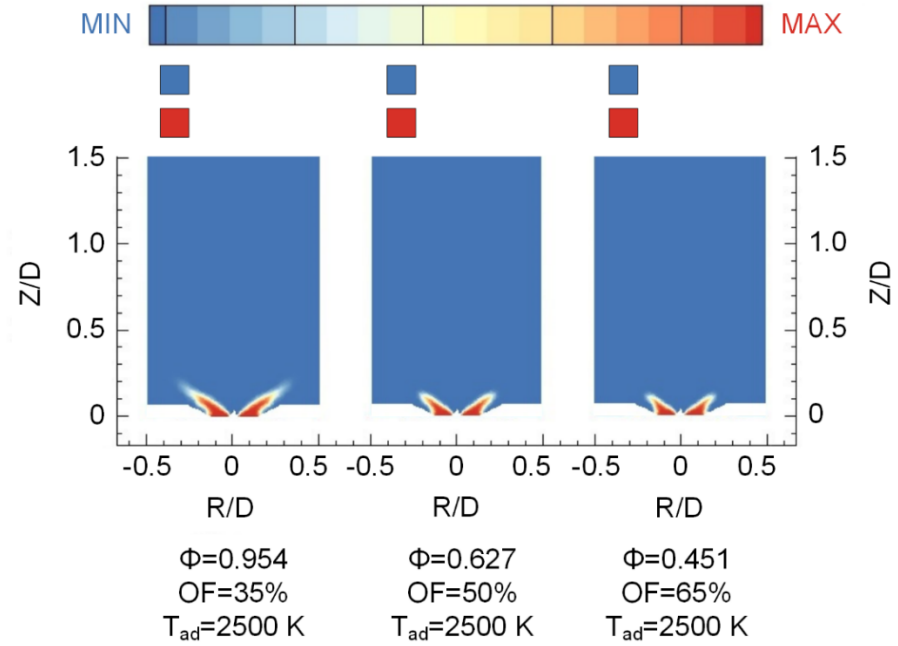


Figure 4.24: Mole fraction contours of CH_4 at fixed AFT of 2500K and OFs of 35% (A1), 50% (A2), and 65% (A3).

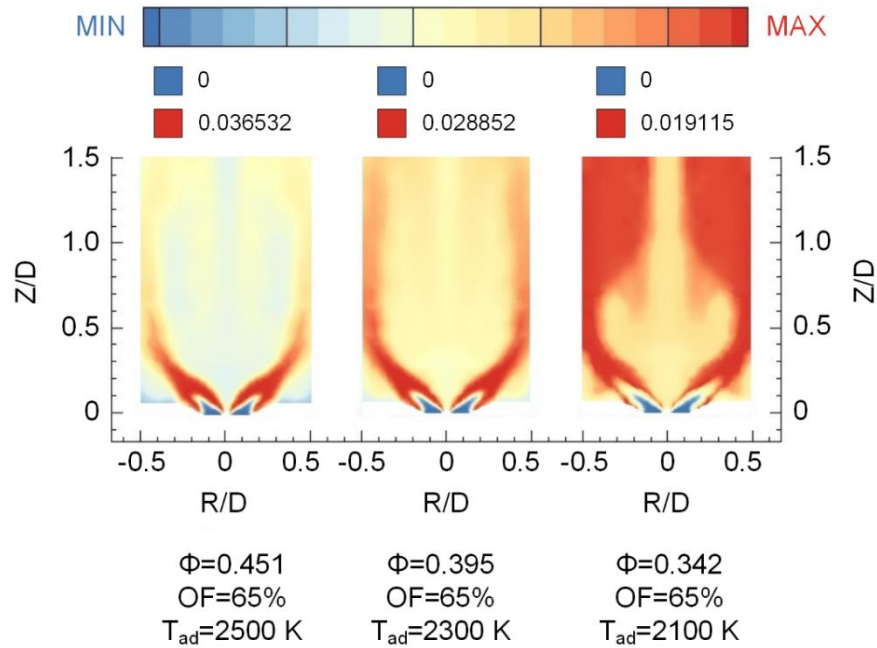


Figure 4.25: Mole fraction contours of OH at fixed OF of 65% and AFTs of 2500K (A3), 2300K (B3), and 2100K (C3).

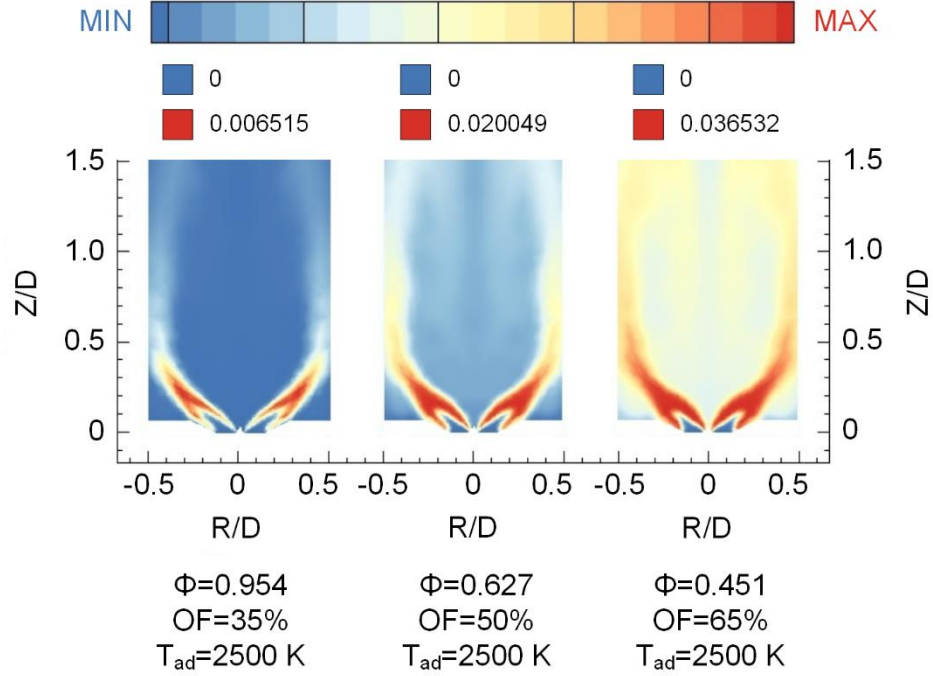


Figure 4.26: Mole fraction contours of OH at fixed AFT of 2500K and OFs of 35% (A1), 50% (A2), and 65% (A3).

4.2.4 Emission attributes of CH₄/O₂/CO₂ flames

The major constituents of the exhaust streams in oxy-methane combustion are CO₂ and H₂O. The CO₂ can be separated from the H₂O by simple condensation, which can later be recirculated back in combustion chamber to control the combustion temperature. The remaining CO₂ can be captured through various carbon captured techniques. Beside CO₂ and H₂O, some harmful CO is also produced during the combustion process. The emission characteristics of the oxy-methane flames are analyzed in this section for the different flames by studying the distributions of CO mole fractions within the combustor, as shown in **Figure 4.27** and **Figure 4.28**. Majority of the CO formation takes place near the inlet

within $0 \leq Z/D \leq 0.5$. Most of the CO converts back to CO_2 as the flame progresses downstream. As shown in **Figure 4.27**, the concentration of CO is the highest in case A3 at AFT of 2500 K. This may be attributed to the higher dissociation rates at higher AFTs. The CO concentration drops as the Φ is decreased to reduce the AFT at fixed OF. Among the atoms C, O and H of the reactant mixture, O and H reacts more quickly compared the C and H. In addition, additional C atoms are present in the combustor due to the more fuel supply at higher Φ . All this attributes to the formation of more CO. At lower Φ , the O atoms are adequate for the C atoms to produce CO_2 , which ultimately reduces the intermediate CO formation. For flames with fixed AFT in **Figure 4.28**, higher CO mole fractions are observed for case A1 and lower fractions are obtained for case A3. As discussed above, both Φ and OF are varied to obtain fixed AFT condition. The Φ is decreased and OF is increased from case A1 to case A2, resulting in higher C and lower O atoms in case A1 that increases the CO concentration levels.

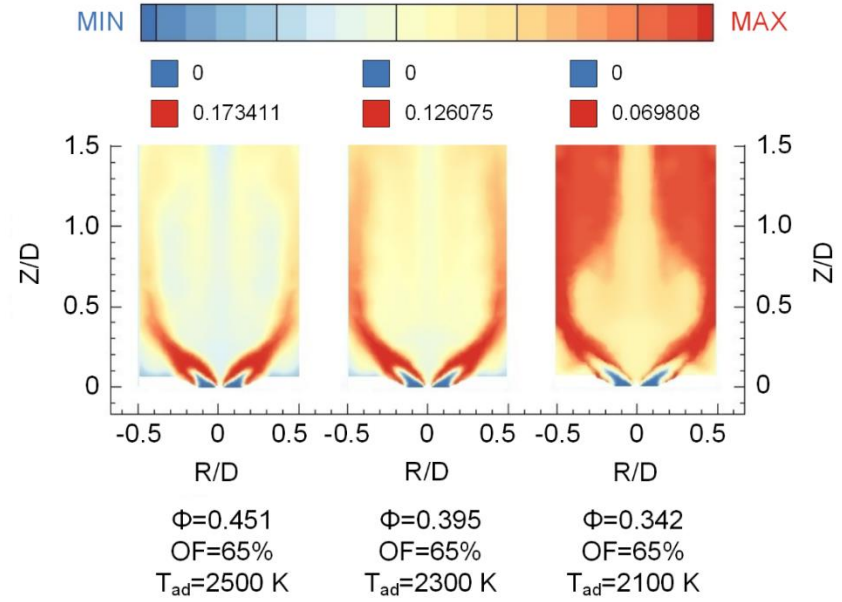


Figure 4.27: Mole fraction contours of CO at fixed OF of 65% AFTs of 2500K (A3), 2300K (B3), and 2100K (C3).

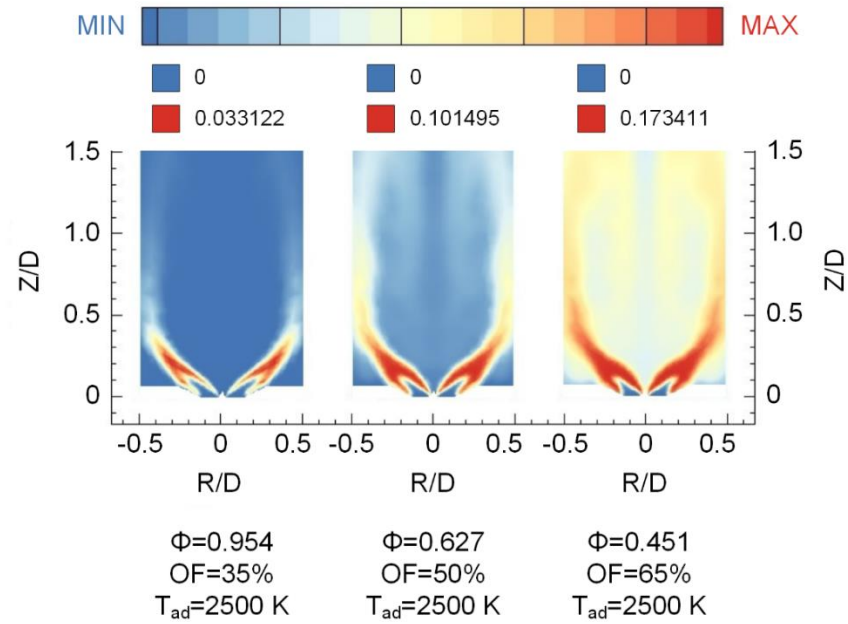


Figure 4.28: Mole fraction contours of CO at fixed AFT of 2500K and OFs of 35% (A1), 50% (A2), and 65% (A3).

Axial profiles of CO concentrations, in parts per million (ppm), are plotted along the combustor centerline in **Figure 4.29**. For fixed OF operation (OF=65%), a maximum value of CO concentration of ~7000 ppm is recorded for case A3 at the highest AFT, and a minimum value of ~700 ppm is observed for case C3 at the lowest AFT. Majority of these formed CO is oxidized to CO₂ downstream of Z/D=1. At fixed AFT of 2500 K, the maximum and minimum axial CO formation is observed to be ~19000 ppm and ~7000 ppm for cases A1 and A3, respectively. Most of the CO produced in fixed AFT cases oxidizes to CO₂ within the zone of $0 \leq Z/D \leq 2$. **Figure 4.30** illustrates the mass weighted averaged CO emissions downstream of the flame core, at axial distance of Z/D=2, where the highest CO emission is ~1.01 ppm for case A3 in fixed AFT and ~22 ppm for case A1 in fixed OF.

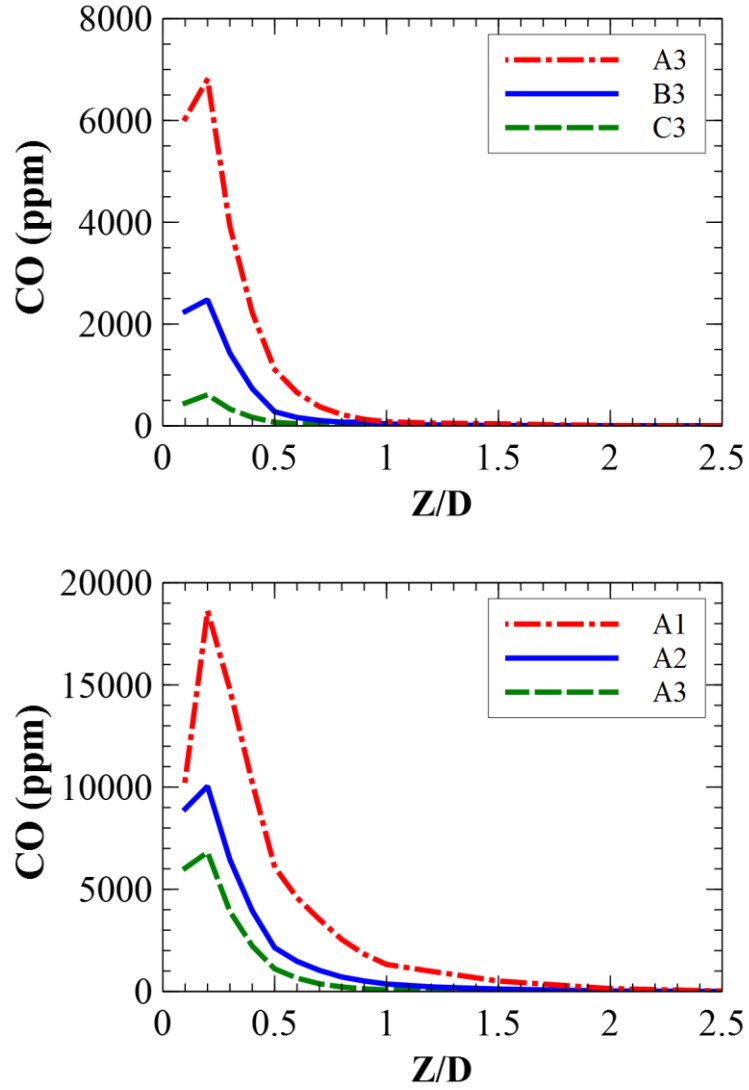


Figure 4.29: Mass weighted averaged CO concentrations in axial direction at (top) fixed OF of 65% and AFTs of 2500K (A3), 2300K (B3), and 2100K (C3); and (bottom) at fixed AFT of 2500K and OFs of 35% (A1), 50% (A2), and 65% (A3).

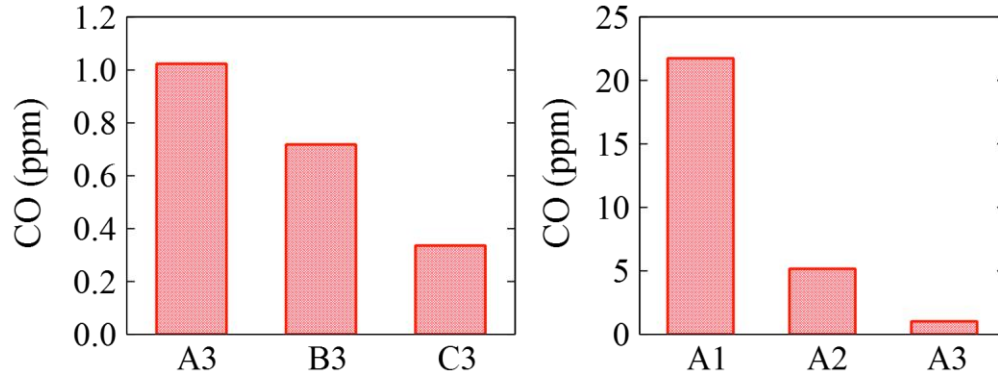


Figure 4.30: Mass weighted averaged CO concentration at $Z/D = 2.5$ for (left) fixed OF of 65% and AFT of 2500K (A3), 2300K (B3), and 2100K (C3); and (right) at fixed AFT of 2500K and OFs of 35% (A1), 50% (A2), and 65% (A3).

4.3 Comparison of propane with methane and syngas under oxy-combustion in a swirl-stabilized combustor

Swirl-stabilized premixed oxy-combustion flames have been examined numerically considering three different fuels (methane, syngas, and propane) in varying equivalence ratio at fixed OF and under atmospheric conditions. The syngas, studied here, consists of CH₄, CO and H₂ at a molar ratio of 0.50:0.25:0.25 (2:1:1) and has a lower heating value (LHV) for the mixture of 57,470 kJ/kg. This specific composition of syngas is adopted from the experimental work by Joo et al. [253]. **Table 4.3** lists the investigated lean premixed cases, where Φ ranges from 0.34 to 0.42 at 60% constant OF. The studied cases are selected carefully so that the cases remain within the stable combustion zone as evaluated in experimental studies by Abdelhafez et al. [107] and Ali et al. [243] for oxy-methane and oxy-propane flames, respectively. The flames are compared in terms of flow fields along with relevant combustion and emission characteristics. The results are expressed in dimensionless manner, where axial and radial directions are presented in relevance to the combustor length and diameter as Z/D and r/R, respectively. All the results from the simulation are obtained at 186 sec where marginal variation in key parameters (like temperatures and species mole fractions) have been observed, thus static-state results are presented and analyzed in this study.

Table 4.3: The inlet conditions considered for oxy-combustion flames for each of the three fuels (i.e., methane, propane, and syngas) under investigation.

Case number	Oxygen fraction (OF)	Equivalence ratio (Φ)
1	60 %	0.34
2	60 %	0.39
3	60 %	0.42

4.3.1 Global flame behavior with different fuels

4.3.1.1 Adiabatic flame temperature, laminar flame speed, and power density

The characteristics of oxy-fuel flames are initially compared in terms of their respective adiabatic flame temperatures (T_{ad}), laminar flame speed (LFS), and power density (PD) as shown in **Figure 4.31**. These parameters are important for gas turbine (GT) combustor design. For the three fuels, the values of these parameters increase with the equivalence ratio, where the change is more significant for LFS. For a fixed equivalence ratio, both T_{ad} and LFS increase from methane to syngas to propane. Power density on the other hand,

reduces slightly while going from methane to syngas and increases again with oxy-propane flames. This can be attributed to the variations in the heating values for the different fuels. In authors previous experimental works [151,172], T_{ad} was identified as a controlling parameter for flame stability and was found directly influencing the LFS.

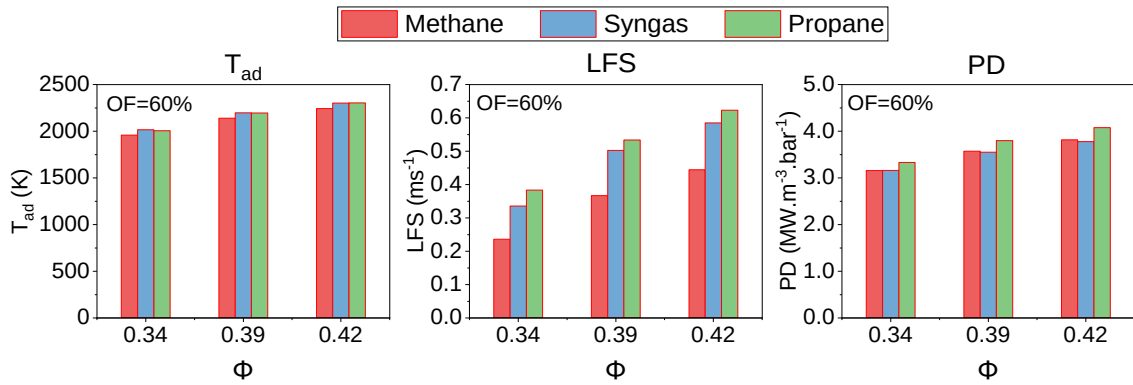


Figure 4.31: Adiabatic flame temperature (T_{ad}), laminar flame speed (LFS), and power density (PD) of the different flames of different equivalence ratios and fixed oxygen fraction (OF) of 60%.

4.3.1.2 Flame macrostructure

Figure 4.32 depicts comparison of the flame shapes in terms of OH contours for each of the fuels. In each of the cases, the flame shapes are almost similar in terms of spread-out, shape, and size, and assuming the characteristic ‘V’ shape. Nevertheless, no reactions take place at the outer recirculation zone (ORZ) in any of the flames. The presence of the OH radicals increase with the increase in equivalence ratio. Higher OH concentration at flame

core is observed with oxy-syngas flames while OH concentration is found lower in oxy-methane flames. This can be attributed to the effect of hydrogen enrichment as reported in previous studies [172,238]. Free hydrogen molecules present in syngas, and higher hydrogen availability in propane (compared to methane) result in elevated OH concentration in syngas and propane flames than that in methane flames. Increased hydrogen content improves the reactivity among the reactants and makes the flame stronger [254]. In the studied cases, flame is dominated by the IRZ resulting in the mixing of burned and unburned species, which reduces the reaction consequently reducing the OH concentration and temperature (temperature distribution discussed in the following section) in the IRZ [246]. The recirculation in the combustion chamber can be observed from the velocity streamlines (in **Figure 4.34**) and vorticity distribution (in **Figure 4.35**) **Error!**

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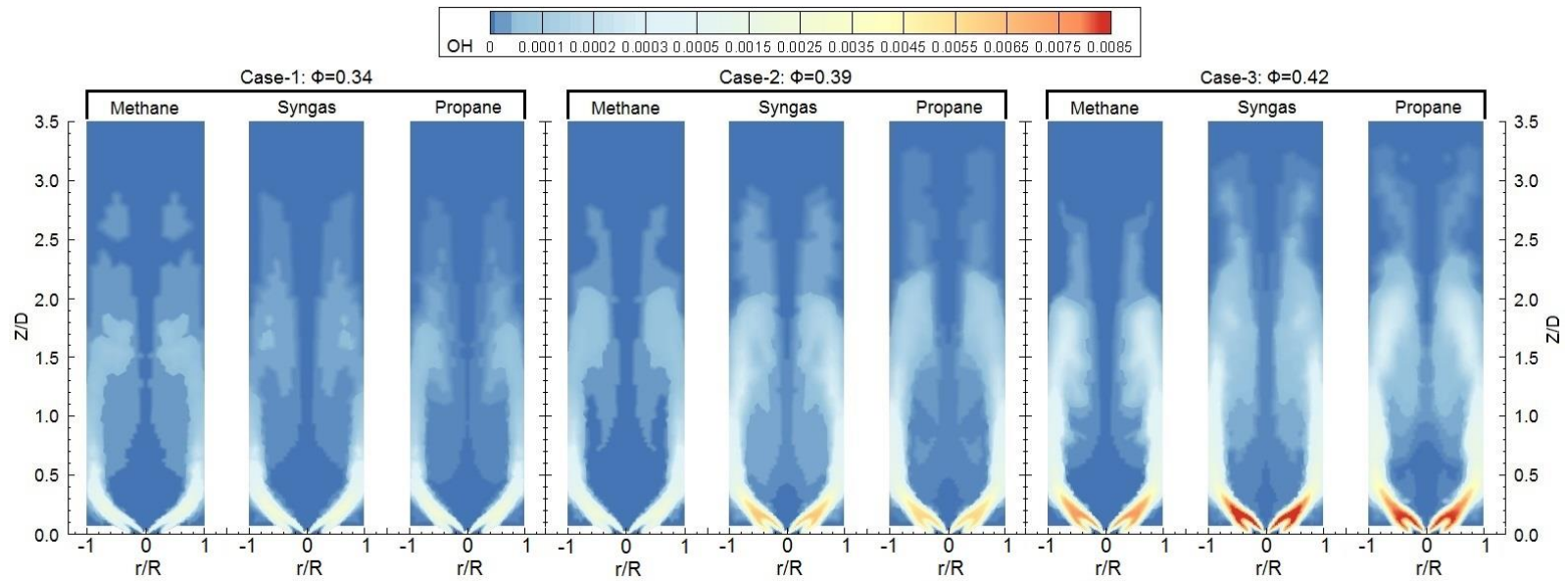


Figure 4.32: Flame shapes of methane, syngas, and propane based on OH contours for the cases 1-3.

4.3.2 Temperature profiles and flow-field structure in oxy-fuel flames of methane, propane and syngas

Combustion temperature is one of the most important parameters for the design and manufacturing of any combustion system. The expected combustion temperature should be as high as possible under the limit constrained by combustor material. Figure 5 illustrates the temperature distribution along the axial direction of the combustor. As shown in **Figure 4.33**, the combustor temperature increases from the inlet to $\sim Z/D=0.7-1.1$ for all the cases and, after that, the temperature starts declining. This can be attributed to the formation of eddies in the inner recirculation zone (IRZ), which circulates convective heat in this zone, as explained in a later section of this study. Moreover, radiation and reaction rates may also influence the temperature drop along axial direction. It worth mentioning that the highest axial temperatures for all equivalence ratios were achieved with propane flames due to the higher rates of reactions.

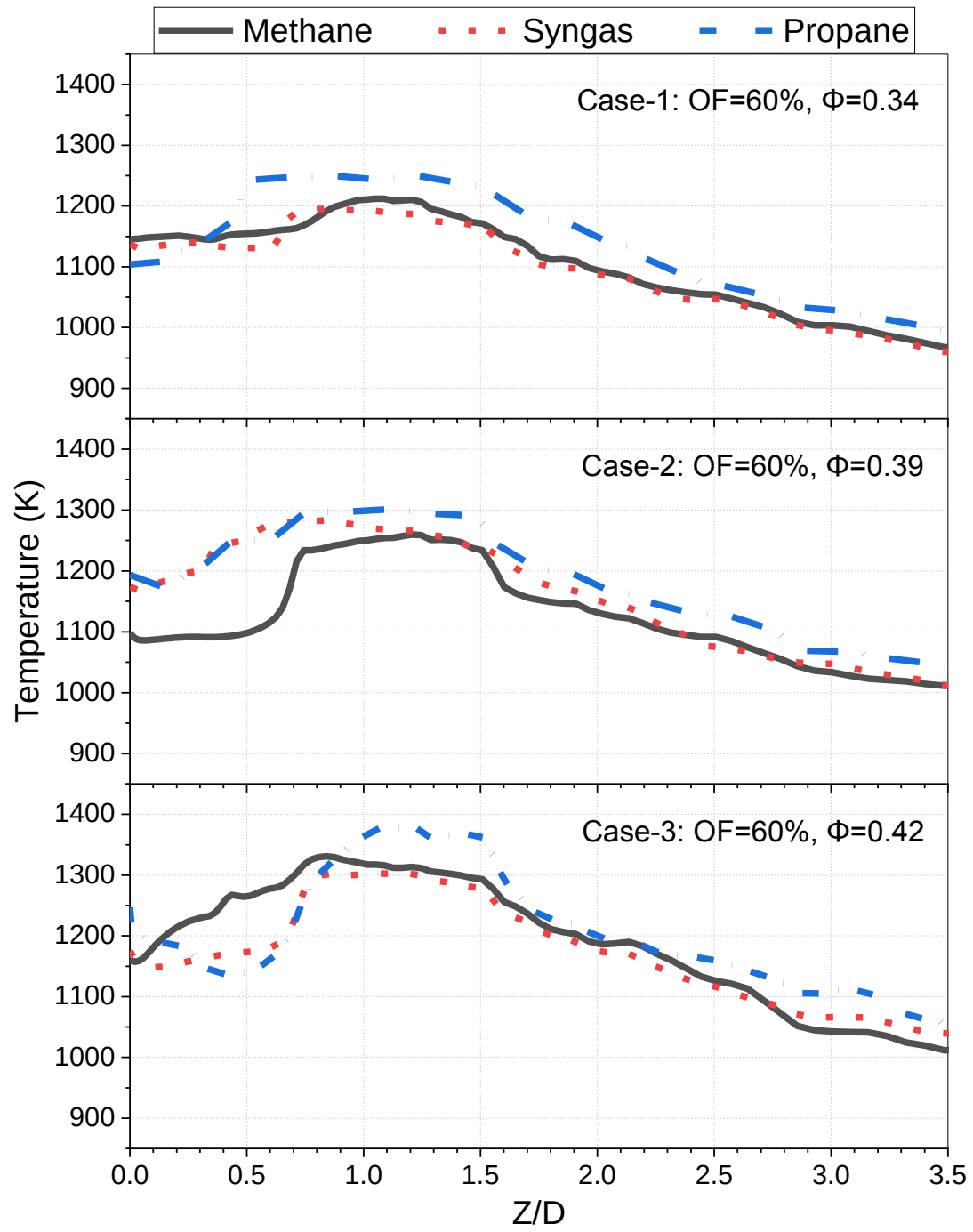


Figure 4.33: Axial temperature distributions for different oxy-fuel flames for cases 1-3.

Besides the axial temperature, flow-field structure can provide deeper insight in understanding flow behavior of the different combustion flames inside the combustor. The flow-fields for the studied flame cases are examined based on their velocity streamlines and vorticity magnitudes. Velocity streamlines demonstrate the formation of outer recirculation zone (ORZ) and inner recirculation zone (IRZ) in a turbulent reacting flow. Vorticity, on the other hand, reveals the rotation tendency in the flow field and plays significant role in turbulent eddy formations inside the combustor. **Figure 4.34** exhibits the velocity streamlines over the temperature contours on center-plane of the combustor. The velocity streamlines are generated at identical time step after reaching a static-state condition, where no variation in different parameters (like temperature, fuel, oxygen, OH, CO) have been observed. The flow-field in the combustion zone is identified by the creation of eddies in both IRZ and ORZ. In all cases, the presence of more than one IRZ is evident, where the larger eddy circulating in counterclockwise direction is observed within the axial distance $0.3 \leq Z/D \leq 2$. Smaller secondary eddies are also present in the IRZ within the axial distance $0 \leq Z/D \leq 0.5$. The IRZ shifts downstream with the increase in Φ and makes the flame stronger, which is reported, as well, in **Figure 4.32** above. For all the fuels, one clockwise-spinning eddy is observed in the ORZ irrespective of the equivalence ratio. Similar eddy formation in the ORZ was reported in a study of air-propane combustion in a backward-facing step combustor [246]. High aspect ratio between the inlet diameter and the diameter of quartz tube (combustion chamber) makes the IRZ more dominant compared to ORZ. However, the formation and recirculation in ORZ is case sensitive for a fixed combustor design and is also a vital parameter for the flame stability. The effect of ORZ in various OF and Φ for individual fuels have been examined in previous sections.

Figure 4.35 exhibits the effect of different fuels on the vorticity magnitude, where the contours of vorticity and temperature is presented for different equivalence ratios. Flame is stabilized in between the outer shear layer (OSL) and inner shear layer (ISL), where the reactions take place. The flame core between ISL and OSL broadens with the increase in Φ rising the core temperature. At $\Phi=0.42$, the highest core temperatures recorded for methane, syngas, and propane are 2176 K, 2224 K, and 2225 K, respectively. High core temperature raises the buoyant force that causes shifting of the IRZ towards the combustor exit as well as increasing the vorticity level. As a result of this elevated vorticity, a slight increase in the ISL thickness is observed as well. The high temperature generated within the flame core reduces to more suitable temperature for turbine blade operation as the flame propagates downstream.

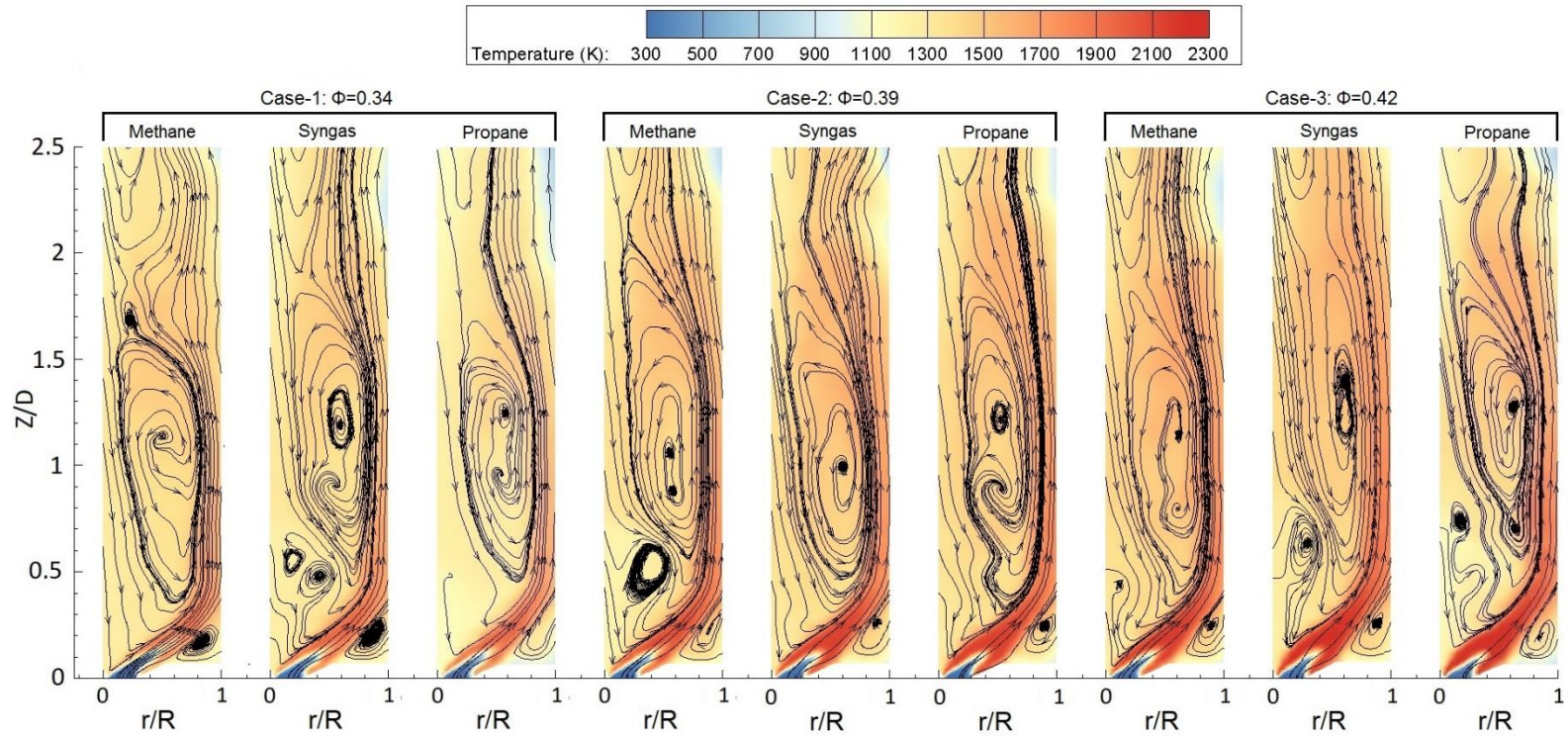


Figure 4.34: Velocity streamline over temperature contours for the different fuels for cases 1-3.

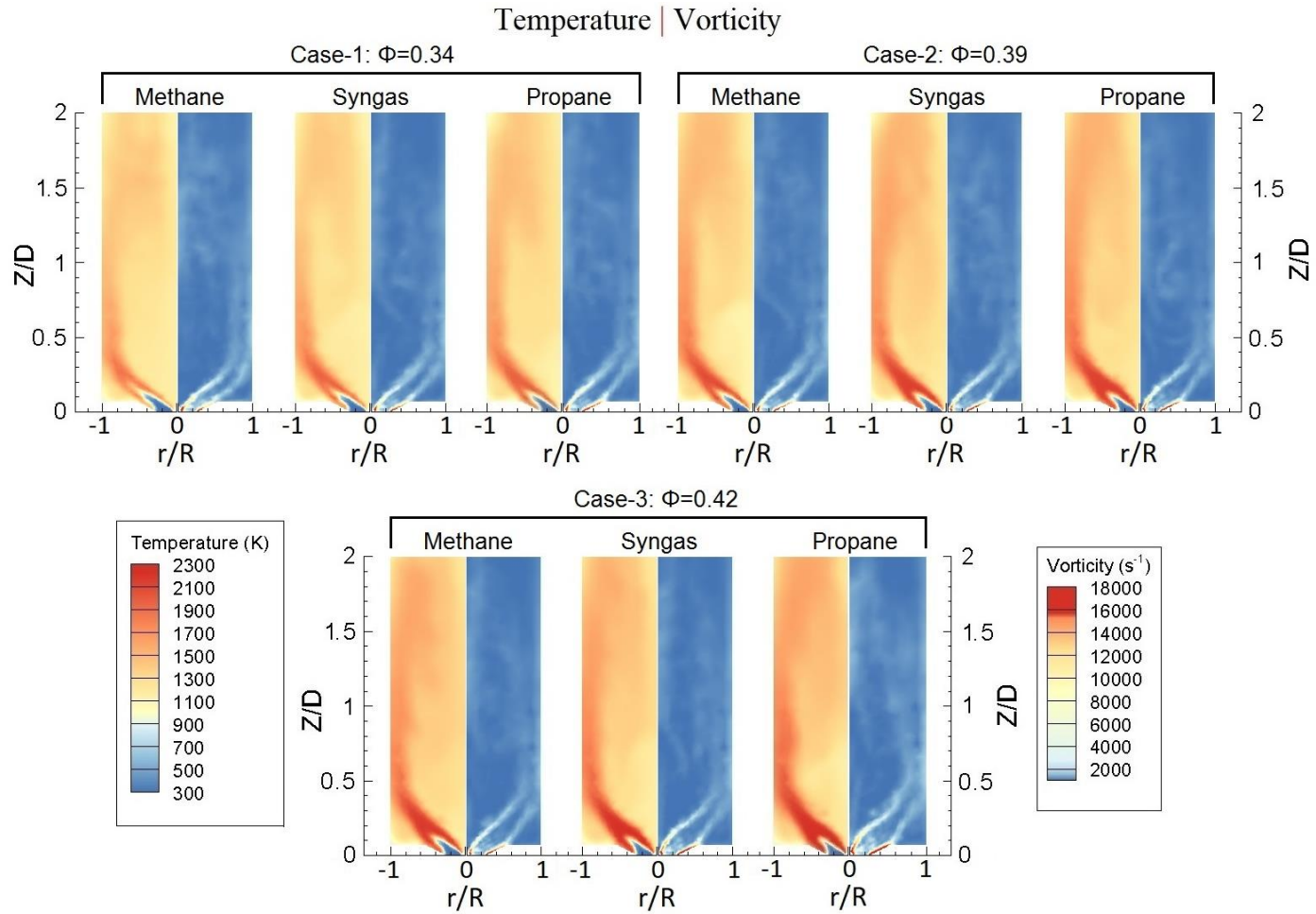


Figure 4.35: Center plane contours of temperature (left) and vorticity magnitude (right) of methane, syngas, and propane flames for the cases 1-3.

4.3.3 Combustion characteristics of methane, propane and syngas

oxy-combustion flames

Combustion attributes of the flames are investigated in this section in terms of product formation rate (PFR), combustion progress variable (PV), flame thickness (δ), Damköhler number (Da), pattern factor (PF), and thermal power (TP). Product formation rate corresponds to the rate at which products are formed from the reactants. Progress variable refers to the transition of unburnt reactants to fully burnt products. Flame thickness represents the thickness within which unburnt reactants are heated to ignition temperature by the reaction zone. Damköhler number is the ratio between reaction rate and diffusion rate. Pattern factor indicates how uniform the temperature distribution is at the outlet of the combustor. Pattern factor is an important parameter in turbine performance and plays a crucial role on the operating life of turbine vanes and blades [255,256]. Lastly, thermal power refers to the power generated by the combustor due to combustion.

Figure 4.36 illustrates the contours of PFR and PV near combustor inlet for different fuels. For all flames, the reaction zone exists between ISL and OSL and the flames are stabilized on both layers. The value of PRF is highest with propane flame followed by syngas and methane, respectively at lower Φ . This causes the oxy-propane flame to be more intense and shorter ($0 < Z/D < 0.175$) than oxy-syngas ($0 < Z/D < 0.18$) and oxy-methane ($0 < Z/D < 0.2$) flames. Furthermore, PFR increases in the ISL and decreases in the OSL from methane to syngas to propane, which results in more compact flame with propane and slightly spread-out flame (towards corner of the combustor) with methane. With higher PFR, oxy-propane flame requires smaller region for unburnt mixture than syngas and methane counterparts,

respectively. As Φ increases, all the flames become stronger while the oxy-propane flame remains more compact than the other two flames. Additionally, the progress variable also shows similar trend and the transition region from unburnt mixture to completely burnt products becomes, as well, more compact for the oxy-propane flames.

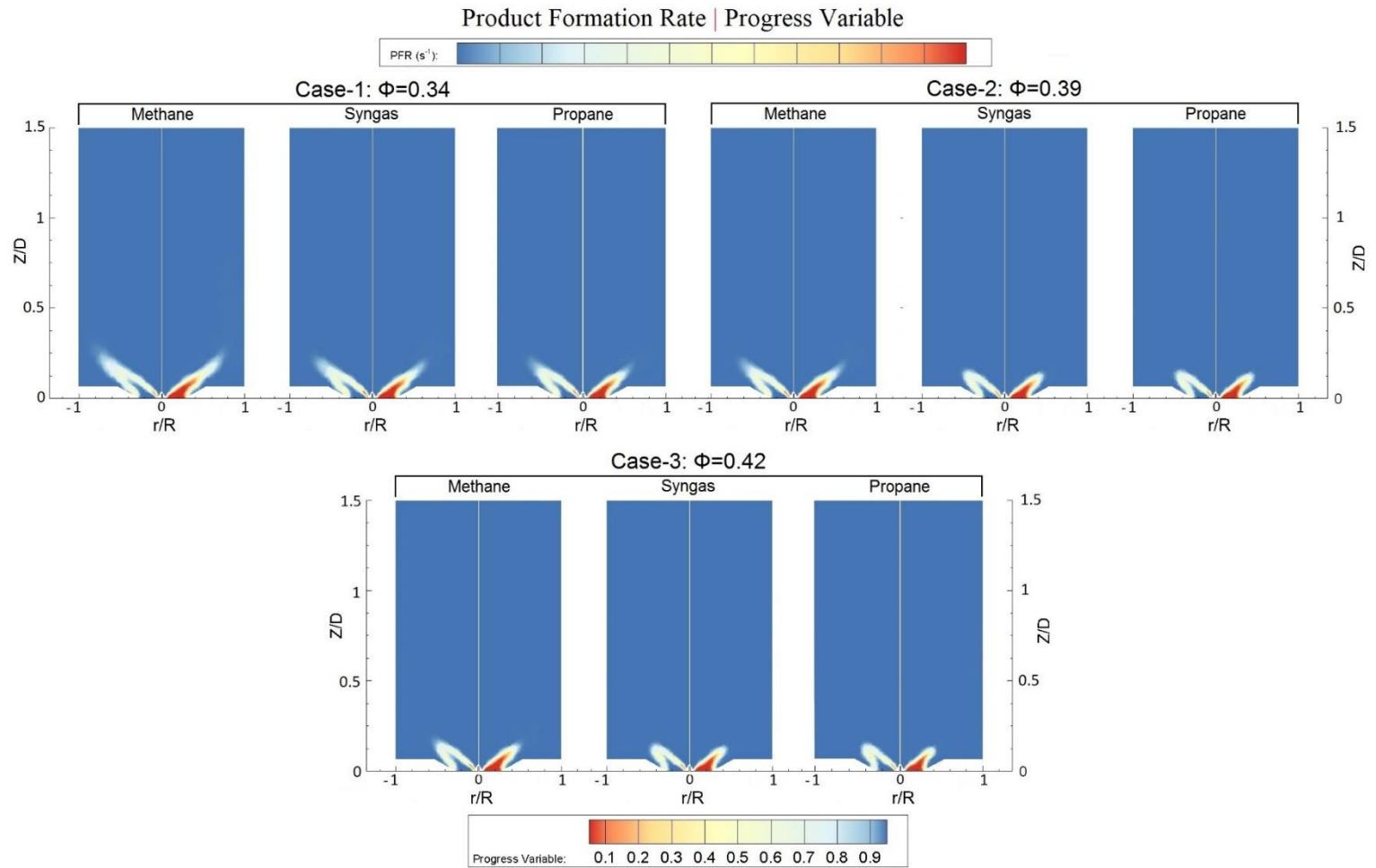


Figure 4.36: Contours of PFR (left) and PV (right) for oxy-combustion flames of methane, syngas, and propane for the case 1-

3.

Figure 4.37 represents the flame characteristics in terms of δ , PF, Da number, and TP. Higher flame thickness is observed for methane, followed by syngas and propane, respectively. Smaller flame thickness refers to compact structure of the flame indicating faster reactions at the flame core. Flame thickness of these fuels decrease in a similar fashion with the increase in Φ , as indicated, as well, in **Figure 4.36** above. Methane, syngas, and propane flames demonstrate flame thicknesses of approximately 144.4 μm , 102.7 μm , and 85.5 μm at $\Phi=0.34$; 92.9 μm , 68.6 μm , and 61.0 μm at $\Phi=0.39$; and 76.7 μm , 58.9 μm , and 52.1 μm at $\Phi=0.42$, respectively. Higher flame thickness of methane flames can be attributed to the reaction rates, as expressed in terms of the Da number. As shown in **Figure 4.37(b)**, methane flames have the lowest Da followed by syngas and propane flames. Lower Da for oxy-methane flames (12.9 at $\Phi=0.34$, 30.2 at $\Phi=0.39$, and 45.7 at $\Phi=0.42$) indicate relatively lower reaction rate for methane combustion than its syngas and propane counterparts. Pattern factor corresponds to the uniformity of temperature at combustor outlet which is observed to be the lowest in case of syngas combustion. This implies that the syngas flames have more uniform temperature distribution than propane and methane flames, respectively (see **Figure 4.37(c)**). Around 22-36% and 4-16% decrease in PF are observed with syngas flames as compared to the methane and propane counterpart, respectively. Oxy-propane flames, on the other hand, demonstrate 7-33% reduction and 4-19% increase in PF in contrast with oxy-methane and oxy-syngas flames, respectively. The thermal power is a good indicator of output energy generated from the combustion. **Figure 4.37(d)** shows the TP for the different flames, where propane flames demonstrate higher values of TP ($\sim 1.29\text{-}1.38$ KW) in all

equivalence ratios, followed by methane (~ 1.09-1.21 KW) and syngas (~ 1.00-1.12 KW) flames.

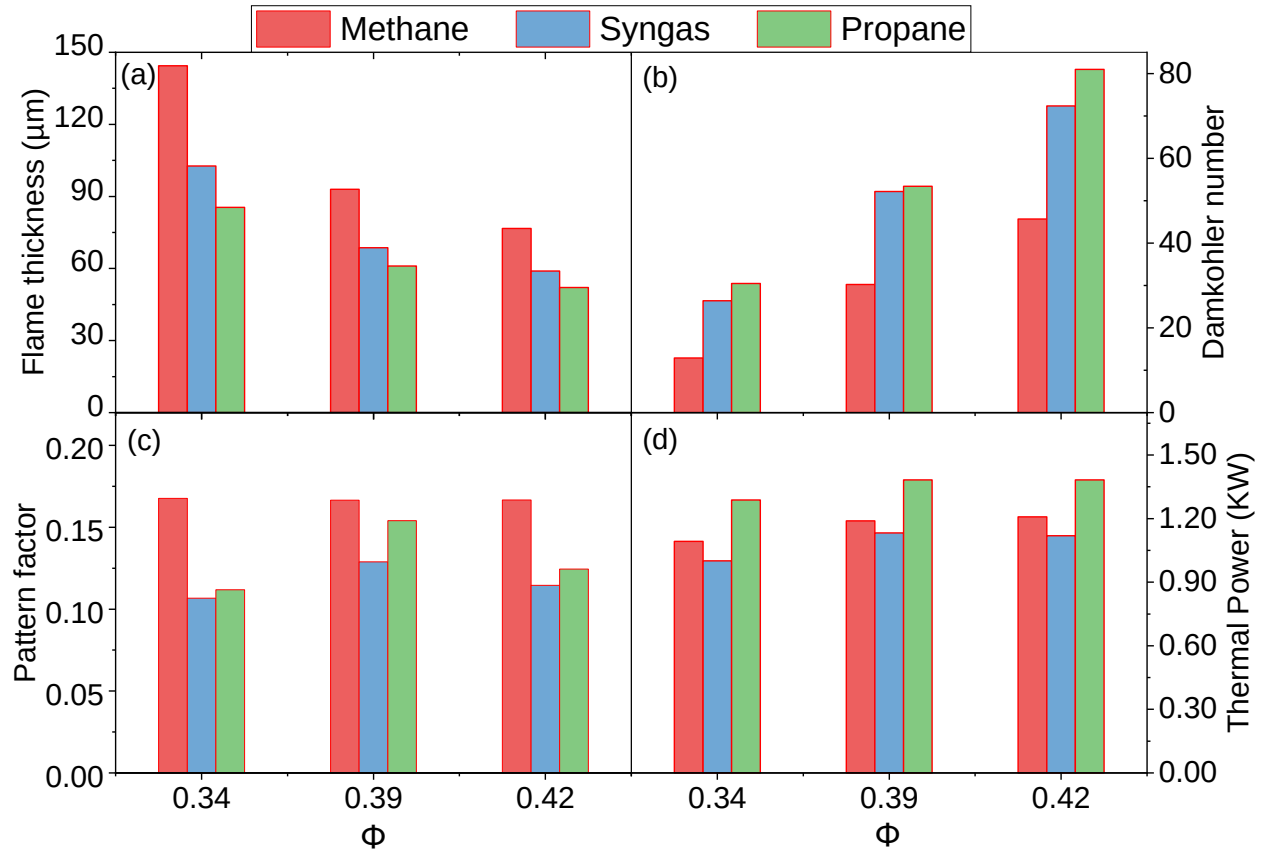


Figure 4.37: Comparisons of the combustion characteristics of the different flames: (a) Flame thickness, (b) Damköhler number, (c) pattern factor, and (d) thermal power.

4.3.4 Emission attributes in oxy-fuel flames of methane, propane and syngas

Oxy-combustion is a NO_x-free combustion technique where the exhaust stream ideally constitutes of CO₂ and H₂O in stoichiometric condition. This CO₂ can be easily extracted from the flue gas through condensation of water vapor, a portion of which can be recirculated back into the combustor and the remaining can be sent for carbon capture processes. Carbon monoxide is one of the major contributors to the existing air pollution problem. This section examines the distribution of CO inside the combustor and emission of CO in parts per million (ppm) at the combustor outlet for the fuels under investigation.

Figure 4.38 shows the distribution of CO (in mole fractions) within the combustion zone. Among the three fuels, syngas has higher CO near combustor inlet due to the presence of CO in the fuel feed. As the reaction progresses, the majority of this feed CO converts into CO₂. The area where most of the CO formation takes place is within the axial distance $0 \leq Z/D \leq 0.4$ for methane, $0 \leq Z/D \leq 0.6$ for syngas, and $0 \leq Z/D \leq 0.7$ for propane, at $\Phi=0.34$. This zone expands in size towards downstream with the increase in equivalence ratio. The rise in fuel supply improves the reactivity and, as a result, CO formation zone grows. At $\Phi=0.42$, most of the CO formation occurs within the axial distances $0 \leq Z/D \leq 1.1$, $0 \leq Z/D \leq 1.2$ and $0 \leq Z/D \leq 1.3$ for methane, syngas, and propane, respectively. This intermediate CO then oxidizes with the remaining oxygen and forms CO₂. Despite the oxidation, a portion of CO remains unchanged in some cases and goes with the exhaust stream. **Figure 4.39** depicts the CO emission at the outlet of the combustor. No CO emission is observed from any of the oxy-fuel flames at lower equivalence ratio ($\Phi=0.34$),

implying sufficient supply of oxidizer. The fuel concentration increases with the increase in the equivalence ratio resulting in increased CO concentration, which is observed at equivalence ratios of 0.39 and 0.42. Among the fuels, the syngas resulted in higher CO emission than the other two fuels because of its higher hydrogen content that competes with CO for oxygen. The emission of CO with methane, syngas, and propane are 0.0009, 0.0083, and 0.0063 ppm at $\Phi = 0.39$ and 0.0059, 0.0140, and 0.0101 ppm at $\Phi = 0.42$, respectively. Compared to methane flames, CO emission increase around 9 times for syngas flame and 7 times for propane flames at $\Phi = 0.39$. At increased Φ of 0.42, CO emission elevates to approximately 2.4 times and 1.7 times those of syngas and propane counterparts. This can be attributed to the varied hydrogen content in the fuel. In an earlier study by Nemitallah et al. [172], the results showed that CO emission often increase with the increase of hydrogen content in the fuel. For fuels of higher hydrogen content, carbon molecules in the fuel have to compete with the hydrogen for oxygen and, concurrently, producing more CO. In this investigation syngas has higher hydrogen content than the other two fuels, hence higher CO emission from syngas flames.

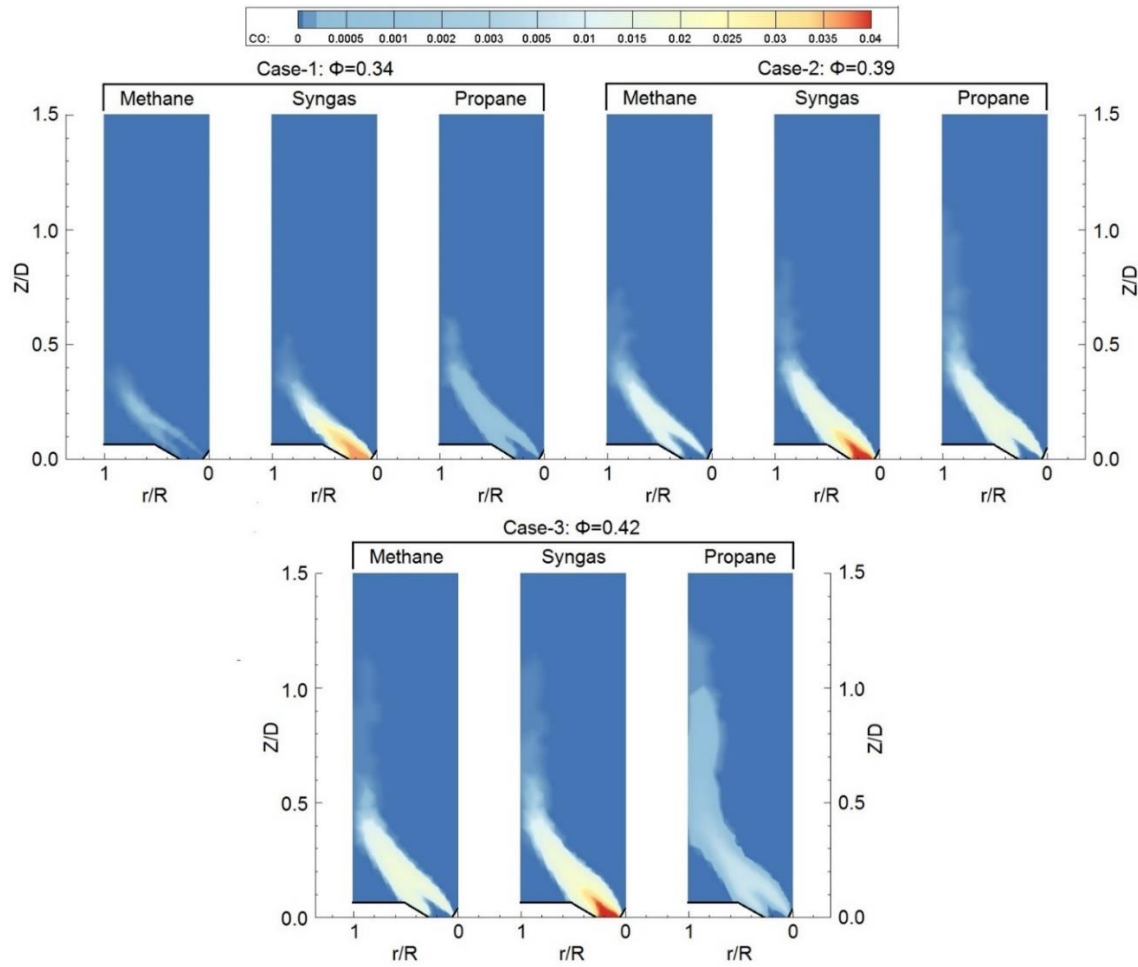


Figure 4.38: Contours of CO mole fractions within the combustor for oxy-combustion flames of methane, syngas, and propane for the case 1-3.

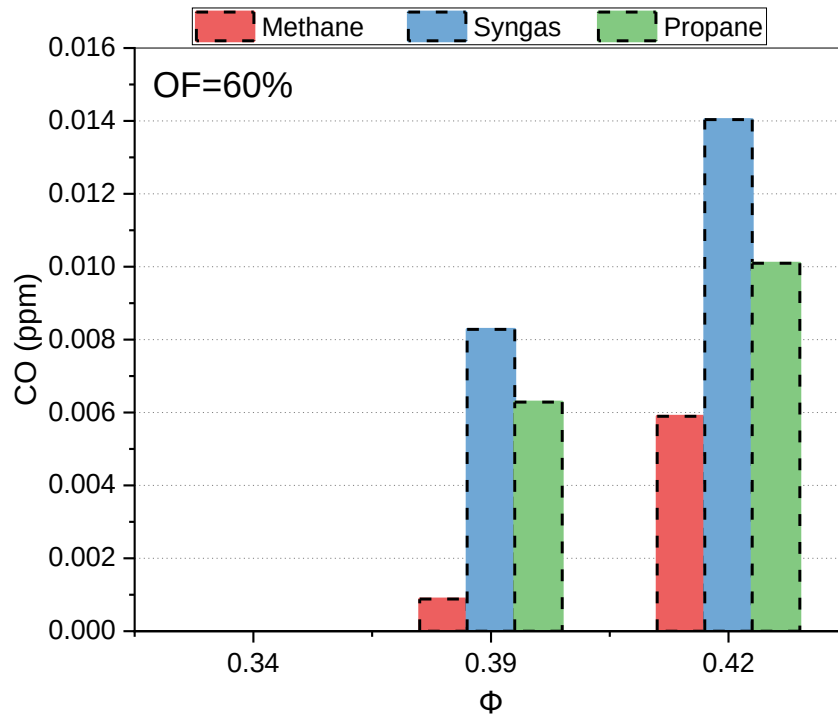


Figure 4.39: CO emission (in ppm) at the combustor outlet for oxy-combustion flames of methane, syngas, and propane for the case 1-3.

4.4 Premixed C₃H₈/O₂/CO₂ flames in multi-hole burner

A range of inlet composition has been investigated numerically for the oxy-propane flames in multi-hole burner with CO₂-dilution. The test matrix considered in this study is listed in **Table 4.4**, where cases are considered in different Ø (0.241-0.50) and OFs (32.4-60.0%). The effects of these parameters are studied in terms of flame shapes, temperature and vorticity distributions, velocity streamlines, along with combustion and emission attributes. Furthermore, the combustion in multi-hole combustor is compared with that in model swirl-stabilized gas turbine combustor at Ø=0.50 and OF=60%.

Table 4.4: Test matrix for C₃H₈/O₂/CO₂ flames in micromixer combustor in different Ø and OFs along with their corresponding T_{ad}.

Cases for the micromixer setup	Equivalence ratio (Ø)	Oxygen fraction (OF)	Adiabatic flame temperature (T _{ad}), K
1	0.241	60.0%	1600
2	0.276	60.0%	1750
3	0.313	60.0%	1900
4	0.392	50.0%	1900
5	0.500	40.8%	1900
6	0.500	36.6%	1750

7	0.500	32.4%	1600
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The results are presented in dimensionless manner in both axial and radial directions. The terms Z/D and r/R are used to express the axial and radial position, respectively. Here, Z , r , R , and D correspond to axial distance, radial distance, combustor radius and diameter, respectively. Furthermore, the contours for various parameters examined in the study is presented on a centerline plane inside the combustor as illustrated in **Figure 4.40**.

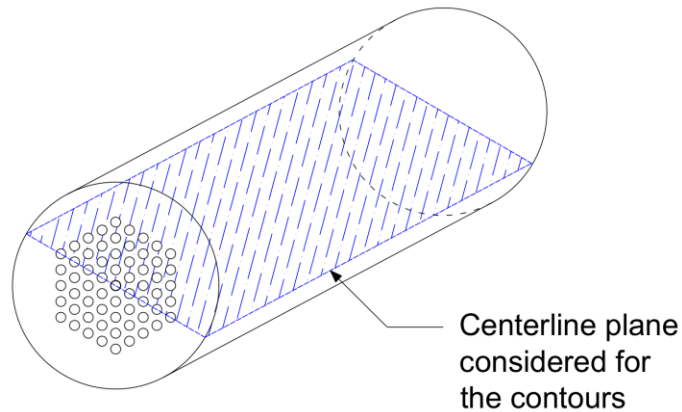


Figure 4.40: Centerline plane in the combustor considered for contour illustrations.

4.4.1 Global flame behavior of oxy-propane flames in multi-hole burner

Premixed $C_3H_8/O_2/CO_2$ flames in multi-hole burner are examined initially in terms of their flame shapes which is a good indicator of combustion behaviors and stability. Typically, particle image velocimetry (PIV) is used to detect the flame structure, heat releases, and

reaction characteristics where OH* chemiluminescence is approach is employed to evaluate the premixed flames [244,245]. In order to make the study on par with the experimental approaches, the flame shapes in this study are represented using their respective OH contours. **Figure 4.41** shows the contours of OH radical in the combustion zone for the studied cases (see **Table 4.4**), while the corresponding laminar flame speeds are presented in Figure 4.42. For a fixed OF=60%, with the increase in ϕ (and T_{ad}), the OH concentrations increase making the flame stronger with high heat release rate and elevated laminar flame speed (in **Figure 4.41**). Case-1, here, illustrates a weaker flame near blow out limit, which attributes to the reduced OH concentration in the middle of the combustion chamber within $0.1 \leq Z/D \leq 1.7$. Low OH concentrations in $0 \leq Z/D \leq 0.1$ are due to the inlet flow of the individual flamelets. The flames assume similar shapes in constant T_{ad} , nevertheless, the OH intensity decreases with the oxygen fraction. Reduced oxygen concentration at constant T_{ad} from cases 5-7, makes the mixture more fuel-rich, subsequently lowering the laminar flame speed. At constant equivalence ratio ($\phi = 0.5$) in cases 5-7, OH concentration and laminar flame speed reduce with OF and T_{ad} . Similar to case-1, case-7 also demonstrate weaker lifted flame in lower T_{ad} near blowout limit. Furthermore, in all cases lower presence OH radicals are observed in the corner of the combustor indicating limited reaction in the outer recirculation zone (ORZ), which is explained in **Figure 4.44** below.

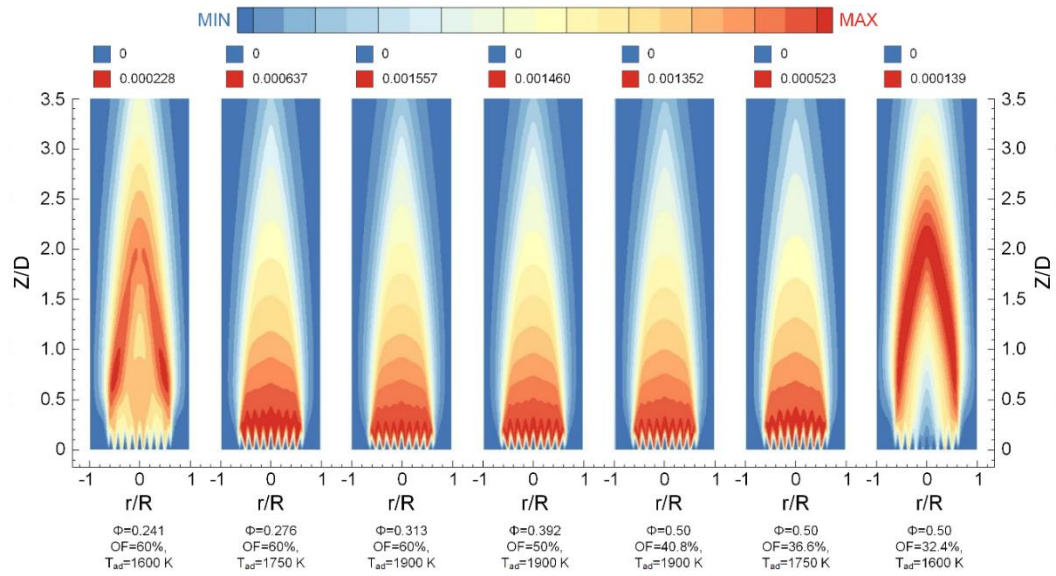


Figure 4.41: Flame shapes based on OH contours for the selected cases.

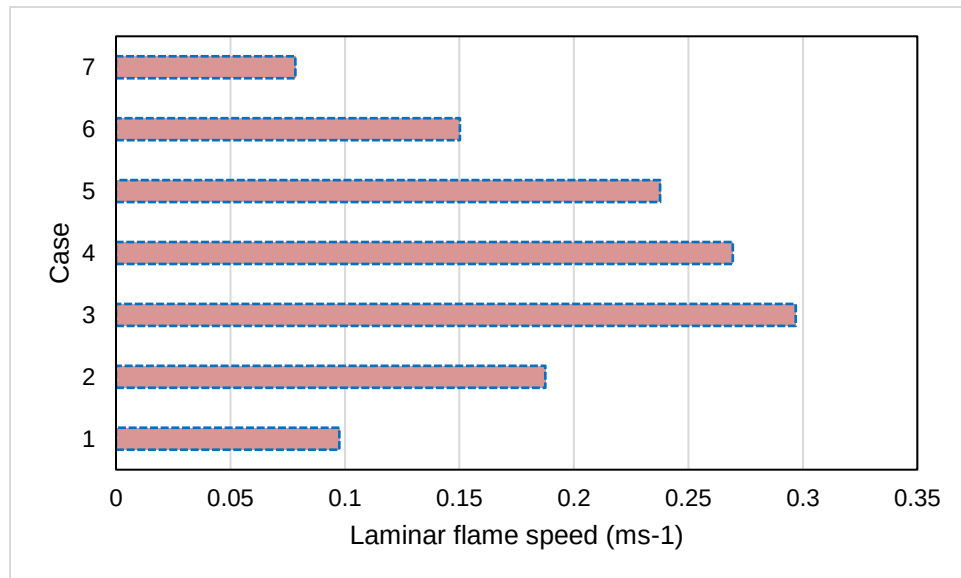


Figure 4.42: Laminar flame speeds for $C_3H_8/O_2/CO_2$ flames.

4.4.2 Temperature and flow-field structure of $C_3H_8/O_2/CO_2$ flames in multi-hole burner

Flame temperatures and velocity streamlines can provide insight in comprehending the flow field and heat release. **Figure 4.43** illustrates the temperature distribution inside the combustion chamber. The temperature inside the combustor increases as the $\emptyset$ is increased in constant OF from cases 1 to 3 and decreases as the OF is increased in constant $\emptyset$ from cases 5 to 7. Similarly, at constant T_{ad} , the changes in combustor temperature is attributed to the variation in $\emptyset$ and OF. Temperature is observed to be significantly lower in the in between $-0.8 \leq r/R \leq 0.8$ and $0 \leq Z/D \leq 2$ as the flame approaches near blowout limit (i.e. cases 1 & 5). A temperature gradient along the radial direction is seen for the flames in multi-hole combustor, which reduces at higher $\emptyset$, OF and T_{ad} .

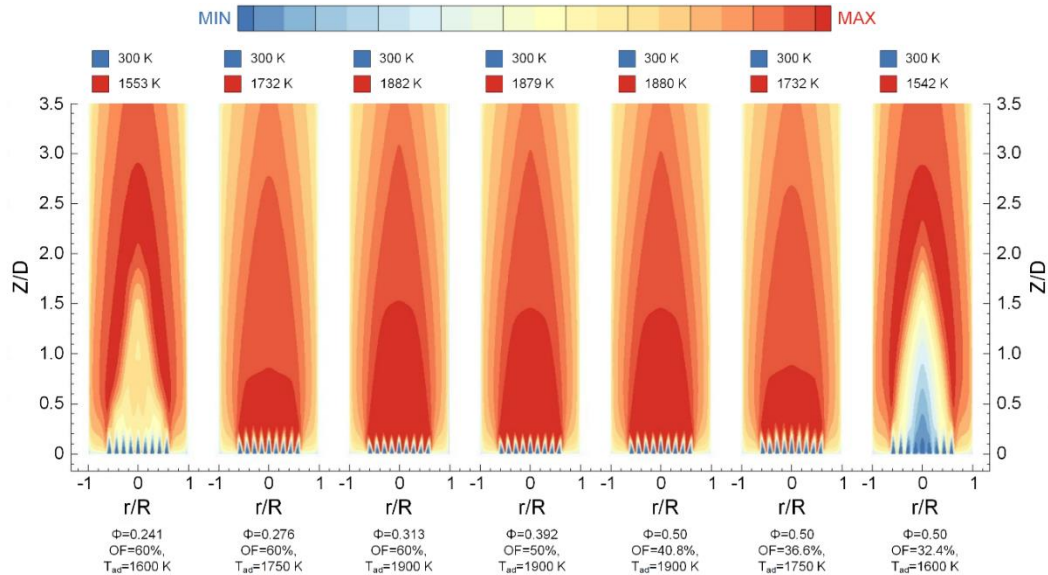


Figure 4.43: Temperature contours for $C_3H_8/O_2/CO_2$ flames in multi-hole combustor.

Figure 4.44 shows the velocity streamlines mapped over temperature contour at the centerline plane of the combustion chamber in $\Phi=0.313$, OF=60%, $T_{ad}=1900$ K. Unlike the swirl stabilized $C_3H_8/O_2/CO_2$ flames, examined in earlier study by Nemitallah et al. [257], where the flames are characterized by two recirculation zones: inner recirculation zone (IRZ) and outer recirculation zone (ORZ), the flow-field in multi-hole combustor can be characterized by the presence of ORZ only. Similar finding was also reported in the experimental study involving $CH_4/O_2/CO_2$ flames in a multi-hole combustor by Hussain et al. [222]. Further comparison between the multi-hole and swirl-stabilized combustors are presented in **section 4.4.4** below.

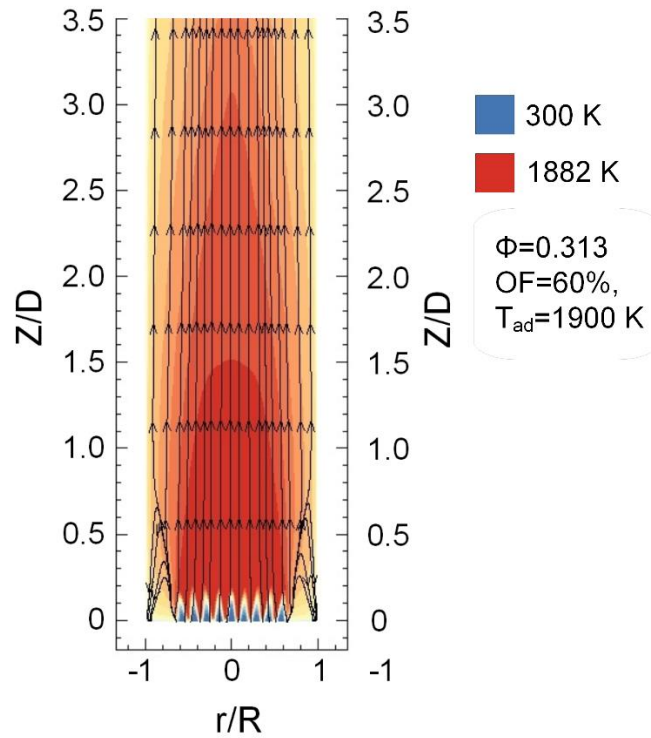


Figure 4.44: Velocity streamlines over temperature contours for $C_3H_8/O_2/CO_2$ flame at 5.2 m/s bulk inlet velocity, 0.313 Φ and 60% OF under atmospheric condition.

4.4.3 Combustion and emission characteristics in multi-hole burner

Combustion and emission attributes of $C_3H_8/O_2/CO_2$ flames in multi-hole combustor are examined in this section in terms of product formation rate (PFR), progress variable (PV) and Damköhler number (Da), flame thickness, distribution of species mole fractions and the CO emission in ppm. The terms PFR corresponds to the rate at which the products are formed, PV refers to transition from unburnt to fully burnt product whereas Da is the ratio of reaction rate and diffusion rate.

Figure 4.45 and **Figure 4.46** illustrate the PFR and PV in the combustor. The reaction zone exists between the inner shear layer (ISL) and outer shear layer (OSL) for each flamelets and the flamelets are stabilized on both ISL and OSL. For the flames near blow out limit in **Figure 4.45**, i.e. cases-1 & 7, the no reaction is taking place in 3 inlet holes in the middle and the production formation occurs within $0 \leq Z/D \leq 2.5$. For the rest of the flames, i.e. cases 2-6, the reaction zone is observed within $0 \leq Z/D \leq 0.35$. Likewise, complete transition from unburnt reactant to burnt production occurs within $0 \leq Z/D \leq 0.35$ for stable flames in cases 2-6 as shown in **Figure 4.46**. The transition requires more axial distance to fully turn into product species in flames near blow out limit, which is $0 \leq Z/D \leq 2.2$ for case-1 and $0 \leq Z/D \leq 2.4$ for case-7.

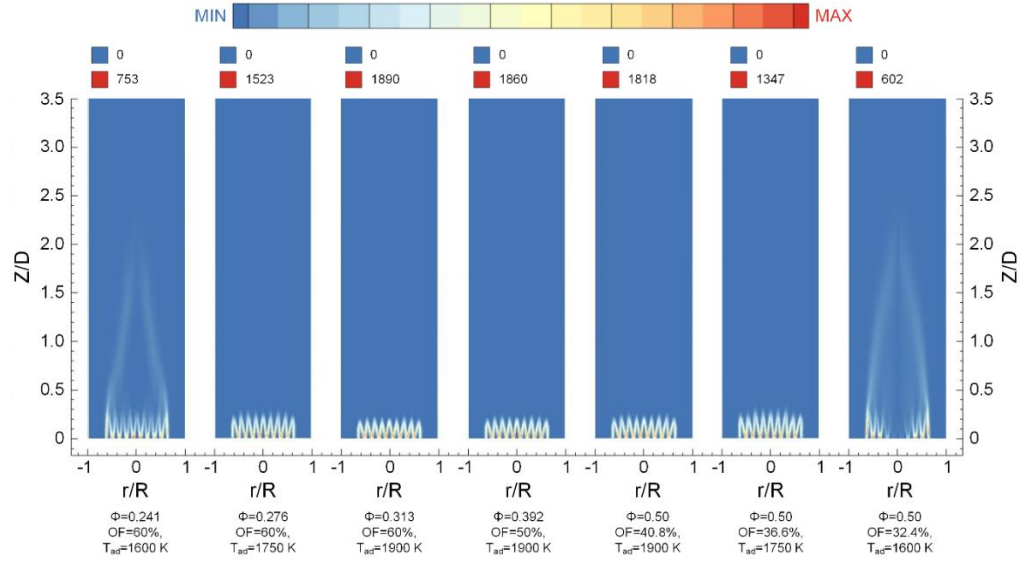


Figure 4.45: PFR contours for the selected cases.

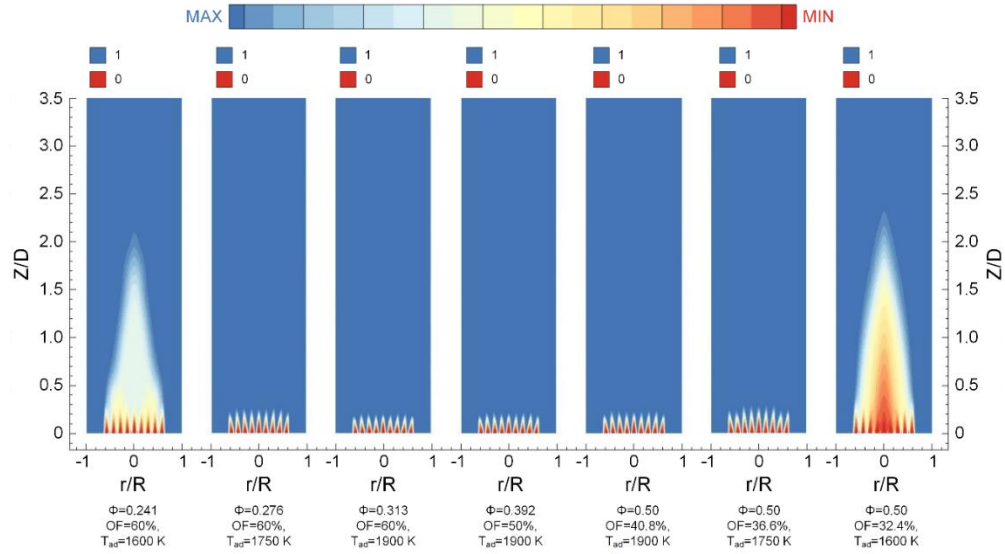


Figure 4.46: PV contours for the selected cases.

Figure 4.47 depicts the Da and flames thickness for the oxy-propane flames. The values of Da in **Figure 4.47(a)** are more than implying the reaction rate in the combustor is dominant over the diffusion rate. Da increases with Φ constant OF, while Da changes with

OF at constant $\emptyset$. At constant T_{ad} , Da depends on the fuel-oxidizer composition, where Da decreases from cases 3-5 with the drop in OF and rise in $\emptyset$. The change in flame thickness, on the other hand, is opposite to the Da as shown in **Figure 4.47(b)**, whereas the flames get stronger the flame becomes compact consequently reducing the flame thickness.

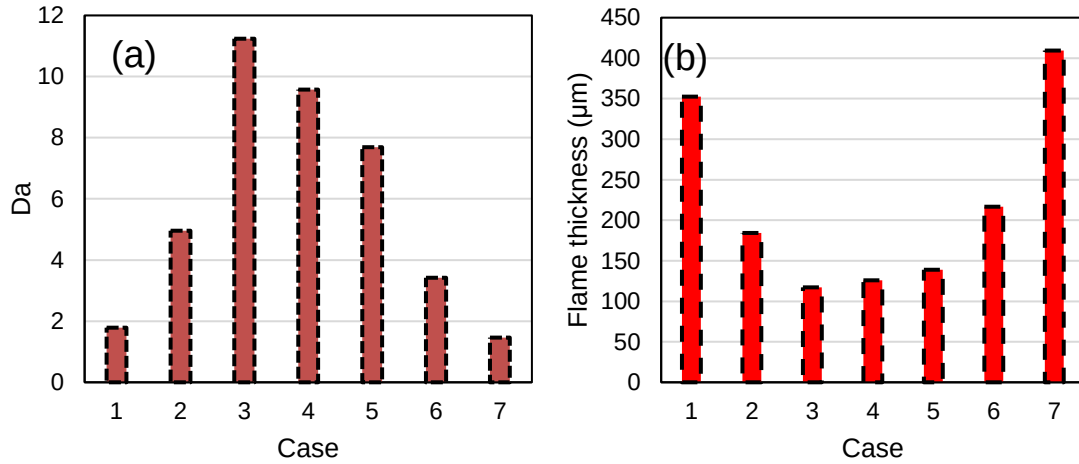


Figure 4.47: (a) Damköhler number, and (b) flame thickness for $C_3H_8/O_2/CO_2$ flames.

Figure 4.48 and **Figure 4.49** present the distributions of C_3H_8 and CO mole fractions within the combustor. As shown in **Figure 4.48**, the concentration of C_3H_8 is higher at the inlet and reacts with oxygen to form the product gases within $0 \leq Z/D \leq 0.3$. Due to the lower PFR in the middle 3 holes and the transition from reactant to product taking place within $0 \leq Z/D \leq 2.1$, the presence of C_3H_8 is observed within axial distance $0 \leq Z/D \leq 2.4$. The mole fraction of CO inside the combustor in **Figure 4.49** mainly depends on the combustor temperature and the availability of oxygen and fuel concentration. The CO concentration increase from Case-1 to 3 with the increase in $\emptyset$ and T_{ad} . CO mole fraction inside the combustor increases from Cases 3 to 5 with the OF. At higher OF and lower $\emptyset$ (case-3), more oxygen is available compared to the fuel in the combustion chamber, which oxidizes

the generated CO and produces CO₂. Alternatively, at lower OF and higher Φ (case-5), the oxygen content is inadequate for complete combustion, which raises the CO in the combustor. Lastly, in cases 5 to 7, the decrease in CO concentration is due to the reduction in OF, which reduces the oxygen availability for the oxidation of CO. The variation of CO in the combustion chamber is also reflected in the CO emission at the combustor outlet, shown in **Figure 4.50**.

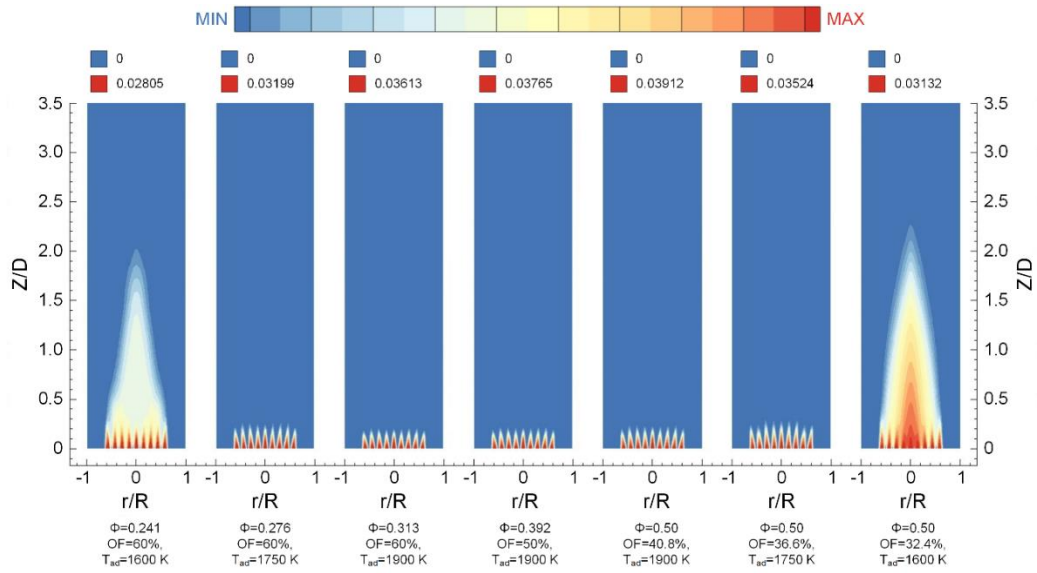


Figure 4.48: C₃H₈ contours for the selected cases.

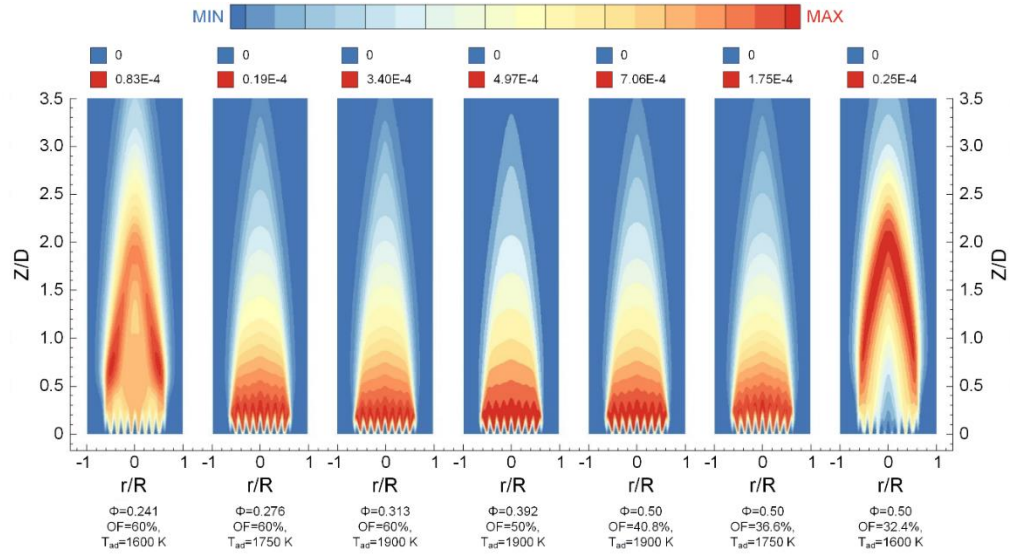


Figure 4.49: CO contours for the selected cases.

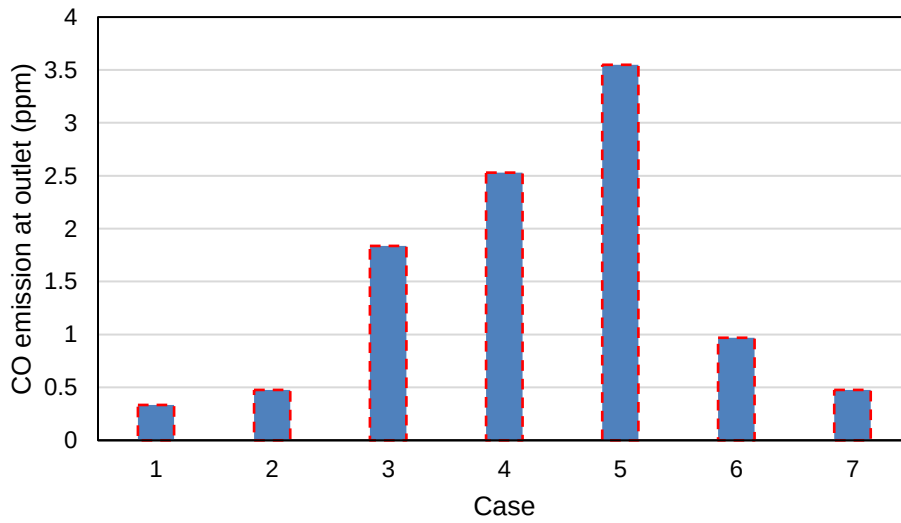


Figure 4.50: CO emission at combustor outlet with the studied $C_3H_8/O_2/CO_2$ flames.

4.4.4 Flame comparison between multi-hole and swirl-stabilized

combustors

The oxy-propane flame in multi-hole combustor is compared with that in a swirl-stabilized combustor with bluff body in this section. The swirl-stabilized burner encompasses a swirler setup with 8 vanes angled at 55° . The swirler surrounds a solid conical center-body with 28° cone angle. The flames in both the combustor have identical inlet reactant composition ($\phi=0.313$, $OF=60\%$, $T_{ad}=1900$ K). Since, these combustors have different cross-sectional areas for fuel-oxidizer inlet, fixing bulk throat velocity at 5.2 m/s will result in variation in total mass flow rates. Thus, to maintain identical power density (8.36 MW/m³/bar) among the combustors, the mass fluxes are fixed ensuring identical mass flow rates.

Figure 4.51 depicts the comparison between multi-hole and swirl-stabilized combustor in terms of temperature distribution, flow-field, vorticity and CO formation within the combustion chamber. High temperature zones is observed in the middle of combustor at upstream of the flow with only ORZ at the corner of the combustor, whereas the high temperature areas are recorded near the combustor wall due to the swirling motion of the flow with both IRZ and ORZ present in the chamber. The highest flame core temperatures are comparable in both the multi-hole (1882 K) and swirl-stabilized (1892 K) combustor. The axial temperatures are slightly higher in multi-hole combustor than the swirl-stabilized counterpart. **Figure 4.52** shows the temperature along combustor length for both types of burner. Sharp increase in temperature is observed within $0 \leq Z/D \leq 0.28$, and $0 \leq Z/D \leq 0.09$ for multi-hole and swirl-stabilized combustor, respectively. Temperature decreases gradually

as the flow progresses downstream (i.e. $0.25 \leq Z/D \leq 3.5$) for multi-hole configuration, whereas a steep reduction in temperature is found in swirl-stabilized counterpart within $0.09 \leq Z/D \leq 0.14$ followed by ~ 255 K temperature drop within the axial position $0.14 \leq Z/D \leq 3.5$.

Reduced temperature downstream of swirl-stabilized combustor are attributed to the effect of swirl flow which enhances the heatflow inside the combustion chamber. This also impacts the pattern factors at the combustor outlet. Multi-hole combustor demonstrate large difference between the average and maximum temperature at the outlet, raising the pattern factor to 0.19, while lower difference in swirl-stabilized combustor results in significantly lower pattern factor of 0.06, as depicted in **Figure 4.53**. This variation in mean and maximum outlet temperatures are due to heat loss through the quartz wall by means of both convection and radiation heat transfer. Furthermore, the swirl effect allows increases residence time and reduces flame temperature as reported in earlier studies [258,259].

Maximum vorticity in multi-hole combustor is observed as 5928.24 s^{-1} , while the value of which is considerably higher (46394.8 s^{-1}) in swirl-stabilized burner. Lower vorticity in multi-hole burner reduces the circulation tendency compared to the swirl-stabilized burner. On the other and, the maximum CO mole fraction is higher in multi-hole combustor than swirl-stabilizes combustor, which oxidizes to CO_2 , resulting in lower CO emission at the outlet, as shown in **Figure 4.54(c)**. Da is lower in multi-hole combustor (**Figure 4.54(a)**) which implies reduced reaction rate over diffusion rate compared to that of swirl-stabilized counterpart. Reduced reaction rate consequently impacts the flame and in turn increase flame thickness, shown in **Figure 4.54(b)**.

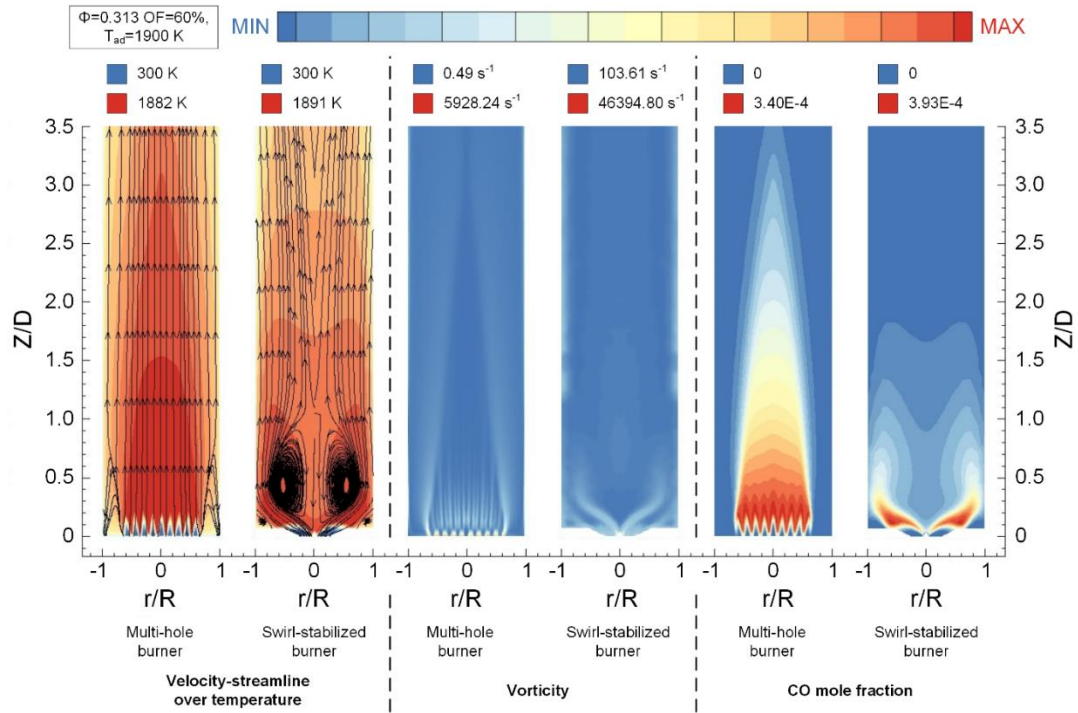


Figure 4.51: Temperature distribution in multi-hole (left), and swirl-stabilized (right) combustor at 0.313 Φ , 60% OF under atmospheric conditions.

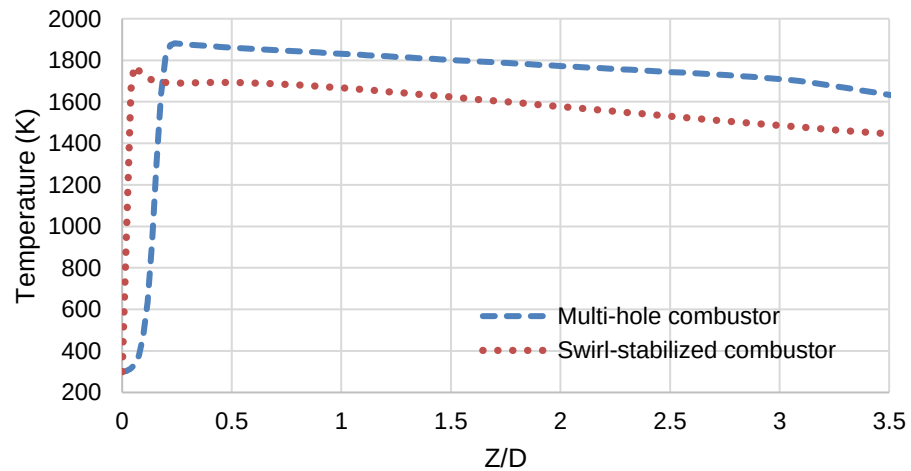


Figure 4.52: Axial temperature distribution in multi-hole, and swirl-stabilized combustor at 0.313 Φ , 60% OF under atmospheric conditions.

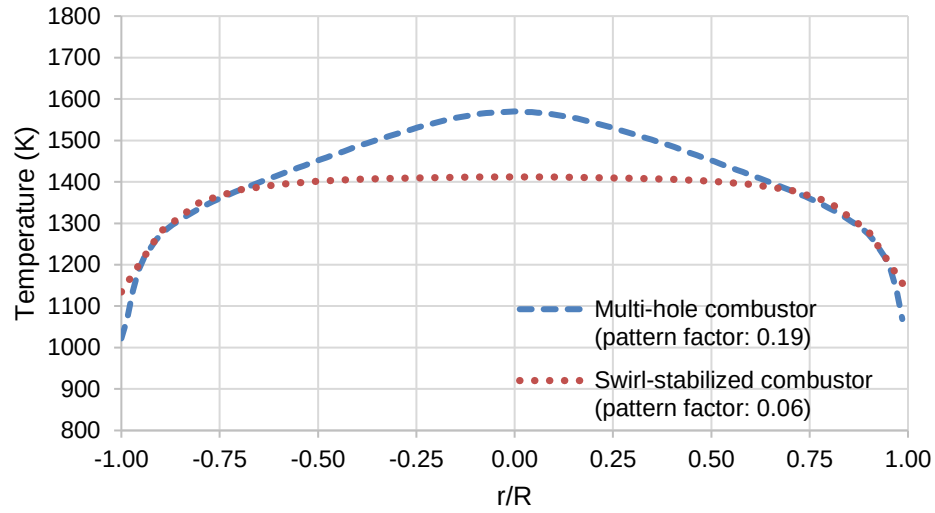


Figure 4.53: Radial temperature distributions at the outlet of the combustors at 0.313 Ø, 60% OF under atmospheric conditions.

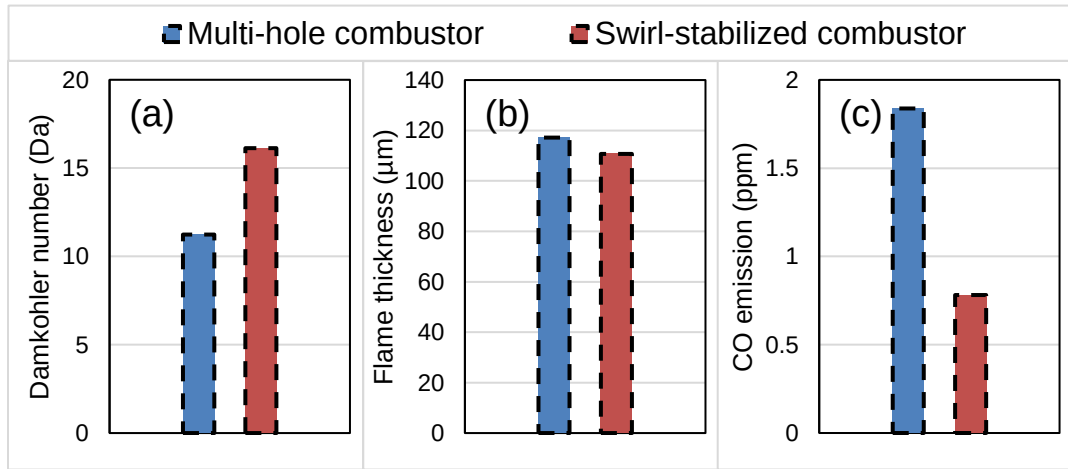


Figure 4.54: Comparison of flames in multi-hole and swirl-stabilized combustor in terms (a), Da , (b) flame thickness, and (c) CO emission at 0.313 Ø, 60% OF under atmospheric conditions.

CHAPTER 5

CONCLUSIONS

Premixed oxy-fuel flames (propane and methane) have been investigated numerically in premixed swirl-stabilized and multi-hole combustors in different feed composition under atmospheric condition. The equivalence ratio (Φ) and oxygen fraction (OF) have been varied from 0.241-0.597 and 32.4-60%, respectively, at a fixed bulk inlet velocity of 5.2 m/s. Swirl-stabilized oxy-propane flames have also been compared with that of methane and syngas. Oxy-propane flames have been further examined in a multi-hole type gas turbine combustor. In addition, a comparison between propane flames in swirl-stabilized and multi-hole setup in identical combustor power density. Based on this study, the following conclusions have been drawn.

For swirl-stabilized premixed $C_3H_8/O_2/CO_2$ flames:

- Adiabatic flame temperature (T_{ad}) has demonstrated a dominant role in controlling flame shape, stability, and combustion and emission characteristics. Flames of similar T_{ad} have similar macro- and flow field-structures for a given swirler setup (swirl angle 55°). At higher T_{ad} , the oxy-propane flames become compact and possess the characteristic V-shape. For the highest T_{ad} at 2303K in case 3, the flame thickness is found the smallest (52.10 μm). Alternatively, at lower T_{ad} , the flames are more spread-out towards the combustor wall, losing the V-shape and stability. Among the studied

cases, the lowest T_{ad} is calculated for case 1 at 1681 K for which shows high flame thickness of 222.86 μm .

- A balance between Φ and OF should be maintained to achieve the optimum T_{ad} and laminar flame speed. At a fixed 60% OF, the change in Φ from 0.26 to 0.42 results in approximately 3.2 times enhancement in laminar flame speed and 37% rise in T_{ad} . Similar effect is also observed with increasing OF at fixed Φ .
- Two inner recirculation zones (IRZ) were observed for oxy-propane flames: one near combustor inlet (primary IRZ) and another further downstream (secondary IRZ). The primary IRZ observed at higher Φ is characterized by the formation of more than one single eddy which is located within $0.1 < Z/D < 0.5$. At higher Φ /OF/ T_{ad} , the secondary IRZ (at $Z/D > 1.7$) shifts further downstream. The role of outer recirculation zone-ORZ (at $Z/D < 0.3$) in enhancing flame stabilization and anchoring is more visible at higher Φ /OF/ T_{ad} ; however, it disappears at lower Φ /OF, making the flame more spread-out, weak, as well as lifted, before eventually blowing out.
- Reaction rates rise at higher Φ /OF due to the increased concentration of chemically active radicals, subsequently increasing the Damköhler number (Da) and reducing the flame thickness. The highest and lowest values of Da are found for case 3 and case 8 at 80.95 and 4.08, respectively. Equivalence ratio plays a vital role in the CO emission of $\text{C}_3\text{H}_8/\text{O}_2/\text{CO}_2$ flames. Zero CO emission is observed with case 1 and 2, meanwhile the highest CO emission calculated in this case is 0.17 ppm for case 5.

For swirl-stabilized premixed CH₄/O₂/CO₂ flames:

- Flame core temperature, the thickness of the reaction zone between inner shear layer (ISL) and outer shear layer (OSL) in CH₄/O₂/CO₂ flames, and vorticity increases with T_{ad} at fixed OF and with OF at fixed AFT. A single IRZ is observed for all the cases, where recirculation intensity increases with the T_{ad} (OF fixed) and OF (T_{ad} fixed). For the studied cases, the counter-clockwise IRZ usually observed within $0 \leq Z/D \leq 1.85$ assuming the characteristic V-shape. The clockwise spinning ORZ is found unaffected with the rise in AFT at constant OF, while the recirculation slightly increased with OF at Fixed AFT.
- Emission of CO and Da values for CH₄/O₂/CO₂ flames increases in higher T_{ad} (OF fixed) and increased OF (T_{ad} fixed). Increasing the AFT from 2100 to 2500 K at 65% OF resulted in approximately 2.9 time rise in CO emission.

For comparison of oxy-fuel flames for propane-methane and syngas under swirl-stabilized condition:

- In comparison with different fuels, T_{ad} and power densities (PD) are almost similar for methane, syngas, and propane flames, where both these parameters show lowest values for oxy-methane flames. Laminar flame speed (LFS) varies significantly with different fuels. Oxy-methane flames demonstrate lower LFS values than syngas and propane, respectively. In addition, more compact flame with lower flame thickness is observed for propane which are around 59-67% of methane flames and 82-88% of syngas flames under studied operating conditions. The concentration of OH radicals are higher with

syngas and lower with methane, indicating higher reactivity at flame core due to the variation in hydrogen content in the fuel. Combustion temperature is slightly higher for oxy-propane flame as compared to methane and propane counterparts.

- The lower value of pattern factor (PF) is observed with syngas flames followed by propane and methane implying more uniform temperature distribution at the combustor outlet for the syngas flames. On the other hand, thermal power is higher with propane, where the lowest thermal powers are observed for syngas in all equivalence ratios.
- Among the fuels, syngas resulted in higher CO emission than the other two fuels because of its higher hydrogen content. The CO emissions at combustor outlet are approximately 7.1 times for syngas and 9.3 times for propane as compared to that with methane flames at $\Phi = 0.39$, while the ratios are 2.4 and 1.7, respectively, at $\Phi = 0.42$.
- To further summarize the parameters in different fuels, in identical bulk throat velocity of 5.2 m/s in atmospheric pressure:
 - LFS: Propane>syngas>methane
 - PD: propane>methane>syngas
 - Flame thickness: methane>syngas>propane
 - Da: propane>syngas>methane
 - PF: methane>propane>syngas
 - CO emission: syngas>propane>methane

For comparison of $C_3H_8/O_2/CO_2$ flames in swirl-stabilized and multi-hole combustors:

- Oxy-propane flames in multi-hole combustor possess only ORZ, while both IRZ and ORZ are present in swirl-stabilized setup. Damköhler number and flame thickness changes similarly with Φ , OF and T_{ad} to swirl-stabilized counterpart.
- Due to the absence of swirling motion inside (IRZ) the chamber the axial temperature is considerably higher with multi-hole combustor compared to the swirl-stabilized one.
- For a given case (flow composition), the Da is lower, while the pattern factor, flame thickness and CO emission are higher in multi-hole combustor than the swirl-stabilized counterpart.

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Vitae

Name	:Md Azazul Haque
Nationality	:Bangladeshi
Date of Birth	:5/22/1993
Email	:h.azazul@gmail.com
Address	:56, Nobabgonj Road, Lalbagh, Dhaka, Postal code-1211, Bangladesh
Academic Background	: M.Sc. in Mechanical Engineering December 2021 King Fahd University of Petroleum and Minerals, Dhahran-31261, Saudi Arabia : B.Sc. in Mechanical Engineering November 2014 Islamic University of Technology, Gazipur-1704, Dhaka, Bangladesh
ORCID:	https://orcid.org/0000-0002-4800-0101

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