OPTIMIZATION OF MILD CHAMBER FOR THE COMBUSTION OF BIOMASS PRODUCER GAS

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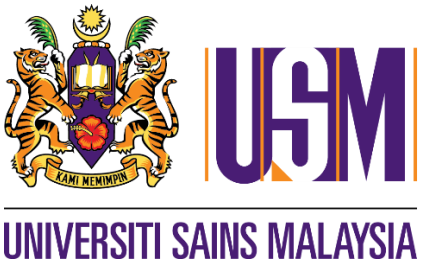

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This thesis is the result of my own investigations, except where otherwise stated.

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ACKNOWLEDGEMENT

In the name of Allah, the Most Gracious, the Most Merciful

First and foremost, I would like to praise Allah the Almighty, the Most Gracious, and the Most Merciful for His blessings given to me during my study and in completing this thesis. May Allah's blessing go to His final messenger Prophet Muhammad (peace be up on him), his family and his companions.

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LIST OF SYMBOLS

D_a	Damköhler number
D_{air}	Air inlet diameter
D_c	Circular combustor diameter
D_e	Equivalent diameter
D_f	Fuel inlet diameter
D_o	Outlet diameter
G_b	Generation of turbulence kinetic energy due to buoyancy
G_k	Generation of turbulence kinetic energy due to the mean velocity
H_s	Square combustor height
k	Turbulence kinetic energy
K_v	Dilution ratio
L_c	Circular combustor length
L_s	Square combustor length
P_{in}	Thermal input
T_c	Chamber temperature
T_{in}	Inlet temperature
t_m	Mean residence time
T_{max}	Maximum combustors temperature
T_{si}	Self-ignition temperature
V	Volume of chamber
V_a	Air inlet velocity
V_f	Fuel inlet velocity
Y_M	Contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate
ΔT	Maximum temperature increase
ε	Dissipation rate
φ	Fuel air equivalence ratio
G_{ij}	Buoyancy production
Z_i	Elemental mass fraction for element (i)
$Z_{i,fuel}$	Value at the fuel stream inlet
$Z_{i,ox}$	Value at the oxidizer stream inlet
f	Mixture fraction
m	Total mass flow rate
ρ	Average density of the gas
ρ_ε	Turbulent Prandtl numbers for ε
ρ_k	Turbulent Prandtl numbers for k

LIST OF ABBREVIATIONS

C_2H_4	Ethylene
C_2H_6	Ethane
CFD	Computational Fluid Dynamics
CH_4	Methane
CH_4	Methane
CO	Carbon Monoxide
CO_2	Carbon Dioxide
DOE	Design of Experiments
EDC	Eddy dissipation concept
EGR	Exhaust gas recirculation
Eq.	Equation
FLOX	Flameless oxidation
FOF	Fuel-oxidant-fuel
H_2	Hydrogen Gas
H_2S	Hydrogen sulfide
HHV	Higher heating value
HiTAC	High temperature air combustion
IGR	Internal exhaust gas recirculation
kg/s	Kilogram/Second
kW	Kilowatt
LHV	Low Heating Value
MA	Mass flow rate of air
ME	Mass flow rate of exhaust gas recirculation
MF	Mass flow rate of fuel
MILD	Moderate or intense low-oxygen dilution
mm	Millimetre
MMF	Mean Mixture Fraction
MT	Total mass flow rate
N_2	Nitrogen Gas
NH_3	Ammonia
NOx	Nitrogen oxides
OFO	Oxidant-fuel-oxidant
OH	Hydroxyl
PCA	Principal component analysis
PDF	Probability Density Function
PG	Producer Gas
ppm	Parts Per Million
T_c	Chamber temperature
T_{in}	Inlet temperature
T_{max}	Maximum combustors temperature
T_{si}	Self-ignition temperature
ΔT	Maximum temperature increase

ABSTRAK

Pengeluaran tenaga masih banyak bergantung pada pembakaran. Pembakaran MILD adalah calon yang menjanjikan untuk menyokong peralihan ke arah sasaran pelepasan sifar bersih, namun ia memerlukan kajian asas lanjut kerana penyelidikan terhad semasa mengenai penggunaannya pada gas pengeluar biojisim (PG) gred rendah. Cabaran utama adalah untuk mencapai pembakaran lengkap dalam pembakaran MILD dengan pelepasan CO dan NO_x yang rendah sambil mengekalkan geometri pembakaran yang ringkas dan padat. Matlamat kajian ini adalah untuk menangani cabaran gas pengeluar biojisim (PG) gred rendah melalui pengoptimuman pembakaran MILD. Kerja ini termasuk menggunakan simulasi ANSYS-FLUENT computational fluid dynamics (CFD) bagi gas pengeluar biojisim (PG) gred rendah daripada pengegasan udara kayu dalam ruang pembakaran MILD. Kajian ini merangkumi dua peringkat Reka Bentuk Eksperimen (DOE), peringkat pertama (DOE1) dan peringkat kedua (DOE2). Parameter geometri, untuk dua bentuk (pembakar keratan rentas bulat dan keratan rentas segi empat sama) telah diuji dengan menggunakan 18 kes simulasi CFD dan keputusan dianalisis melalui alat pengoptimuman DOE1. Geometri optimum untuk pembakar bulat ialah diameter pembakar 200mm, D_c dan 1000mm panjang pembakar, L_c dengan peningkatan suhu maksimum 710°C, pelepasan CO 3.3 ppm, pelepasan NO_x 15.2 ppm dan nombor Damköhler 0.99 dan geometri optimum untuk pembakar persegi ialah 548.86mm panjang pembakar, L_s dan ketinggian pembakar 1500mm, H_s dengan peningkatan suhu maksimum 718°C, pelepasan CO 6.41 ppm, pelepasan NO_x 342.24 ppm dan nombor Damköhler 0.34. Pembakar bulat dengan ketara melebihi segi empat sama dalam pelepasan CO dan NO_x dan nombor Damköhler dengan pengecualian peningkatan suhu maksimum. DOE2 melibatkan pembakar bulat optimum kerana pembakar bulat secara amnya mengatasi pembakar persegi dan mempunyai ciri pembakar optimum yang lebih baik. DOE2 mempunyai 9 simulasi CFD berdasarkan arahan DOE. DOE2 bertujuan untuk mengoptimumkan kebuk pembakaran MILD untuk keadaan operasi. Pada akhirnya, pembakar keratan rentas bulat 200mm diameter pembakar, D_c dan 1000mm panjang pembakar, L_c dengan nisbah kesetaraan bahan api-udara, $\varphi = 0.9$ dan halaju masuk bahan api, V_f = 200m/s mempunyai suhu maksimum 733°C peningkatan, 2.5 ppm pelepasan CO, 11.1 ppm pelepasan NO_x dan 0.76 nombor Damköhler dianggap sebagai ruang MILD yang optimum.

ABSTRACT

Energy production still heavily relies on combustion. MILD combustion is a promising candidate to support the transition towards the net zero emission target, however it needs further fundamental study due to the current limited research on its application on low-grade biomass producer gas (PG). The main challenge is to achieve complete combustion in MILD combustion with low CO and NOx emissions while maintaining simple and compact combustor geometry. The aim of this study was to tackle the challenges of low-grade biomass producer gas (PG) through optimization of MILD combustion. The work included using ANSYS-FLUENT computational fluid dynamics (CFD) simulation of low-grade biomass producer gas (PG) from wood air-gasification in a MILD combustion chamber. The study included two stages of Design of Experiments (DOE), first-stage (DOE1) and second-stage (DOE2). Geometry parameters, for two shapes (circular cross-section and square cross-section combustors) were tested by using 18 CFD simulation cases and results were analysed through DOE1 optimization tool. Optimum geometry for circular combustors was 200mm in combustor diameter, D_c and 1000mm in combustor length, L_c with 710°C maximum temperature increase, 3.3 ppm CO emissions, 15.2 ppm NO_x emissions and 0.99 Damköhler number and the optimum geometry for square combustors was 548.86mm combustor length, L_s and 1500mm combustor height, H_s with 718°C maximum temperature increase, 6.41 ppm CO emissions, 342.24 ppm NO_x emissions and 0.34 Damköhler number. The circular combustors significantly surpassed the square ones in, terms of performance, for CO and NO_x emission and Damköhler number with the exception of maximum temperature increase. DOE2 involved the optimum circular combustor since circular combustors generally outperformed the square combustors and had better optimum combustor characteristics. DOE2 had 9 CFD simulations based on the instruction of DOE. DOE2 aimed to optimize the MILD combustion chamber for operating conditions. In the end , the circular cross-section combustor of 200mm in combustor diameter, D_c and 1000mm in combustor length, L_c with fuel-air equivalence ratio, $\varphi = 0.9$ and fuel inlet velocity, $V_f = 200$m/s having 733°C maximum temperature increase, 2.5 ppm CO emissions, 11.1 ppm NO_x emissions and 0.76 Damköhler number was considered the optimum MILD chamber .

CHAPTER 1
INTRODUCTION

1.1 General

Energy security is growing more significant as the usage of energy has been critical in the growth of the human society, as well as concerns about fossil fuel reserves depletion. By 2042, fossil fuels will be depleted due to the existing supply and demand [1]. Because of the world's growing population and significant economic development in places like Southeast Asia, China, and India, energy demand is surging. About 80% of these energy requirements are expected to be met by fossil fuel burning[2]. In 2012, global energy consumption was 549 quadrillion Btu, and by 2040, it is anticipated to rise to 815 quadrillion Btu [3]. Large volumes of fuel are required due to the increased demand for energy. Furthermore, Northern Europe and North America relied heavily on fossil fuels to create their economies throughout the 18th, 19th, and 20th centuries [4].

Biomass energy is a renewable energy source. Examples of biomass include crops waste, livestock manure, municipal solid waste, and industrial waste [5]. Biomass is an environmentally friendly fuel since it is carbon neutral, producing no net CO_2 through the natural carbon cycle[6]. Biomass is carbon neutral because the amount of CO_2 emitted after combustion is equal to the amount of CO_2 absorbed while alive. Many countries use biomass energy for heat and electricity generation, and because most countries have forest resources and a forest industry, biomass energy use will be significant in the future [7]. Because Malaysia is an agricultural producer, biomass can be employed as a renewable energy source. Empty fruit bunches, fruit fibers, palm shell, palm oil mill effluent, wood chips, rice husks, bagasse, and other biomass resources are available in Malaysia[8]. Biomass can be turned into producer gas (PG) for use in power plants via the gasification process. CO_2, CO, H_2, O_2, N_2, and CH_4 make up the majority of PG's composition. Because of the dilution of CO_2 and N_2 in PG, its heating value is low, ranging from 4 to 6 MJ/m^3[9]. Better fuel-air mixing and a longer residence time are necessary to totally burn low-grade PG. While biomass fuel is environmentally friendly, it has a low heating value. As a result, operating a combustor using biomass

fuel presents numerous challenges. The following are the primary difficulties of burning low-grade PG[10]:

1. Low-grade PG combustion instability.
2. Burning low-grade PG results in a low temperature.
3. Low-grade PG burning necessitates a large combustor capacity.

To address this problem, researchers are focusing on new technology and combustion modelling in order to improve combustion efficiency while lowering emissions[11], [12] . Preheating the reactant with a hot flue gas is one way to improve combustion efficiency. Moderate or Intense Low-oxygen Dilution (MILD) combustion of PG, which yields high combustion efficiency with very low emissions, has been developed as a solution to this problem. DOE, using MINITAB software, will be used extensively to optimize the combustion variables, this will be done to two shapes of combustion chambers designs and later a new optimized design shall emerge, and further DOE will be performed on the latter to optimize for operating conditions. The performance of low-grade PG burning can be improved and minimal emissions emitted by using the MILD combustion method.

1.2 Problem statement

The low quality of producer gas (PG) from biomass gasification with low heating value 4-6 MJ/m^3 and high dilution with non-combustible gases such as N_2 and CO_2, is a major obstacle. Therefore, researchers are looking into new technologies to achieve efficient and complete combustion of PG. One of the recent innovative methods for clean and efficient combustion of low-grade fuels is MILD combustion method [13]. However, the current challenge for MILD is to develop further understanding about the combustion characteristics. Therefore, an optimization of MILD combustion, using DOE simulation, to determine the major parameters impacting the emission performance is essential.

1.3 Objectives

1. To design and optimize the geometry of MILD combustion chambers, using DOE method and ANSYS FLUENT simulation to determine the significant variables that achieve complete combustion of biomass PG with low CO and NO_x emissions.

2. To optimize the operating conditions of MILD optimum combustion chamber obtained in first-stage DOE, using second-stage DOE and ANSYS FLUENT simulation, that achieves MILD requirement.

1.4 Scope of work

The literature on the use of biofuels in the flameless mode, also known as MILD, is extremely scarce. In a study by Abuelnuor [14] and a more recent review by Budzianowski [15], they state that there are relatively few studies in this area. Therefore, the aim is to incorporate the use of biomass PG in MILD combustion while overcoming its main challenges of burning and performing optimization using DOE simulation to achieve optimum results with no experimental approach.

There are a few limitations to this research, which are:

1. Because the simulation is limited to a boundary condition, unforeseen factors outside of the boundary condition (for example, factors in real scenarios) are not considered.

2. The research was limited to DOE methods. Due to time constraint, the experimental test of the optimum geometry was not conducted.

CHAPTER 2
LITERATURE REVIEW

2.1 Introduction

This chapter provides an overview of MILD combustion and gasification. It also covers the requirements to achieve MILD combustion. The chapter also includes research on MILD combustion design requirements including oxygen dilution and reactant preheating. Later in this section, MILD combustion modelling is also discussed.

2.2 MILD Combustion

Fuel, oxidizer, and a heat or ignition source are required for combustion processes. A turbulent mixing process is required before the ignition process to mix the fuel and oxidizer on a molecular level. During studies with a self-recovery burner, Wünning (1991)[16] noticed an unexpected behaviour. No flame could be observed, and no UV-signal could be identified at furnace temperatures of 1000°C and roughly 650°C air preheat temperature. The fuel was totally burned, and the CO level in the exhaust was less than one part per million. With smooth and consistent combustion, NO_x emissions were nearly non-existent. Milani and Wünning (2007) [17] dubbed the situation "flameless oxidation," or FLOX[18].

MILD combustion is another name for this innovative combustion technique[19]. Apart from functioning at higher temperatures, Katsuki and Hasegawa (1998) and Tsuji (2003) [20], [21] discovered that high-temperature air combustion (HiTAC) is substantially identical to MILD combustion. MILD combustion has several advantages, including the ability to produce a uniform temperature distribution, superior combustion stability, high efficiency, and low NO_x emissions.

Because the temperature of the reactant must be higher than the mixture's self-ignition temperature (Table 2.1), MILD combustion relies on the recirculation of hot flue gas to preheat the reactants while also diluting oxygen [21]. The maximum temperature increase caused by combustion is lower than the temperature at which the mixture self-ignites[19].

Common MILD combustion appears to be summarized as:

1. The essential prerequisites for accomplishing MILD combustion are high-temperature pre-heating of combustion air and high-speed injection of air and fuel.
2. The crucial technique for maintaining MILD combustion is strong entrainments of high-temperature exhaust gases, which dilute the fuel and air jets.
3. Important environmental parameters for the creation of MILD combustion include a local oxygen content of less than 5–10% and a temperature in the reaction zone that is higher than that of fuel self-ignition. The significant dilution of reactants with flue gas (N_2 and CO_2-rich exhaust gases) is required to achieve these goals.
4. The thermal efficiency of MILD combustion can be increased by 30% while NO_x emissions are reduced by 50% when the regenerator is used to recycle the waste heat of flue gases[21].

Table 2.1: Summary of different combustion modes. [19]

Combustion mode	**Inlet conditions**	**Working conditions**
Mild Combustion (MILD)	$T_{in} > T_{si}$	$\Delta T < T_{si}$
High Temperature Air Combustion (HiTAC)	$T_{in} > T_{si}$	$\Delta T > T_{si}$
Feedback Combustion	$T_{in} < T_{si}$	$\Delta T > T_{si}$

MILD combustion differs from regular combustion mostly due to the low oxygen content (3–13 percent) and a mixture temperature above the autoignition point of the fuel [22]. To absorb the waste heat from the flue gas, the supply air must be heated using a recuperator or regenerator. A recuperator can heat the air to 1000 degrees Fahrenheit, whereas a regenerator can heat the combustion air to around 1600 degrees Fahrenheit [21]. There are four main regimes: a clean MILD combustion region, where MILD can be easily maintained without significant emissions; an unstable flame region, where low-emission MILD conditions can be achieved by appropriately selecting key operating parameters, such as the combustion air temperature; a conventional (normal) flame combustion region, and a no-combustion or extinction zone.

Wünning (1997) [18] distinguishes between stable and unstable flame combustion regimes, as well as a flameless oxidation area. The comparison of MILD and ordinary flames is shown in Figure 2.1. The MILD combustion range for oxygen dilution ratio is about 2.5 and above, and the reactant temperature is higher than the self-ignition temperature, as shown in Figure 2.2.

The colour of the MILD flame is affected by the oxygen concentration and temperature of the preheated air, as shown in Figure 2.3. When the oxygen level drops to 2%, the flame turns green and becomes less visible [23]. Parente (2009, 2011)[24], [25] investigated the essential features for characterization of the MILD combustion regime using a unique methodology based on Principal Component Analysis (PCA). The CH_4/H_2 experimental dataset's low-dimensional representations can be identified using PCA. Based on [OH] contours, Figure 2.4 depicts the flame zone for MILD and conventional combustion. In comparison to the conventional case, the MILD scenario's reacting and non-reacting zones are significantly larger.

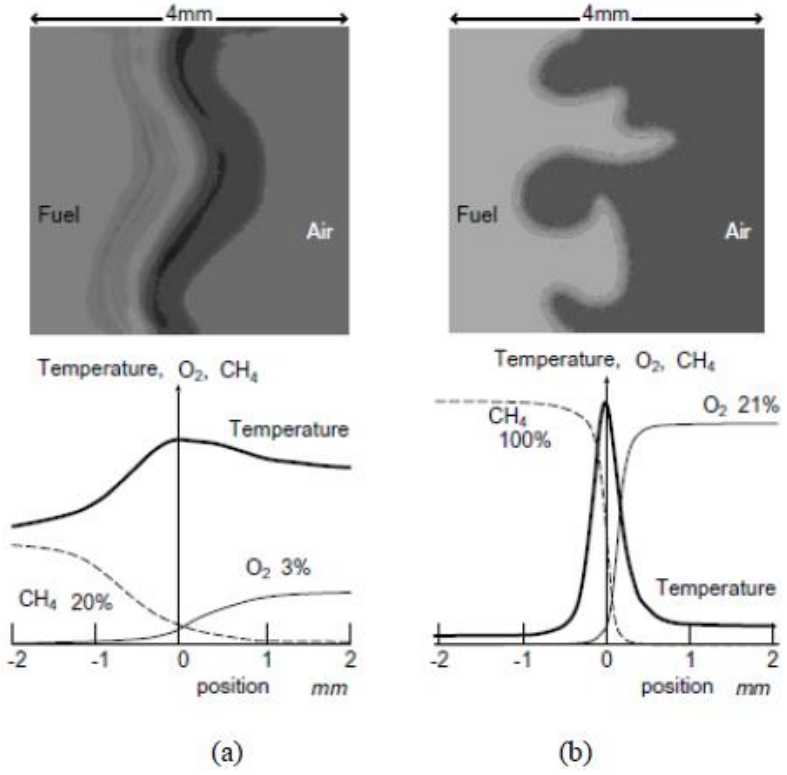

Figure 2.1: Comparison of the temperature and mass fraction (a) MILD combustion (b) Conventional Combustion[21]

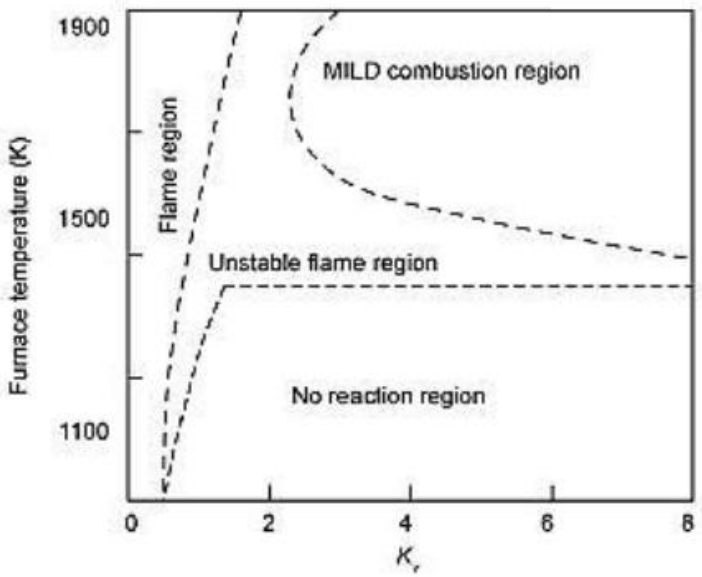

Figure 2.2: The relationship between furnace temperature and dilution ratio [18]

Figure 2.3: Combustion air temperature of 1100 °C and percentage of O_2 concentration [23]

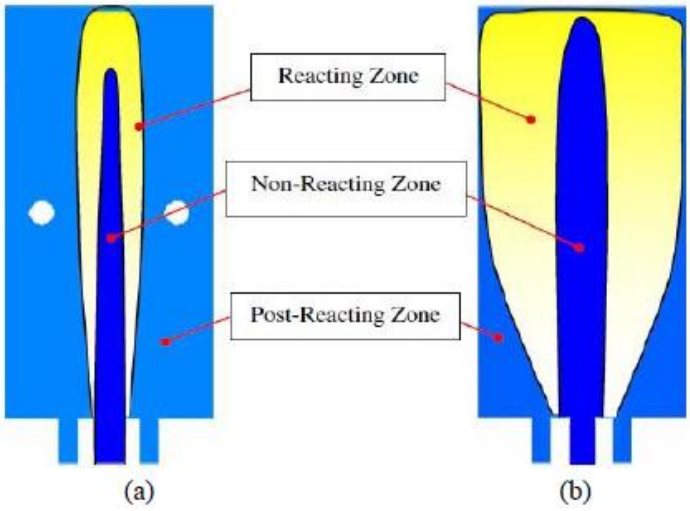

Figure 2.4: Closed furnace reacting zone for (a) conventional and (b) MILD combustion [26]

Low NO_x emissions were attained given the low combustion temperature in recent experiments on low calorific value fuels employed in MILD combustion [27], [28]. The average combustion chamber temperature (T_c), dilution ratio (K_v), and jet velocity are the three most important parameters in MILD combustion [29]. For the MILD combustion working conditions, K_v is an important parameter. Dilution ratio was described by several other researchers [18], [24], [30], [31] as the ratio of recycled exhausts to incoming air and fuel flow rates. MILD combustion has a number of advantages, including high thermal efficiency and minimal NO_x emissions. It has been dubbed one of the new-generation, clean, and efficient combustion technologies because it creates a consistent temperature distribution and great combustion stability. It has the potential to be used in a wide range of industrial applications.

2.2.1 Oxidant Dilution

One of the most important components in achieving the MILD regime is oxygen dilution. Figure 2.2 (from the previous section) depicts the MILD combustion regime with furnace temperature against dilution ratio[18].

It reveals four basic regimes: a clean MILD combustion region, in which MILD can be easily sustained without considerable emissions; an unstable flame region; a conventional (regular) flame combustion region; and a no-combustion or extinction zone. The more common presentations distinguish between stable and unstable flame combustion regimes, as well as a flameless oxidation zone [18], [30]. The MILD combustion range for oxygen dilution is around 3 to 13%, and the reactant temperature is above the self-ignition temperature, as shown in Figure 2.5. To dilute and preheat the oxidant with EGR, Wünning and Winning (1997) calculated the dilution ratio (Kv) as follows:

$$K_v = \frac{M_E}{(M_F + M_A)} = \frac{(M_T - M_F - M_A)}{(M_F + M_A)} \tag{2.1}$$

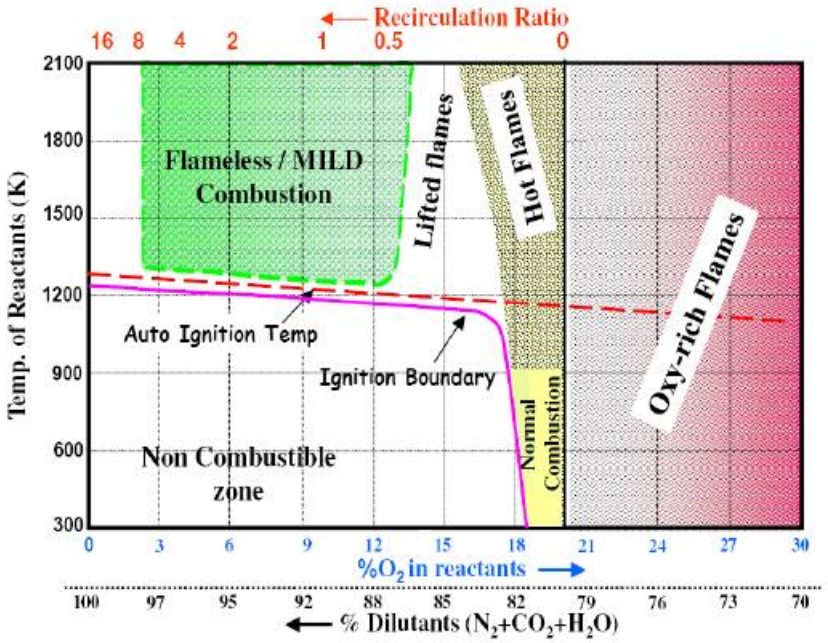

Figure 2.5: Schematic regime diagram for methane-air JHC flames[32]

By adding the exhaust gas recirculation (EGR) mass flow rate, ME, the fuel mass flow rate, MF, and the fresh air mass flow rate, MA, the total mass flow rate, MT, is obtained. When combustion reaches steady state, the dilution ratio and temperature inside the combustion chamber should be measured. For constant-density processes, mass and volume flow rates are equivalent. The dilution ratio must be at least 2.5.

2.2.2 Reactants Preheating

To limit waste and flue gas release to the atmosphere in diffusion or non-premixed combustion, heat from the flue gas can be recirculated by preheating the supply air with exhaust heat from the burned products. According to Lloyd and Weinberg (1975) [33], preheating the combination by heat recirculation can provide stable combustion with a lean combustion mixture and broaden the flammability limits of the combustion.

2.2.2(a) Exhaust Gas Recirculation

MILD combustion requires rapid mixing of exhaust gas recirculation (EGR), fresh air, and fuel in the combustion chamber before the combustion process can commence. The recirculation of hot exhaust gas into the fresh air and fuel stream raises

the temperature of the mixture over the self - ignition temperature, creating multiple simultaneous ignitions. Homogeneous combustion produces very low NO_x emissions due to the avoidance of tiny reaction zones and locally high peak temperatures.

2.3 Gasification Process

Gasification is a thermochemical process that produces producer gas (also known as product gas, syngas, synthetic gas, or synthesis gas) from the interactions between the fuel and the gasification agent. CO, H_2, N_2, CO_2, and certain hydrocarbons (CH_4, C_2H_4, C_2H_6, etc.) make up the majority of the producer gas. H_2S, NH_3, and tars may also be present in trace concentrations [34].

Biomass gasification is the thermochemical conversion of organic (waste) feedstock in a high-temperature environment to create producer gas for energy generation, in addition producing chemicals such as methane, ethylene, adhesives, fatty acids, surfactants, detergents, and plasticizers [35].

According to the gasification agent used, the different gasification processes get their names, if air is utilised it is called air gasification, if oxygen is utilised it is called oxygen gasification, same goes to steam gasification, carbon dioxide gasification, supercritical water gasification and so on. In general, higher HHVs of producer gas are obtained by other gasification process (such as oxygen, water, carbon dioxide and steam) however, because the gasification agent (air) is of low cost and abundant, the reaction process is simple, the reactor construction is simple, and so on, air gasification is the most commonly studied and implemented process.

The total gasification reaction for biomass gasification with steam, carbon dioxide, or supercritical water is often endothermic, requiring external heating throughout the process. The overall gasification of biomass gasification using air or oxygen, on the other hand, might be exothermic or endothermic. Variations in air or oxygen levels can affect or change these reactions. If no external heat is provided, a specific air or oxygen content equates to a specific gasification temperature. External heat should be added, or a greater air or oxygen content is necessary if a higher gasification temperature is required or intended [36]. A gasifier is the location where the gasification reactions take place [34], [37].

2.4 MILD Combustion Modelling

Many researchers have been successful in their modelling of MILD combustion [38]–[41]. CFD modelling for MILD (HiTAC) firstly originated from the Japanese heating industry, in which a few researchers performed simulations for the NO_x formation using an experimental continuous slab reheating furnace [42]–[44]. In this study, MILD combustion will be numerically studied and optimized using biomass producer gas. MILD combustion is a rather emerging topic with several unresolved concerns that require additional research and study [45]. Although MILD combustion technology has begun to be commercialised, it is still not well accepted in the furnace industry. As a result, doing extensive fundamental and practical research to increase combustion performance and efficiency is critical [25], [46], [47]. One of the most intriguing research projects is fuel-air mixing in MILD combustion [48]. This is due to the turbulence caused by air-fuel mixing in the MILD condition. Because turbulent mixing has such a big impact on the flow field and the turbulence-chemistry interaction, precise prediction of turbulent mixing is critical for modelling turbulent combustion [49]. One of the key criteria determining the quality of the air-fuel combination are the reactants' jet velocity and angles [50].

2.4.1 Damköhler Number

The Damköhler number, D_a is a dimensionless number that can be defined as the ratio of the characteristic mixing time to the characteristic chemical time, or in other words, it is the how long the fluid takes to mix divided by how long chemical reaction takes to occur.

The main parameter that controls the combustion regime is the interaction between turbulent mixing and chemical kinetics: only a thorough understanding of this interaction can provide insight into the physics of the flame and aid in the selection and/or creation of modelling tools. The Damköhler number distribution, which depicts the flow to chemical time-scale ratio, can be used to assess the turbulence-chemistry interaction. Large Damköhler readings suggest mixing controlled flames. Low Damköhler values, on the other hand, correspond to slow chemical reactions: turbulence quickly mixes reactants and products, making the system behave like a perfect stirred

reactor. The definition of correct flow and chemical timescales is required for the calculation of the Damköhler number[51].

The chemistry and mixing time scales are comparable in MILD circumstances, hence the Damköhler number is often low and often approaches unity [52]. Galletti looked at turbulence and chemical timescales and found that in MILD combustion, the high-temperature area has Damköhler values that are lower than those seen in flame mode [53]. The Damköhler numbers for MILD combustion are in the range of 0.01-5.35, indicating that this regime is governed by both flow and chemical time scales, according to Li [54]. Zhang [55] has explored the impact of various injection settings on Damköhler number quantitatively. They employed the EDC combustion model and found that lowering the D_a value is critical for achieving the non-premixed MILD combustion regime. Tu [56] researched MILD combustion in different gas atmospheres, using the Damköhler and turbulent Reynolds values to create diagrams to get quantitative insight into the reaction regimes. The majority of earlier studies used simple approaches to estimate chemical time scales. There are, however, more sophisticated techniques to obtaining this amount, as demonstrated by Isaac [51], for example.

2.5 Literature Summary

In a review, Pino Sabia [57] pointed out that large-scale burners and furnaces have employed mild combustion. However, it necessitates appropriate changes to the overall plant architecture as well as a complete revision of the burner geometry. Many innovative concepts have been developed and proved to achieve optimal burning conditions in a wide range of operating situations (in a wide range of working load ranges). However, real experience with MILD biofuel combustion is limited, and further research and development is needed to design geometries and flow configurations capable of assuring satisfactory load flexibility at large scale facilities. The literature on the use of biofuels in the flameless mode, also known as MILD, is extremely scarce. In a study by Abuelnuor [14] and a more recent review by Budzianowski [15], they state that there are relatively few studies in this area. Therefore, the aim is to incorporate the use of biomass PG in MILD combustion while overcoming its main challenges of burning and performing optimization using DOE simulation to achieve optimum results with no experimental approach.

CHAPTER 3
METHODOLOGY

3.1 Overview

In this chapter, fuel selected for the simulation is described, in addition to procedures leading to the optimization of the MILD chamber will be discussed and a detailed flowchart has been drawn to highlight the flow of the procedures and is shown in Figure 3.1, beginning with the procedures to produce CFD simulation results for first and second stages of DOE which includes, for both stages, the SolidWorks 3D modelling followed by the ANSYS FLUENT meshing and setup and later the design of experiments (DOE) is performed to analyse the factors and carry out the response optimizer.

In the current burner layout, air and fuel are injected at high speeds from the bottom to the top, causing reversal flow and hence gas recirculation inside the combustor. Strong exhaust gas recirculation aids in the spontaneous ignition of uniformly distributed reactants as well as the increase of the reactants oxidation rate, lowering CO emissions and avoiding the locally high temperatures that cause high NO_x, lowering NO_x emissions.

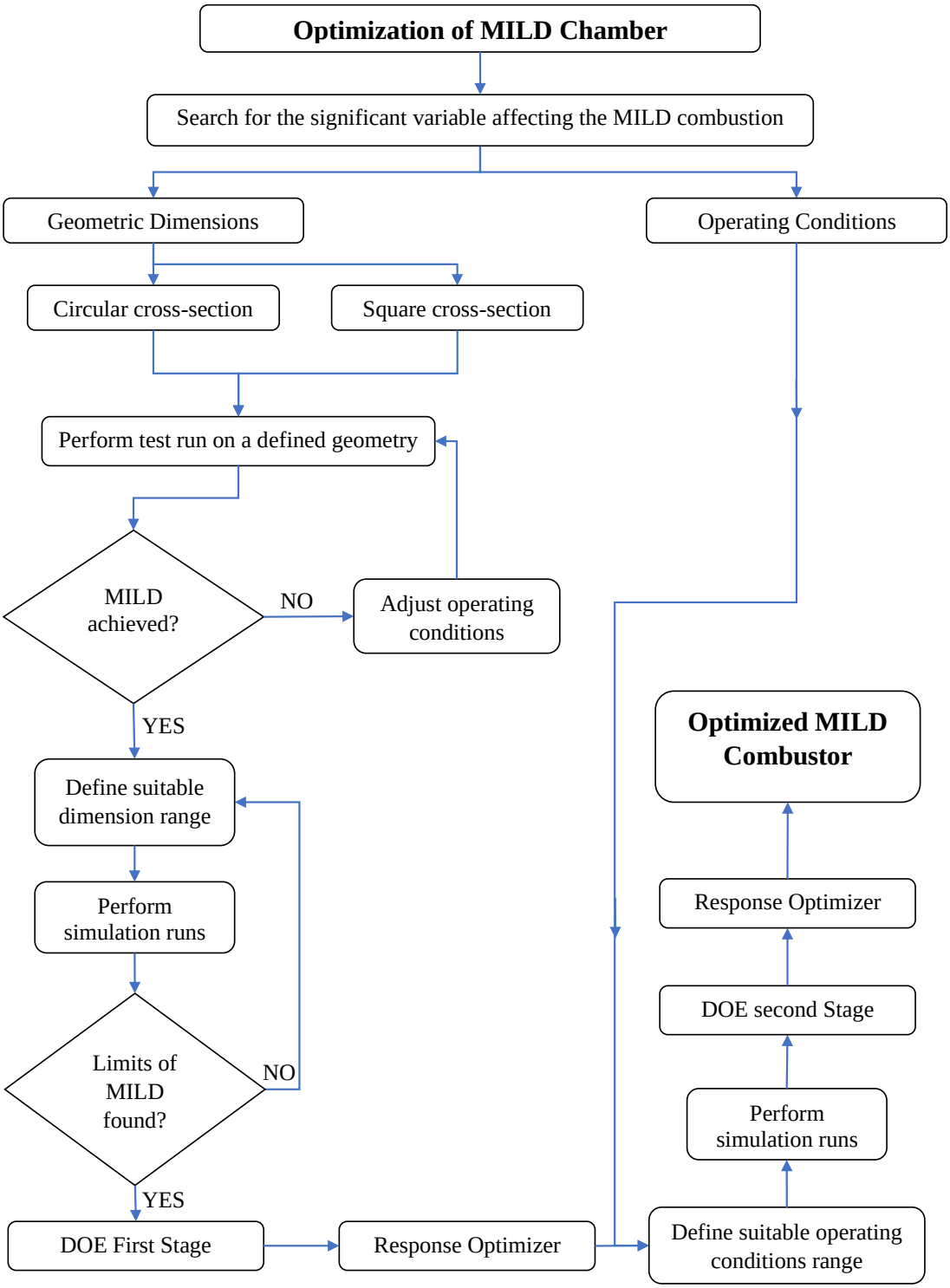

Figure 3.1: Methodology chart of the research study

3.2 Fuel Selection

To produce low-grade diluted PG, standard air-gasification of biomass wood was employed. The lowest value was chosen for the optimization of the PG MILD combustion since the range of PG lower heating value (LHV) is around 4-6MJ/m^3[58]. H_2= 5.0%; CO_2= 2.1%; O_2= 0.9%; N_2= 62.5%; CH_4= 0.3%; CO= 29.2% were derived from experimental results in the literature for the lowest quality (but still combustible) gas with an LHV of 3.99MJ/m^3[59].

3.3 Data Analysis

The key performance indicating parameters used for the characterization of the chamber, including both operating and geometrical variables, are discussed in this section.

3.3.1 Equivalence Ratio

The ratio of the actual fuel–air ratio to the stoichiometric fuel–air ratio is known as the equivalence ratio. Fuel air equivalence ratio (φ) is important in operating any combustor. By adjusting fuel air equivalence ratio of combustor, the outcomes of the combustion can be changed. When φ more than 1, combustion runs rich, which means excess fuels exist in the combustor. When φ less than 1, combustion runs lean, which means excess air exist in the combustor. When φ equals to 1, stoichiometric combustion occurs, which means the fuels are burnt completely without excess air. The formula of fuel air equivalence ratio (φ) is shown in Eq. (3.1):

$$\varphi = \frac{Actual\ Fuel/Air}{Stoichiometric\ Fuel/Air} \tag{3.1}$$

3.3.2 Damköhler Number

Discussed previously in section 2.4.1, Damköhler number is a dimensionless number that can be defined as the ratio of the characteristic mixing time to the characteristic chemical time. The Damköhler numbers for MILD combustion are in the range of 0.01-5.35, indicating that this regime is governed by both flow and chemical time scales, according to Li [54].

3.3.3 Residence Time

One of the most critical parameters that can affect combustion performance is residence time. To achieve complete combustion, fuel molecules must have enough time to break down and interact with oxidizer molecules in order to complete the reaction.

According to a study conducted by Chanphavong [60], mean residence time (t_m) can be calculated as Eq. (3.2):

$$t_m = \frac{\rho V}{m} \tag{3.2}$$

Therefore, by taking the average density of the gas (ρ) across the chamber, total volume of the chamber (V) and the total mass flow (m), the average residence time for the gas when crossing the chamber length can be calculated. With a fixed flow rate (m), the dominant factor that can affect the residence time is the total volume of the chamber that can be represented in the diameter/length and length/height of the chamber.

3.4 Design and Optimization of MILD Combustor Geometry

First part includes the design and optimization of MILD combustor geometry to determine the optimum geometric dimensions with MILD combustion achievement and low CO and NO_x emissions. Most combustors either take on a circular or a square cross-section and these were adopted in this research.

3.4.1 Chamber Geometry

Although ANSYS software contains a built-in design modeller, using SolidWorks software to design the chambers is more convenient since it allows for easy changes to satisfy the different runs. Furthermore, the SOLIDWORKS file can be exported in a highly portable file format called Parasolid and is imported directly into the ANSYS DesignModeler where the geometry is quickly generated using DesignModeler function. The 3D model in SOLIDWORKS is a solid model and not a

hollow model, where the fluid occupies, later in ANSYS it is calculated as the fluid domain.

Figure 3.2 and Figure 3.3 shows the 3D geometry of circular and square cross-section combustors, respectively which were drawn by using SOLIDWORKS 2021 software. The fuel-air inlets follow the fuel-oxidant-fuel (FOF) configuration (2 fuel inlets and 1 air inlet) as illustrated in Figure 3.6 that Cheong [41] employed in his research, although it was pointed out that the oxidant-fuel-oxidant (OFO) configuration promoted better occurrence of MILD combustion, for the present research the thermal input of the combustor, P_{in} = 50 kW and therefore would have a high fuel rate which requires more inlets. For the before mentioned reason the FOF was adopted. Air and fuel are injected at high speeds from the bottom to the top, causing reversal flow and hence flue gas recirculation inside the combustor. The air, fuel and exhaust ports sizes are the same in circular and square cross section combustors. The diameter of the air inlet, D_{air} = 9 mm, the diameter of fuel inlets, D_f = 5.5 mm and the diameter of the outlet D_o = 80 mm.

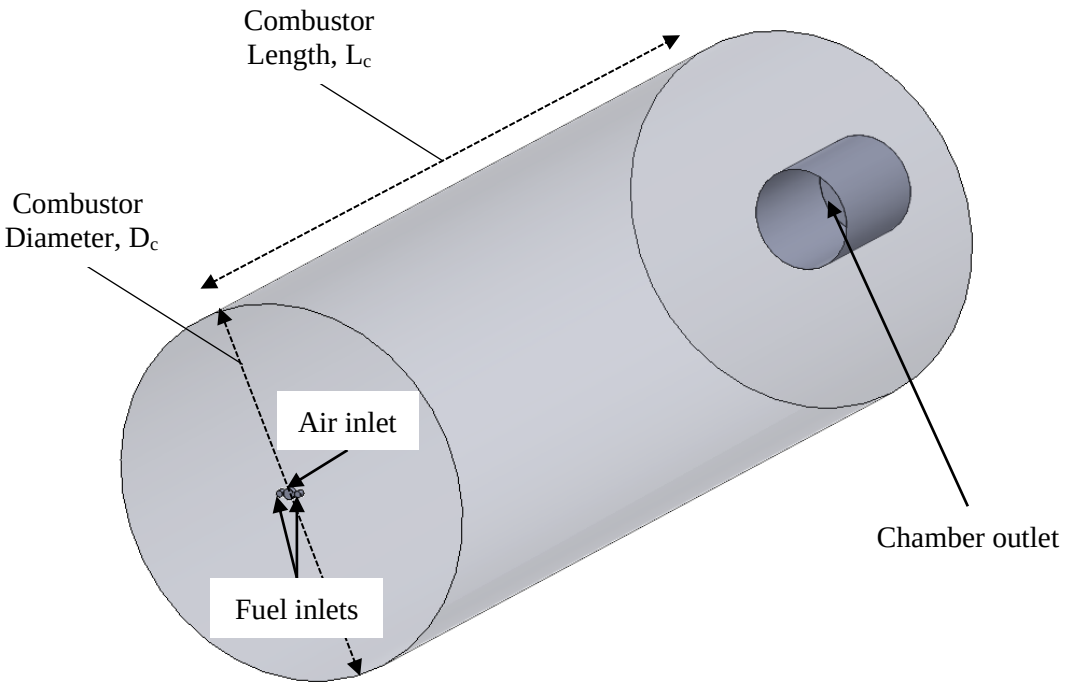

Figure 3.2: Geometry of circular cross-section combustor

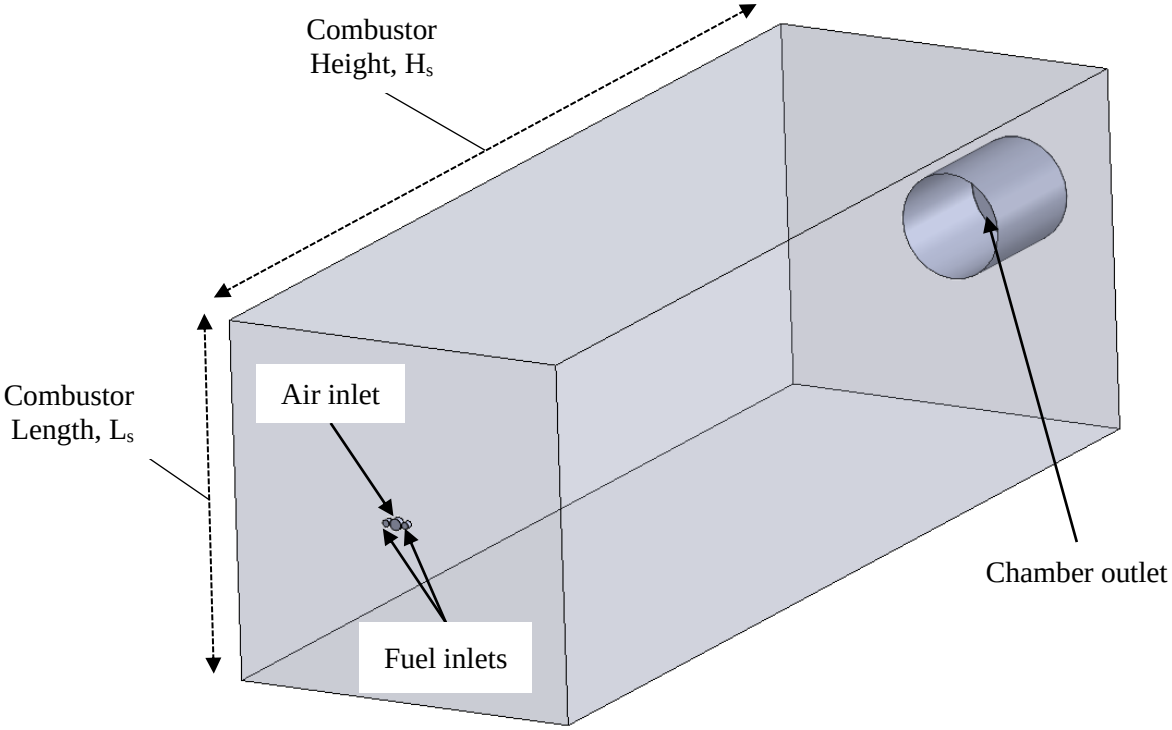

Figure 3.3: Geometry of square cross-section combustor

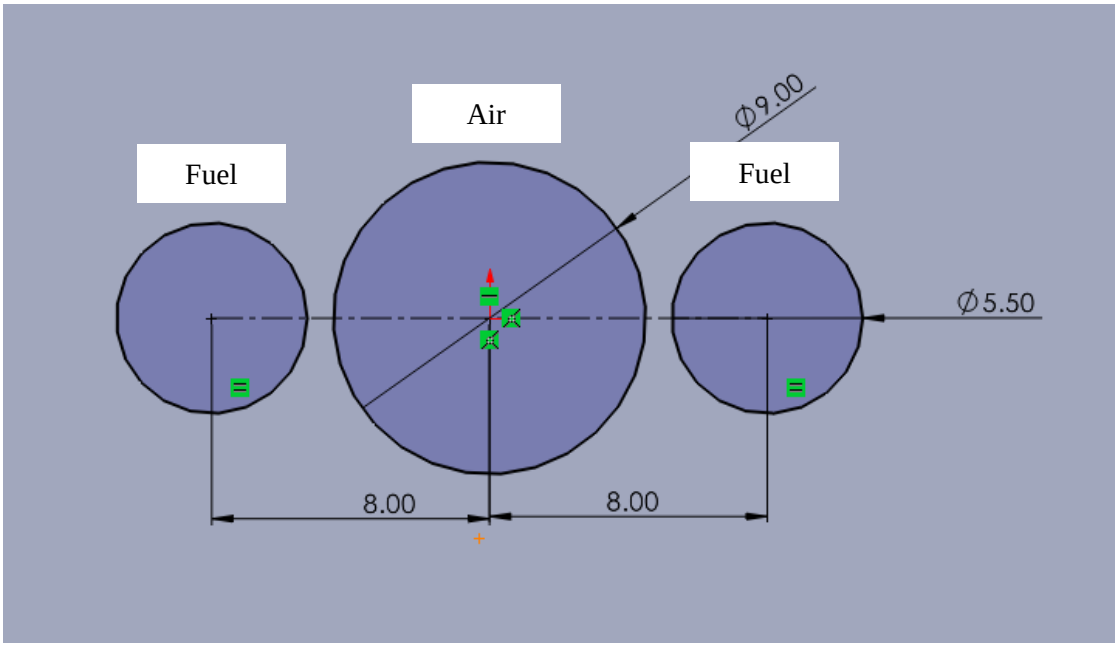

Figure 3.4: Fuel-Oxidant-Fuel (FOF) configuration (circular and square)

3.4.2 Meshing Setup

Model meshing is the most important step in the CFD process. The meshing process will determine the meshing quality. The grid of cells or elements created by meshing will allow all desired fluid flow equations to be solved. The computational time, which directly affects the cost of the simulations, will be significantly impacted by the size of the grid. The grid will also have a considerable impact on the rate of convergence and the precision of the solutions.

Skewness and aspect ratio on the mesh metric are the necessary qualities to be examined. The solution will easily generate a divergence error and won't converge as anticipated if the maximum skewness is above 0.98. The aspect ratio is calculated by dividing the longest edge length to shortest edge. The ideal aspect ratio is 1.0, which indicates that any shape's edge lengths are equal. From mesh independence test in section 4.2, the mesh size that gives approximately ~ 413040 elements was used for all simulations. Sample meshing and statistics are shown in Figure 3.5 and Figure 3.6, and Table 3.1 and Table 3.2, respectively.

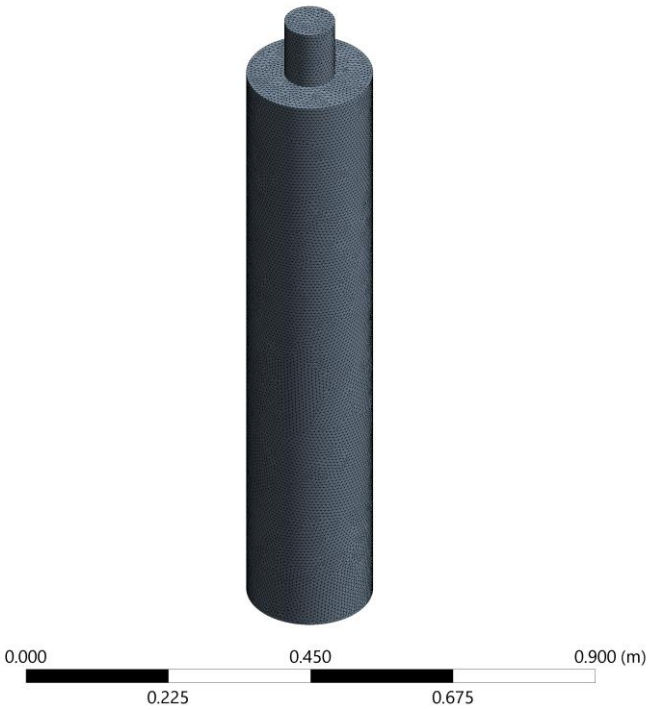

Figure 3.5: 3D view of model after meshing (circular combustor)

Table 3.1: Statistic on nodes, elements and mesh metric for skewness and aspect ratio for a circular combustor

Item	Setting
Nodes	80292
Elements	417229
Mesh Metric	Skewness
Min	1.1384e-7
Max	0.84402
Average	0.22243
Standard Deviation	0.11555
Mesh Metric	Aspect Ratio
Min	1.1577
Max	9.7779
Average	1.8356
Standard Deviation	0.44425

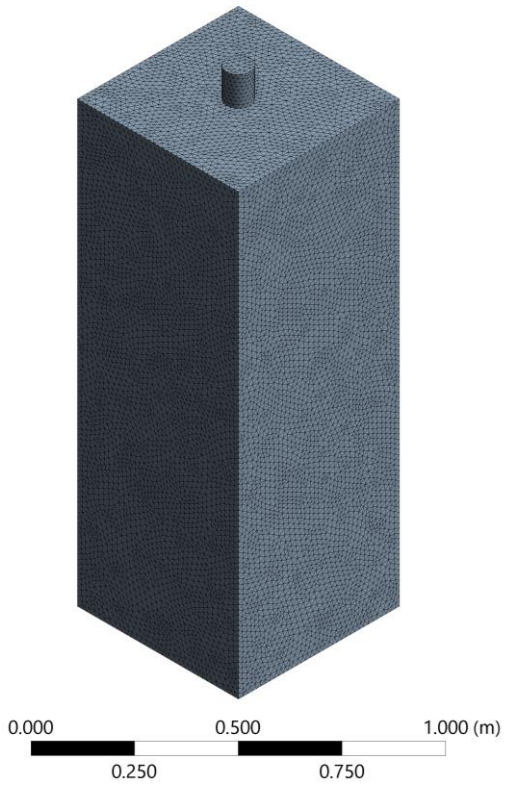

Figure 3.6: 3D view of model after meshing (square combustor)

Table 3.2: Statistic on nodes, elements and mesh metric for skewness and aspect ratio for a square combustor

Item	Setting
Nodes	78593
Elements	414252
Mesh Metric	Skewness
Min	1.0892e-4
Max	0.84027
Average	0.22447
Standard Deviation	0.11743
Mesh Metric	Aspect Ratio
Min	1.1617
Max	40.88
Average	1.8392
Standard Deviation	0.45729

3.4.3 Turbulence Model

Standard k-ε model was used in current study to simulate the turbulent flow conditions inside the combustor as it can well predict the turbulent flow behaviour in combustion and heat transfer simulations. Standard k- ε model worked based on model transport equations for the turbulence kinetic energy (k) and its dissipation rate (ε) [61]. Few assumptions were made in standard k- ε model, such as the flow is fully turbulent, and the effects of molecular viscosity are negligible. Turbulence kinetic energy (k) and its dissipation rate (ε) can be obtained from the following transport Equations (3.3) & (3.4):

$$\frac{\partial}{\partial \mathrm{t}}(\rho k)+\frac{\partial}{\partial x_i}(\rho k u_i)=\frac{\partial}{\partial x_j}\left[\left(u+\frac{u_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right]+G_k+G_b-\rho\varepsilon-Y_M+S_k \qquad (3.3)$$

$$\frac{\partial}{\partial \mathrm{t}}(\rho\varepsilon)+\frac{\partial}{\partial x_i}(\rho\varepsilon u_i)$$

$$=\frac{\partial}{\partial x_j}\left[\left(u+\frac{u_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right]+C_{1\varepsilon}\frac{\varepsilon}{k}(G_k+C_{3\varepsilon}G_b)-C_{2\varepsilon}\rho\frac{\varepsilon^2}{k}+S_\varepsilon \qquad (3.4)$$

Where G_k is the kinetic energy of turbulence produced as a result of mean velocity gradients, and G_b is the kinetic energy of turbulence produced as a result of buoyancy. Y_M is the portion of the overall dissipation rate that the fluctuating dilatation in compressible turbulence makes up; Constants $C_{1\varepsilon}$, $C_{2\varepsilon}$, $C_{3\varepsilon}$ exist; ρk, $\rho\varepsilon$ are the turbulent Prandtl numbers for k, ε; and S_k, S_ε are user-defined source terms.

3.4.4 Combustion Model

In this study, the partially premixed combustion model was used since this model has shown good results with producer gas combustion[62], [63] and is also the model adopted in the validation process as shown upcoming in section 4.2.

3.4.4(a) Probability Density Function Approach

In ANSYS FLUENT, the partially premixed model is a simple combination of the non-premixed and premixed models. The position of the flame front is determined by the premixed reaction progress variable, c. The mixture is burned behind the flame front (c = 1), and the equilibrium or laminar flamelet mixture fraction solution is utilised. The species mass fractions, temperature, and density are determined from the mixed but unburnt mixture fraction ahead of the flame front (c = 0). A linear combination of the unburned and burnt materials is employed within the flame (0 < c < 1).

For the combustion modelling in Fluent, the partially combustion model was used, essentially air and fuel streams were separated therefore it can be regarded as non-premixed combustion model, however the partially premixed model was used since it is able to compute the turbulence-chemistry interaction of PG combustion more accurately. The model included probability density function (PDF) that allowed the user to predefine the fuel and oxidizer species. Thus, the composition of PG and air were defined before running the simulation. In partially premixed modelling, solution of transport equations for mixture fractions was included and is calculated using Eq.(3.5).

If the chemistry is rapid enough in turbulent combustion flames, the fluid's instantaneous thermochemical state can be characterised as a function of a conserved scalar quantity known as mixture fraction [64], [65]. The mixture fraction in a fuel/oxidizer binary system can be calculated as follows:

$$f = \frac{Z_i - Z_{i,ox}}{Z_{i.fuel} - Z_{i,ox}} \tag{3.5}$$

Where, Z_i is the elemental mass fraction for element (i); $Z_{i,ox}$ is the value at the oxidizer stream inlet; and $Z_i,fuel$ is the value at the fuel stream inlet. For the fuel species (in comparison to the other species in PDF) the Mean mixture fraction (MMF) is calculated as a special case of the mixture fraction. MMF value starts at 1 for 100% concentration of the fuel with no dilutants or oxidizer, and the value drop below 1 (MMF<1) with the presence of dilutants down to zero at the air inlet boundary

condition. Therefore, MMF is a useful tool to indicate the quality of air-fuel mixing process by tracing the reduction in MMF values at the different zones.

3.4.5 Boundary Conditions

Boundary conditions were needed to predefine the simulation constraints and operating parameters. In order to test on how the geometry changes affect the combustion, the boundary conditions were predetermined, as shown in Table 3.3, based on a test run which achieves MILD combustion and kept constant throughout all the simulations for both the circular and square cross section combustors. The mass flowrate of fuel needed to achieve the thermal input of 50 kW can be calculated from the volume flow rate obtained from the following equation:

$$P_{in} = (\dot{V})(lhv) \tag{3.6}$$

Where P_{in} is the thermal power input, $\dot{V}$ is the volume flowrate of the fuel and lhv is the low heating value of the fuel.

Table 3.3: Boundary conditions of the circular and square cross-section combustors

Air inlet	Velocity = 265.5 m/s, mass flow rate = 0.012602272 kg/s
	Initial gauge pressure = 0 atm
	Temperature = 473K
	Mean mixture fraction = 0
Fuel inlets	Velocity = 263.7 m/s, mass flow rate = 0.00610202 kg/s
	Initial gauge pressure = 0 atm
	Temperature = 673K
	Mean mixture fraction = 1
Pressure outlet	Back flow temperature = 1000K