

**APPLICATION OF FLUENT TO PREDICT COMBUSTION PERFORMANCE  
FOR PURE PROPANE**

**MUHAMMAD AMINUDDIN BIN ABD RAHMAN**

**UNIVERSITI MALAYSIA PAHANG**

# UNIVERSITI MALAYSIA PAHANG

## BORANG PENGESAHAN STATUS TESIS

JUDUL : APPLICATION OF FLUENT TO PREDICT COMBUSTION PERFORMANCE FOR PURE PROPANE

SESI PENGAJIAN: 2008/2009

Saya MUHAMMAD AMINUDDIN BIN ABD RAHMAN  
(HURUF BESAR)

mengaku membenarkan tesis PSM ini disimpan di Perpustakaan Universiti Malaysia Pahang dengan syarat-syarat kegunaan seperti berikut:

1. Tesis adalah hakmilik Universiti Malaysia Pahang.
2. Perpustakaan Universiti Malaysia Pahang dibenarkan membuat salinan untuk tujuan pengajian sahaja.
3. Perpustakaan dibenarkan membuat salinan tesis ini sebagai bahan pertukaran antara institusi pengajian tinggi.
4. \*\*Sila tandakan (✓)

SULIT

(Mengandungi maklumat yang berdarjah keselamatan atau kepentingan Malaysia seperti yang termaktub di dalam AKTA RAHSIA RASMI 1972)

TERHAD

(Mengandungi maklumat TERHAD yang telah ditentukan oleh organisasi/badan di mana penyelidikan dijalankan)

TIDAK TERHAD

Disahkan oleh

\_\_\_\_\_  
(TANDATANGAN PENULIS)

Alamat Tetap: **No 516, Kpg Jelai,  
34520 Batu Kurau,  
Perak.**

Tarikh: Dicember 2008

\_\_\_\_\_  
(TANDATANGAN PENYELIA)

**PENYELIA**  
Mr Arman Bin Abdullah

Tarikh: Dicember 2008

CATATAN:

\* Potong yang tidak berkenaan.

\*\* Jika tesis ini SULIT atau TERHAD, sila lampirkan surat daripada pihak berkuasa/organisasi berkenaan dengan menyatakan sekali sebab dan tempoh tesis ini perlu dikelaskan sebagai SULIT atau TERHAD.

◆ Tesis dimaksudkan sebagai tesis bagi Ijazah Doktor Falsafah dan Sarjana secara penyelidikan, atau disertai bagi pengajian secara kerja kursus dan penyelidikan, atau Laporan Projek Sarjana Muda (PSM).

“I hereby declare that I have read this thesis and in my opinion this thesis is sufficient in terms of scope and quality for the award of the degree of Bachelor of Chemical Engineering”

Signature : .....

Supervisor : Mr Arman Bin Abdullah

Date : .....

APPLICATION OF FLUENT TO PREDICT COMBUSTION PERFORMANCE FOR  
PURE PROPANE

MUHAMMAD AMINUDDIN BIN ABD RAHMAN

A thesis submitted in fulfillment  
of the requirements for the award of the degree of  
Bachelor of Chemical Engineering  
(Gas Technology)

Faculty of Chemical & Natural Resources Engineering  
Universiti Malaysia Pahang

DICEMBER 2008

## DECLARATION

I declare that this thesis entitled “APPLICATION OF FLUENT TO PREDICT COMBUSTION PERFORMANCE FOR PURE PROPANE” is the result of my own research except as cited in references. The thesis has not been accepted for any degree and is not concurrently submitted in candidature of any other degree.”

Signature : .....

Name of Candidate : Muhammad Aminuddin Bin Abd Rahman

Date : Dicember 2008

## **DEDICATION**

*Special Dedication to my beloved parents, siblings and my beloved friend for their love and encouragement.*

*And,*

*Special Thanks to supervisor (Mr Arman), my fellow course mate and all faculty members.*

*For all your Care, Support and Best Wishes.*

*Sincerely,*

*Muhammad Aminuddin Bin Abd Rahman*

## ACKNOWLEDGEMENTS

First and foremost, I would like to express my sincere appreciation to my supervisor, Mr Arman Abdullah, for constantly guiding and encouraging me throughout this study. Thanks a lot for giving me a professional training, advice and suggestion to bring this project to its final form.

I am very thankful to the all staff of Chemical & Natural Resources Engineering Faculty, Universiti Malaysia Pahang for their cheerfulness and professionalism in handling their work. In preparing this project, I was in contact with many people, researches, academicians and practitioners. They have contributed towards my understanding and thoughts.

In particular, my sincere thankful is also extends to all my colleagues and others who have provided assistance at various occasions. Their views and tips are useful indeed. Unfortunately, it is not possible to list all of them in this limited space. Last, but not least a special thanks to my parents and other family members for their continuous support while completing this project.

## ABSTRACT

Computational Fluid Dynamic (CFD) is a used tool in optimizing propane burner for emissions issues and to study combustions characteristics of flame temperature and flame velocity in furnace system. Using CFD simulation, cost and time can reduce in development new furnace and burner. Studies are aimed at improving combustion performance with reduce pollutant emissions. Also focus on the combustion patterns in the form of measured contours of temperature and species concentrations. Pure propane used as a fuel in this research. Before doing computer simulation, several experiments were running first. Only the best data will choose. This data is use in boundary setting when doing simulation process. In experimental work, practical combustor C492 gas burner is used. The data from the experimental work will analyze and compare to get a constant and stable data. For simulation work 2D design for practical combustor was done in Gambit software. In this software, the design was mesh and export to Fluent 6.3. Fluent 6.3 is one of CFD software that uses to study combustion and flow characteristics. The result from experimental work and computer simulation then compared. The comparison shows in the Table 4.2 in term of percentage differences. Best result depends on small percentage between this two data.

## ABSTRAK

Pengaturcaraan Computational Fluid Dynamic (CFD) digunakan untuk mendapatkan kesan pencemaran dan ciri-ciri pembakaran seperti suhu dan halaju api di dalam sistem pembakar gas propana. Penggunaan CFD juga dapat menjimatkan masa dan kos di dalam pembinaan pembakar (furnace) baru. Ujikaji ini difokuskan kepada peningkatan prestasi pembakaran disamping mengurangkan pencemaran. Ia juga bagi mendapatkan bentuk gambar perubahan suhu dan kepekatan spesis hasil daripada pembakaran. Gas propana (tulen) digunakan sebagai bahan bakar. Sebelum simulasi menggunakan komputer dilakukan, beberapa ujikaji makmal dilakukan menggunakan pembakar dari model C492 yang sedia ada. Data daripada beberapa ujikaji dianalisa dan dibuat perbandingan bagi mendapatkan data yang malar dan stabil. Untuk kerja-kerja simulasi pembakar dari jenis jenis C942 akan dilukis secara 2 dimensi di dalam perisian Gambit. Kemudian hasil lukisan itu akan dimasukkan ke dalam perisian Fluent 6.3. untuk mendapatkan hasil simulasi, data yang dikumpulkan daripada ujikaji makmal akan dibandingkan dengan data yang dikumpul hasil proses simulasi. Perbezaan data dapat dilihat di dalam Jadual 4.2 dalam bentuk peratusan. Peratusan yang kecil adalah hasil yang terbaik.

**TABLE OF CONTENTS**

<b>CHAPTER</b>	<b>TITLE</b>	<b>PAGE</b>
	<b>COVER PAGE</b>	i
	<b>DECLARATION</b>	v
	<b>DEDICATION</b>	vi
	<b>ACKNOWLEDGEMENT</b>	vii
	<b>ABSTRACT</b>	viii
	<b>ABSTRAK</b>	ix
	<b>TABLE OF CONTENTS</b>	x
	<b>LIST OF FIGURES</b>	xiii
	<b>LIST OF TABLES</b>	xv
	<b>LIST OF SYMBOLS</b>	xvi
	<b>LIST OF APPENDIX</b>	xviii
<b>1</b>	<b>INTRODUCTION</b>	
	1.1 Introduction	1
	1.2 Background of Study	3
	1.3 Problem Statement	4
	1.4 Objective	4
	1.5 Scope of Research Work	5
	1.6 Thesis Organization	5
<b>2</b>	<b>LITERATURE REVIEW</b>	
	2.1 Introduction	6
	2.2 Combustion	7

2.3	Combustion Efficiency	8
2.4	Combustion Process	9
2.5	Pure Propane as Fuel for Combustion	10
2.6	Reynolds Number, $Re$	12
2.7	Navier- Stokes Equations	13
2.8	Turbulence Model	13
2.8.1	Irregularity	14
2.8.2	Diffusivity	14
2.8.3	Large Reynolds Numbers	14
2.8.4	Dissipation	15
2.9	Eddy Dissipation	15
2.10	Boyle's Law	15
2.11	Charles's Law	16
2.12	Ideal Gas Law	17
2.13	Turbulence Intensity	19
2.14	Hydraulic Diameter	20
2.14.1	Hydraulic Diameter for Different Duct Geometries	20
2.14.1.1	Circular Pipe	21
2.14.1.2	Rectangular Tube	21
2.14.1.3	Coaxial Circular Tube	21
2.15	Problem Investigation of the Combustion Process	22
2.15.1	Experimental Study	22
2.15.2	Numerical Study	24
2.15.3	Comparison Predicted and Numerical Data	25
2.15.3.1	Energy Balance	26
2.15.3.2	Furnace Wall Temperature	27
2.15.3.3	Gas Species	28

3	<b>METHODOLOGY</b>	
3.1	Introduction	33
3.2	Overall of Research Methodology	34
3.3	Experimental Work	35
3.3.1	Combustion Laboratory Unit C492	35
3.3.2	Gas Burner	36
3.3.3	Flue Gas Analyzer	38
3.4	CFD Modeling and Simulation	39
3.4.1	Problem Solving Step	40
4	<b>RESULT AND DISCUSSION</b>	
4.1	Introduction	42
4.2	Experimental Results	43
4.3	Simulation Results	44
4.4	Comparison Data	52
5	<b>CONCLUSION AND RECOMMENDATION</b>	
5.1	Introduction	53
5.2	Conclusions	54
5.2.1	CFD Modeling	54
5.3	Recommendation for Future Research	54
	<b>REFERENCES</b>	56
	<b>APPENDICES</b>	
A1:	Safety Data Sheet for Propane	58
B1:	Experimental Data	70

## LIST OF FIGURES

FIGURE NO.	TITLE	PAGE
2.1	Configuration of the HiTAC test furnace: (a) furnace geometry, (b) arrangement of air and fuel inlets and flue gas outlets .	23
2.2	Wall temperature distribution along the side wall of the furnace at $x = 0.8$ m, and $y = -0.3$ m.	28
2.3	Predicted and measured O <sub>2</sub> profiles in the furnace: (a) $x = 0$ , $z = 0.3$ m, (b) $x = 0$ , $z = 0.6$ m, (c) $x = 0$ , $z = 1.2$ m.	30
2.4	Predicted and measured CO profiles in the furnace: (a) $x = 0$ , $z = 0.3$ m, (b) $x = 0$ , $z = 0.6$ m, (c) $x = 0$ , $z = 1.2$ m, (d) $x = 0$ , $z = 2.15$ m.	32
3.1	Flowchart of research methodology	34
3.2	Combustion laboratory unit C492	35
3.3	C492 Gas Burner	36
3.4	Nozzle and air outlet	37
3.5	Fuel and air adjustment	37
3.6	System of flue gas analyzer	38
3.7	Program structure for Gambit	39
3.8	Meshing boundary in Gambit	40
3.9	Step of CFD analysis .	41
4.1	Temperature contours at constant Cp, K	44
4.2	Temperature contours at variable Cp, K	45

4.3	Contours of specific heat, J/kg.K	46
4.4	Velocity vector (m/s) at variable Cp	47
4.5	Stream function contours (kg/s) at variable Cp	48
4.6	C <sub>3</sub> H <sub>8</sub> mass fraction	49
4.7	CO <sub>2</sub> mass fraction test mixtures.	50
4.8	H <sub>2</sub> O mass fraction	51

**LIST OF TABLES**

<b>TABLE NO.</b>	<b>TITLE</b>	<b>PAGE</b>
2.1	Properties of propane	11
2.2	The value of the ideal gas constant, $R$ ,	18
2.3	Fuel characteristic and operation condition	24
2.4	Energy balance from measurements and from modeling data (reference temperature: 298 K)	27
4.1	Average data collected from experimental work	43
4.2	Comparison data between experimental work and simulation process	52

## LIST OF SYMBOLS

$n_c$	-	Combustion efficiency
$\mathbf{v}$	-	Mean fluid velocity
$D$	-	Characteristic diameter
$\mu$	-	Dynamic fluid viscosity
$\nu$	-	Kinematic fluid viscosity
$\rho$	-	Density
$\lambda$	-	Second viscosity coefficient
$\delta_{ij}$	-	Kronecker delta
$\Sigma \nabla \cdot \mathbf{u}$	-	Divergence
$\Sigma \mu_B$	-	Black viscosity
$P$	-	Pressure of the system
$V$	-	Volume of the gas
$K$	-	Constant value representative pressure and volume
$T$	-	Temperature
$\alpha$	-	Cubic expansivity
$n$	-	Number of mole
$R$	-	Universal gas constant
$u'$	-	Root mean square of turbulent velocity fluctuation
$U$	-	Mean velocity
$Re_{d_h}$	-	Reynolds number based on the pipe hydraulic diameter
$d_h$	-	Hydraulic diameter

$a$	-	Width
$b$	-	Height
$d_i$	-	Inner diameter
$d_o$	-	Outer diameter
CFD	-	Computational Fluid Dynamic
2D	-	Two dimension

**LIST OF APPENDICES**

<b>APPENDIX</b>	<b>TITLE</b>	<b>PAGE</b>
A1	Safety data sheet for propane	58
B1	Experimental data	70

## CHAPTER 1

### INTRODUCTION

#### 1.1 Introduction

A furnace is a device that produces heat. Not only are furnaces used in the home for warmth, they are used in industry for a variety of purposes such as making steel and heat treating of materials to change their molecular structure.

Central heating with a furnace is an idea that is centuries old. One of the earliest forms of this idea was invented by the Romans and called a hypocaust. It was a form of under-floor heating using a fire in one corner of a basement with the exhaust vented through flues in the walls to chimneys. This form of heating could only be used in stone or brick homes. It was also very dangerous because of the possibility of fire and suffocation.

Furnaces generate heat by burning fuel, but early furnaces burned wood. In the seventeenth century, coal began to replace wood as a primary fuel. Coal was used until the early 1940s when gas became the primary fuel. In the 1970s, electric furnaces started to replace gas furnaces because of the energy crisis. Today, the gas furnace is still the most popular form of home heating equipment.

Wood and coal burning furnaces required constant feeding to maintain warmth in the home. From early morning to late at night, usually three to five times a day, fuel

needed to be put in the furnace. In addition, the waste from the ashes from the burnt wood or coal must be removed and disposed.

Today's modern furnace uses stainless steel, aluminized steel, aluminum, brass, copper, and fiberglass. Stainless steel is used in the heat exchangers for corrosion resistance. Aluminized steel is used to construct the frame, blowers, and burners. Brass is used for valves, and copper in the electrical wiring. Fiberglass is used to insulate the cabinet.

## 1.2 Background of Study

An industrial furnace or direct fired heater, is an equipment used to provide heat for a process or can serve as reactor which provides heats of reaction. Furnace designs vary as to its function, heating duty, type of fuel and method of introducing combustion air. However, most process furnaces have some common features.

Fuel flows into the burner and is burnt with air provided from an air blower. There can be more than one burner in a particular furnace which can be arranged in cells which heat a particular set of tubes. Burners can also be floor mounted, wall mounted or roof mounted depending on design. The flames heat up the tubes, which in turn heat the fluid inside in the first part of the furnace known as the radiant section or firebox. In this chamber where combustion takes place, the heat is transferred mainly by radiation to tubes around the fire in the chamber. The heating fluid passes through the tubes and is thus heated to the desired temperature. The gases from the combustion are known as flue gas. After the flue gas leaves the firebox, most furnace designs include a convection section where more heat is recovered before venting to the atmosphere through the flue gas stack. HTF=Heat Transfer Fluid. Industries commonly use their furnaces to heat a secondary fluid with special additives like anti-rust and high heat transfer efficiency. This heated fluid is then circulated round the whole plant to heat exchangers to be used wherever heat is needed instead of directly heating the product line as the product or material may be volatile or prone to cracking at the furnace temperature. [1]

A computer code for simulating combustion gas flow is a powerful tool in the initial stage of combustor design. Currently there are various commercial computational fluid dynamics (CFD) codes in the market. One of the CFD's software is FLUENT 6.3. FLUENT 6.3 is a computational fluid dynamics (CFD) software package to simulate combustion process. Using FLUENT 6.3 a study for flame temperature, flue gases, velocity vector and concentration of the combustion products can be developed.

The simulation process for this research will continued with experimental study. The experimental work will use a standard C492 gas burner. The gas burner is a device to burn fuels under control to produce useful heat. Function of the burner are to deliver fuel and air to a combustion chamber, mix fuel and air, and provide continuous and stable ignition of air/fuel mixture. For this project pure propane used as a fuel for combustion. Result from experimental work and CFD simulation will compare, and then analyze.

### **1.3 Problem Statement**

Computational fluid dynamics (CFD) has proven being a valuable tool in optimizing combustion equipments and gas burners. Using CFD simulation, is easy to get accurate data measurement. It is also reduces the times and cost of development new burner. The main reason for doing the simulation is the measurement of the detailed distributions of velocity, temperature and gas composition are very difficult for practical combustor. In this study, therefore, the numerical simulation for the prediction of local combustion properties of pure propane by the standard C492 gas burner in the experimental combustor is described. The accuracy of the simulation is discussed by comparing of the calculated and measured results.

### **1.4 Objective of the Project**

The objective of the project is to develop a CFD simulation to predict combustion performance for pure propane in term of emissions, flame temperature, velocity vectors and concentration of the combustion products, and validate with experimental data.

## **1.5 Scope of Research Work**

The scopes of research are:

1. To mesh the 2D drawing of C492 gas burner in Gambit.
2. To develop the CFD simulation using FLUENT 6.3 software.
3. To compare the expected result from simulation with experimental work.

## **1.6 Thesis Organization**

This thesis consists of five chapters summarized as follows:

Chapter 2 comprises a literature survey on the subject of combustion performance using CFD simulation. This chapter briefly discuss about the natural gas combustion and CFD simulation.

Chapter 3 concentrates on the methodology of this research, flowchart, experimental setup instrumentation and measurement.

Chapter 4 provides the result from experimental work and simulation process.

Chapter 5 summaries the results and provides conclusions and recommendation for future work.

## **CHAPTER 2**

### **LITERATURE RIVIEW**

#### **2.1 Introduction**

The purpose of this chapter is to provide a review of past research effort related to furnace, gas burner, combustion, computational fluid dynamics (CFD) analysis, two dimensional and three dimensional modeling. A review of other relevant research studies is also provided. Substantial literature has been studied on experimental and numerical study. However, little information can be found on formulated how to applied the boundary condition (BC) from experimental data to the three dimensional modeling analysis. The review is organized chronologically to offer insight to how past research efforts have laid the groundwork for subsequent studies, including the present research effort. The review is detailed so that the present research effort can be properly tailored to add the present body of literature as well as to justify the scope and direction of the present research effort.

## 2.2 Combustion

All of uses are dependent on the combustion of fossils fuels, whether for generating electricity, heating domestic water, or within an internal combustion engine. As they are a finite resource, using them efficiently and with minimum pollution is increasingly important.

Combustion is a chemical reaction (oxidisation) between combustible components of the fuel and oxygen in the air. The reaction is rapid and heat, light and energy are released as flame, which one started by an ignition source, is self-propagating. The process requires a substance that will burn, and this is usually a fossil fuel, such as coal, oil and gas. They contain a mixture of hydrogen and carbon and so are known as hydrocarbons.

For each hydrocarbon fuel there is a chemical equation of the reactants (fuel and air) forming the product of combustion. From this the theoretical air to fuel ratio can be determined as well as the constituents of the products of combustion.

In perfect combustion of hydrocarbons all the hydrogen and carbon in the fuel are oxidised to produce mainly carbon dioxide ( $\text{CO}_2$ ) and water ( $\text{H}_2\text{O}$ ), although there may be small amounts of carbon monoxide and partially reacted flue constituents. This is call stoichiometric combustion where the exact theoretical air quantity is supplied. Therefore the exhaust gas contains neither incompletely oxidised fuel constituents nor oxygen. So this means the  $\text{CO}_2$  in the flue gas is the maximum attainable.

If insufficient air is supplied, incomplete combustion will result, with part of the fuel remaining unoxidised. This will mean increased levels of carbon monoxide (CO) in the flue gas which can be dangerous and also pollutes the air. In oil burner this will also produce higher smoke number with sooting of the heat transfer surfaces, reducing their effectiveness.

In practice, to ensure complete combustion, excess air is supplied beyond that theoretically required for full oxidization of the fuel. This express as a percentage of the

theoretical air needed i.e. 10% excess air is 1.1 times the theoretical air quantity. Having excess air ensures no fuel is wasted, and variations in fuel quality or air and fuel rates can be tolerated and still guarantee complete combustion.

The control of the excess air is the key to combustion efficiency – too little will cause incomplete combustion with the problems mentioned above, whilst too much will cool the combustion chamber and carry a larger percentage of the heat out of the flue, reducing combustion efficiency.

Air consists of 21% oxygen and 79% nitrogen is inert and takes no part in the combustion process. It will enter the appliance at the ambient temperature, and leave through the flue, several hundred degrees higher, wasting heat in the process. This is a basic inefficiency which has to be accepted as there is no economical way of separating the oxygen and nitrogen.

The only reliable way of determining what is happening in a given combustion process is to take a flue gas sample using an analyzer. These vary in complexity, but will have as a minimum an oxygen sensor. Others may have sensors for other gases such as CO, NO and SO. From the oxygen sensor, knowing the particular fuel characteristics, the CO<sub>2</sub> and excess air values can be derived.

### **2.3 Combustion Efficiency**

Failure to achieve high level of combustion efficiency is generally regarded as unacceptable, partly because combustion inefficiency represents a waste of fuel, but mainly because it is manifested in the form of pollutant emissions such as unburned hydrocarbons and carbon monoxide. That is why current emissions regulations call for combustion efficiencies in excess of 99 percents. For the aircraft engine, an additional requirement is that combustion efficiencies should be fairly high, say from 75 to 80 percents, when the engine is being accelerated to its normal rotational speed after a

flameout in flight. A high combustion efficiency is necessary at this “off design” point because, with the engine wind milling, the pressure and the temperature of the air flowing through the combustor are close to ambient values. At high altitudes, these are so low that the stability limits are very narrow. This means that when the engine control system attempts to compensate for combustion inefficiency by supplying more fuel to the combustor, this extra fuel may cause a “rich extinction” of the flame. [2]

## 2.4 Combustion Process

The primary purpose of combustion is to raise the temperature of the airflow by efficient burning of fuel. From a design viewpoint, an important requirement is a means of relating combustion efficiency to the operating variables of air pressure, temperature and mass flow rate, and to the combustor dimensions. Unfortunately, the various process taking place within the combustion zone are highly complex and a detailed theoretical treatment is precluded at this time. Until more information is available, suitable parameters for relating combustion performance to combustor dimensions and operating conditions can be derived only through the use of very simplified models to represent the combustion process. One such model starts from the well establish and widely accepted notion that the total time required to burn a liquid fuel is the sum of the times required for fuel evaporation, mixing of fuel vapor with air and combustion products, and chemical reaction. Because the time available for combustion is inversely proportional to the airflow rate, the combustion efficiency may be expressed as

$$n_c = f(\text{airflow rate})^{-1} (1/\text{evaporation rate} + 1/\text{mixing rate} + 1/\text{reaction rate})^{-1}$$

In practical combustion systems, the maximum of heat release under any given operating conditions may be governed by either evaporation, mixing or chemical reaction, but rarely by all three at the same time. However, when the combustion process is in transition from one regime to another, two of the three keys rates will participate in determining the overall combustion efficiency. [2]

## 2.5 Pure Propane as a Fuel for Combustion

Propane is a three-carbon alkane, normally a gas, but compressible to a transportable liquid. It is derived from other petroleum products during oil or natural gas processing. It is commonly used as a fuel for engines, barbecues, and home heating systems.

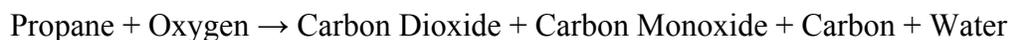
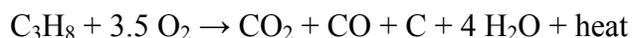
When used as vehicle fuel, it is commonly known as liquefied petroleum gas (LPG or LP-gas), which can be a mixture of propane along with small amounts of propylene, butane, and butylene. The odorant ethanethiol is also added so that people can easily smell the gas in case of a leak. [3]

Propane is produced as a byproduct of two other processes: natural gas processing and petroleum refining. The processing of natural gas involves removal of butane, propane and large amounts of ethane from the raw gas to prevent condensation of these volatiles in natural gas pipelines. Additionally, oil refineries produce some propane as a by-product of production of cracking petroleum into gasoline or heating oil. Table 2.1 shows the properties of propane in general.

Propane undergoes combustion reactions in a similar fashion to other alkanes. In the presence of excess oxygen, propane burns to form water and carbon dioxide.



When not enough oxygen is present for complete combustion, incomplete combustion occurs when propane burns and forms water, carbon monoxide, carbon dioxide, and carbon.



Unlike natural gas, propane is heavier than air (1.5 times as dense). In its raw state, propane sinks and pools at the floor. Liquid propane will flash to a vapor at atmospheric pressure and appears white due to moisture condensing from the air. When properly combusted, propane produces about 50 MJ/kg. The gross heat of combustion of one normal cubic meter of propane is around 91 mega joules

Propane is nontoxic; however, when abused as an inhalant it poses a mild asphyxiation risk through oxygen deprivation. Commercial products contain hydrocarbons beyond propane, which may increase risk. Commonly stored under pressure at room temperature, propane and its mixtures expand and cool when released and may cause mild frostbite.

Propane combustion is much cleaner than gasoline combustion, though not as clean as natural gas combustion. The presence of C-C bonds, plus the multiple bonds of propylene and butylene, create organic exhausts besides carbon dioxide and water vapor during typical combustion. These bonds also cause propane to burn with a visible flame.

Greenhouse gas emissions factors for propane are 62.7 kg CO<sub>2</sub>/ mBTU or 1.55 kg of CO<sub>2</sub> per liter or 73.7 kg / GJ.

Table 2.1: Properties of propane

Molecular formula	C <sub>3</sub> H <sub>8</sub>
Molar mass	44.1 g mol <sup>-1</sup>
Appearance	Colorless gas
Density	1.83kg/m <sup>3</sup> ,gas 0.5077 kg/L, liquid
Melting point	-187.6 °C (85.5 K)
Boiling point	-42.09 °C (231.1 K)

In this research, pure propane used as fuel. The fuel characteristic from laboratory is 96% propane and 4% mixture of butane, methane and ethane. Appendix A1 use as guideline for safety precaution when running this research.

## 2.6 Reynolds Number, Re

The Reynolds number is a measure of the ratio inertial forces ( $v\rho$ ) to viscous forces ( $\mu/L$ ) and consequently, it quantifies the relative importance of these two types of forces for given flow conditions. It is the most important dimensionless number in fluid dynamic and is used, usually along with other dimensionless numbers, to provide a criterion for determining dynamic similitude. When two geometrically similar dimensionless numbers, they are said to be dynamically similar, and will have similar flow geometry. It is also used to identify and predict different flow regimes, such as laminar or turbulent flow. Laminar flow occurs at low Reynolds numbers, where viscous forces are dominant, and is characterized by smooth, constant fluid motion, while turbulent flow, on the other hand, occurs at high Reynolds numbers and is dominated by inertial forces, which tend to produce random eddies, vortices and other flow fluctuations. Typically it is given as follows: [4]

$$\text{Re} = \frac{\text{Dynamic Pressure}}{\text{Shearing stress}} = \frac{\rho v D}{\mu} = \frac{v D}{\nu}$$

Where:

$v$  is the mean fluid velocity in  $\text{m.s}^{-1}$

$D$  is the characteristics diameter in m

$\mu$  is the (absolute) dynamic fluid viscosity in  $\text{N.s.m}^{-2}$  or Pa.s

$\nu$  is the kinematic fluid viscosity, defined as  $\nu = \mu/\rho$ , in  $\text{m}^2.\text{s}^{-1}$

$\rho$  is the density of the fluid in  $\text{kg.m}^{-3}$

## 2.7 Navier-Stokes Equations

The Navier-Stokes equations are the fundamental partial differential equations that describe the flow of incompressible fluids. Using the rate of stress and rate of strain tensors, it can be shown that the components  $F_j$  of the viscous force  $F$  in a nonrotating frame are given by:[5]

$$\begin{aligned} \frac{F_i}{V} &= \frac{\partial}{\partial x_j} \left[ \eta \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \lambda \delta_{ij} \nabla \cdot \mathbf{u} \right] \\ &= \frac{\partial}{\partial x_j} \left[ \eta \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \nabla \cdot \mathbf{u} \right) + \mu_B \delta_{ij} \nabla \cdot \mathbf{u} \right], \end{aligned}$$

(Tritton 1988, Foher 1995), where  $\eta$  is the dynamic viscosity,  $\lambda$  is the second viscosity coefficient,  $\delta_{ij}$  is the Kronecker delta,  $\nabla \cdot \mathbf{u}$  is the divergence,  $\mu_B$  is the bulk viscosity and Einstein summation  $\Sigma$  has been used to sum over  $j = 1, 2$  and  $3$ .

## 2.8 Turbulence Model

Almost all fluid flow which we encounter in daily life is turbulent. Typical examples are flow around (as well as in) cars, aeroplanes and buildings. The boundary layers and the wakes around and after bluff bodies such as cars, aeroplanes and buildings are turbulent. Also the flow and combustion in engines, both in piston engines and gas turbines and combustors, are highly turbulent. Air movements in rooms are also turbulent, at least along the walls where wall-jets are formed. Hence, when we compute fluid flow it will most likely be turbulent.

In turbulent flow we usually divide the variables in one time-averaged part  $\bar{U}$ , which is independent of time (when the mean flow is steady), and one fluctuating part  $u$

so that  $U = \check{U} + u$ . There is no definition on turbulent flow, but it has a number of characteristic features such as:[6]

### **2.8.1 Irregularity**

Turbulent flow is irregular, random and chaotic. The flow consists of a spectrum of different scale (eddy sizes) where largest eddies are of the order of the flow geometry (i.e. boundary layer thickness, jet width, etc). At the other end spectra we have the smallest eddies which are by viscous forces (stresses) dissipated into internal energy. Even though turbulence is chaotic it is deterministic and is described by the Navier-Stokes equations.

### **2.8.2 Diffusivity**

In turbulent flow the diffusivity increases. This means that the spreading rate of boundary layers, jets, etc. increases as the flow becomes turbulent. The turbulence increases the exchange of momentum in e.g. boundary layers and reduces or delays thereby separation at bluff bodies such as cylinders, airfoils and cars. The increased diffusivity also increases the resistance (wall friction) in internal flows such as in channels and pipes.[7]

### **2.8.3 Large Reynolds Numbers**

Turbulent flow occurs at high Reynolds number. For example, the transition to turbulent flow in pipes occurs that  $Re D \approx 2300$ , and boundary layers at  $Re_x \approx 10000$ .

#### **2.8.4 Dissipation**

Turbulent flow is dissipative, which means that kinetic energy in the small (dissipative) eddies are transformed into internal energy. The small eddies receive the kinetic energy from slightly larger eddies. The slightly larger eddies receive their energy from even larger eddies and so on. The largest eddies exact their energy from the mean flow. This process of transferred energy from the largest turbulent scales (eddies) to the smallest is called cascade process.

#### **2.9 Eddy Dissipation**

The eddy dissipation model is based on the concept that chemical reaction is fast relative to the transport processes in the flow. When reactants mix at the molecular level, they instantaneously form products. The model assumes that the reaction rate may be related directly to the time required to mix reactants at the molecular level. In turbulent flows, this mixing time is dominated by the eddy properties and, therefore, the rate is proportional to a mixing time defined by the turbulent kinetic energy,  $k$ , and dissipation. This concept of reaction control is applicable in many industrial combustion problems where reaction rates are fast compared to reactant mixing rates.[8]

#### **2.10 Boyle's Law**

Boyle's law states that at constant temperature, the absolute pressure and the volume of a gas are inversely proportional. The law can also be stated in a slightly different manner, that the product of absolute pressure and volume is always constant.

Most gases behave like ideal gases at moderate pressures and temperatures. The limited technology of the 1600s could not produce high pressures or low temperatures.

Hence, the law was not likely to have deviations at the time of publication. As improvements in technology permitted higher pressures and lower temperatures, deviations from the ideal gas behavior would become noticeable, and the relationship between pressure and volume can only be accurately described employing real gas theory. The deviation is expressed as the compressibility factor.[9]

The mathematical equation for Boyle's law is:

$$PV = k$$

Where:

$P$  denotes the pressure of the system.

$V$  is the volume of the gas.

$k$  is a constant value representative of the pressure and volume of the system.

## 2.11 Charle's Law

In thermodynamics and physical chemistry, Charles's law is a gas law and specific instance of the ideal gas law, which states that:

At constant pressure, the volume of a given mass of an ideal gas increases or decreases by the same factor as its temperature (in Kelvin) increases or decreases. [10]

The formula for the law is:

$$\frac{V}{T} = k$$

Where:

$V$  is the volume of the gas

$T$  is the temperature of the gas (measured in Kelvin)

$k$  is a constant.

In other more thermodynamics-based definitions, the relationship between the fixed mass of a gas at constant pressure is inversely proportional to the temperature applied to the system, which can be further used by stipulating a system where  $\alpha$  represents cubic expansivity of a gas, with  $\theta$  representing the temperature measured of the system in Kelvins:

$$V \propto T$$

$$V = V_0(1 + \alpha\theta)$$

To maintain the constant,  $k$ , during heating of a gas at fixed pressure, the volume must increase. Conversely, cooling the gas decreases the volume. The exact value of the constant need not be known to make use of the law in comparison between two volumes of gas at equal pressure:

$$\frac{V_1}{T_1} = \frac{V_2}{T_2} \quad \text{or} \quad \frac{V_2}{V_1} = \frac{T_2}{T_1} \quad \text{or} \quad V_1 \cdot T_2 = V_2 \cdot T_1$$

Therefore, as temperature increases, the volume of the gas increases. Theoretically as a temperature reaches absolute zero the volume will also reach a point of zero.[9]

## 2.12 Ideal Gas Law

The ideal gas law is the equation of state of a hypothetical ideal gas, first stated by Benoît Paul Émile Clapeyron in 1834. Table 2.2 shows the value of the ideal gas constant,  $R$ . [11]

The state of an amount of gas is determined by its pressure, volume, and temperature according to the equation:

$$PV = nRT$$

Where:

$P$  is the absolute pressure of the gas,

$V$  is the volume of the gas,

$n$  is the number of moles of gas,

$R$  is the universal gas constant,

$T$  is the absolute temperature.

Table 2.2: The value of the ideal gas constant,  $R$ ,

Value	Unit
8.314472	$\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$
8.314472	$\text{m}^3\cdot\text{Pa}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
8.314472	$\text{kPa}\cdot\text{L}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$
0.08205746	$\text{L}\cdot\text{atm}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
62.36367	$\text{L}\cdot\text{mmHg}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
10.73159	$\text{ft}^3\cdot\text{psi}\cdot\text{R}^{-1}\cdot\text{lb}\cdot\text{mol}^{-1}$
53.34	$\text{ft}\cdot\text{lb}_f\cdot\text{R}^{-1}\cdot\text{lb}_m^{-1}$ (for air)

The ideal gas law mathematically follows from a statistical mechanical treatment of primitive identical particles (point particles without internal structure) which do not interact, but exchange momentum (and hence kinetic energy) in elastic collisions.

Since it neglects both molecular size and intermolecular attractions, the ideal gas law is most accurate for monoatomic gases at high temperatures and low pressures. The neglect of molecular size becomes less important for larger volumes, i.e., for lower pressures. The relative importance of intermolecular attractions diminishes with increasing thermal kinetic energy i.e., with increasing temperatures. More sophisticated equations of state, such as the van der Waals equation, allow deviations from ideality caused by molecular size and intermolecular forces to be taken into account.

### 2.13 Turbulence Intensity

The turbulence intensity, also often referred to as turbulence level, is defined as:

$$I \equiv \frac{u'}{U}$$

Where:

$u'$  is the root-mean-square of the turbulent velocity fluctuations.

$U$  is the mean velocity (Reynolds averaged).

If the turbulent energy,  $k$ , is known  $u'$  can be computed as:

$$u' \equiv \sqrt{\frac{1}{3} (u_x'^2 + u_y'^2 + u_z'^2)} = \sqrt{\frac{2}{3} k}$$

$U$  can be computed from the three mean velocity components  $U_x$ ,  $U_y$  and  $U_z$  as:

$$U \equiv \sqrt{U_x^2 + U_y^2 + U_z^2}$$

When setting boundary conditions for a CFD simulation it is often necessary to estimate the turbulence intensity on the inlets. To do this accurately it is good to have some form of measurements or previous experience to base the estimate on. Here are a few examples of common estimations of the incoming turbulence intensity: [12]

**High-turbulence case:** High-speed flow inside complex geometries like heat-exchangers and flow inside rotating machinery (turbines and compressors). Typically the turbulence intensity is between 5% and 20%

**Medium-turbulence case:** Flow in not-so-complex devices like large pipes, ventilation flows etc. or low speed flows (low Reynolds number). Typically the turbulence intensity is between 1% and 5%

**Low-turbulence case:** Flow originating from a fluid that stands still, like external flow across cars, submarines and aircrafts. Very high-quality wind-tunnels can

also reach really low turbulence levels. Typically the turbulence intensity is very low, well below 1%.

For fully developed pipe flow the turbulence intensity at the core can be estimated as:

$$I = 0.16 Re_{d_h}^{-\frac{1}{8}}$$

Where:

$Re_{d_h}$  is the Reynolds number based on the pipe hydraulic diameter  $d_h$ .

## 2.14 Hydraulic Diameter

The hydraulic diameter,  $d_h$ , is commonly used when dealing with non-circular pipes, holes or ducts. [13]

The definition of the hydraulic diameter is:

$$d_h \equiv 4 \frac{\text{cross-sectional-area of duct}}{\text{wetted perimeter of duct}}$$

### 2.14.1 Hydraulic Diameters for Different Duct-Geometries

Using the definition above the hydraulic diameter can easily be computed for any type of duct-geometry. Below follows a few examples.

### 2.14.1.1 Circular Pipe

For a circular pipe or hole the hydraulic diameter is:

$$d_h = 4 \frac{\frac{\pi d^2}{4}}{\pi d} = d$$

Where:

$d$  is the real diameter of the pipe. Hence, for circular pipes the hydraulic diameter is the same as the real diameter of the pipe.

### 2.14.1.2 Rectangular Tube

For a rectangular tube or hole with the width  $a$  and the height  $b$  the hydraulic diameter is:

$$d_h = 4 \frac{ab}{2a + 2b} = 2 \frac{ab}{a + b}$$

### 2.14.1.3 Coaxial Circular Tube

For a coaxial circular tube with an inner diameter  $d_i$  and an outer diameter  $d_o$  the hydraulic diameter is:

$$d_h = 4 \frac{\frac{\pi d_o^2}{4} - \frac{\pi d_i^2}{4}}{\pi d_o + \pi d_i} = d_o - d_i$$

## 2.15 Problem Investigation of the Combustion Process

### 2.15.1 Experimental Study

The HiTAC test furnace, used in this study is equipped with a one-flame HiTAC, and the internal dimensions of the furnace body are 2850×1600×1600mm. Four pipes of a 110mm external diameter of 110mm cooled with air have been installed horizontally in each corner of the furnace to remove heat from the combustion chamber. Figure 2.1 show the dimension of the test furnace. On the wall opposite to the burner, there are two flue gas ducts of 110mm external diameter for removing hot flue gases from the furnace. The walls of the test furnace consist of two layers: an outer steel cover 5.0mm thick, and an inner layer of fibrous ceramic insulation 300mm thick with a thermal conductivity of  $0.14\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ . The emissivity of the insulation was set to 0.5 according to the manufacturer's specifications, and the emissivity of the air-cooled tubes was set to 0.8 to represent an oxidized steel surface. A 200 kW one-flame HiTAC system with honeycomb regenerative burner was used in this study. The regenerator preheats the combustion air using heat from exhaust gases that would normally be just discharged into the atmosphere in a conventional furnace. The one-flame HiTAC system features one fuel nozzle surrounded by air inlets and fuel gas outlets. Each of these inlets or outlets contains a ceramic honeycomb regenerator that absorbs heat from exhaust gases during the exhaust cycle, and releases this heat into the combustion air during the firing cycle.

Figure 2.1 sketches the dimensions of the burner and locations of fuel and air injection ports. There are 12 regenerators in all, working in pairs and organized into two groups separated by intervals. Air is preheated by one of the groups (six regenerators working in pairs) with a set switching time of 10 seconds, while the other group functions as an exhaust-gas extractor and storage bed. When the combustion air passes though the honeycomb regenerator it is preheated to a temperature close to that of the

exiting flue gas before it enters the furnace. Fuel is supplied continuously through the same nozzle, but the air nozzles switch from inlets to outlets and back again during a switch interval. This enables a single flame to be formed with a permanent position. This flame position is almost constant during each switch interval because the regenerators are placed around the fuel-jet nozzle. Only 80% of the exhausting flue gases through the burner outlets. The remainder of the exhaust gases flow out from the furnace through the chimney located on the rear wall of the furnace. The fuel used in the study was propane gas, the composition of which has been provided in Table 2.3, along with the operating conditions tested.[14]

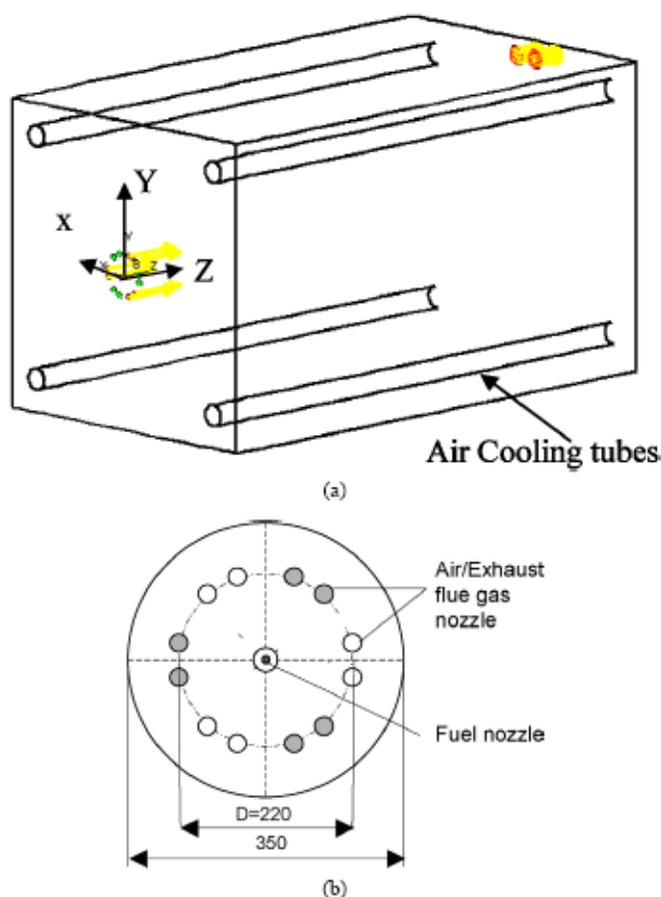


Figure 2.1: Configuration of the HiTAC test furnace: (a) furnace geometry, (b) arrangement of air and fuel inlets and flue gas outlets.

Table 2.3 : Fuel characteristic and operation condition

Characteristics	HiTAC mode
Fuel flow rate, [Nm <sup>3</sup> ·h <sup>-1</sup> ]	7.7
Fuel inlet temperature, [K]	2.98
Fuel composition (Mass fraction [%])	CH <sub>4</sub> (0.02), C <sub>2</sub> H <sub>6</sub> (0.95), C <sub>3</sub> H <sub>8</sub> (98.35), C <sub>4</sub> H <sub>10</sub> (0.67)
Combustion air flow rate, [Nm <sup>3</sup> ·h <sup>-1</sup> ]	200
Combustion air temperature, [K]	1211 K
Combustion air composition, [Vol%]	N <sub>2</sub> (79), O <sub>2</sub> (21)

### 2.15.2 Numerical Study

In the calculations, the origin of the coordinate is always at the central axis of the fuel-nozzle inlet, and the positive  $z$  axis is in the direction of the hearth, and the length of the furnace is the horizontal distance from the burner face. The whole chamber was modeled because there are no planes of symmetry in the furnace. The three dimensional grids have 86420 cells within the domain. The highest concentration of the cells is near the burner and in the flame zone. The furnace used in these investigations operated periodically with a switching time of 10 seconds. Normally the combustion process would reach steady state after 2–3 seconds. This means that the process has already reached steady-state long before the cycle is reversed. In addition, the studied flame almost has permanent position during the switching interval as explained above. Thus, in this work, steady-state simulations have been performed in which the exhaust/firing cycles will not be reversed. Therefore, the burner configuration had to be frozen with respect to the air and gas orifices. Figure 2.1(b) shows the configuration of the burner. Therefore, care should be paid when comparing the predicted and experimental values. Simulations of the combustion at steady-state gives anyway very valuable information on the in-furnace gas velocity field and flow pattern, in-furnace gas temperature field, and in-furnace gases composition and heat flow. The

HiTAC test furnace used is equipped with two different burner systems; in particular, there are 13 measured holes on the top wall, although they are covered. Uniform distribution of heat losses at the furnace wall has not been assumed. In the present paper, heat losses at the furnace wall were obtained by measurement. The cooling air in tubes flows from the front side (burner side) to hidden side (main chimney side), based on the measured surface temperatures in three points the temperature distribution on the cooled tubes is approximated with the following relationships:

$$T = 1337.3 + 18.14 \times Z + 0.18246 \times Z^2 \text{ K}$$

The Computational Fluid Dynamics code, STAR-CD, was employed to evaluate the physical properties the HiTAC test furnace. A control volume approach is used in which a nonstaggered grid arrangement is employed to discretize the differential governing equations. The discretized governing equations are solved using SIMPLEC algorithms with an interactive line-by-line matrix solver and multigrid acceleration.

### **2.15.3 Comparison Predicted and Numerical Data**

In this regarding, validation of the prediction is undertaken by comparing the predicted and measured values of:

- energy balance
- wall temperature profiles
- in-furnace gas species

### 2.15.3.1 Energy Balance

The reference temperature is set at  $T = 298$  K, so the sensible heat flow rate at the fuel inlets was zero. The overall thermal energy (only including the fuels' chemical energy) input to the test furnace in this study was 182 kW. The thermal input of the fuel for the simulation was calculated according to the chemical reaction steps (R1)–(R5). The heat of exhaust after the burner for simulation was approximately calculated as the value of heat of flue gas through the burner minus combustion sensible heat of the combustion air. The summary of the energy balance of the semi-industrial furnace at the operation condition is given in Table 2.4.

A figure of 54.65% of the predicted fuel thermal input passed through the burner, and 83.6 percent of the sensible heat carried by the flue gases through the burner outlets was used to preheat the combustion air from 300 to 1211 K. This means the thermal efficiency of the regenerator is 83.6%. This value is about 45.71% of the total thermal input. This implies that a very high level of energy utilization efficiency is achieved. Reiterating here, 8.94% of the predicted total fuel thermal input is removed by flue gas through the burner. This value is higher than measured value of 5.21%. Possible reasons for this could be one or a combination of the following: heat loss in the burner, or the measurement point being on the outside of the burner.

The predicted amount of heat taken by the air-cooling tubes occupies 51.67% of the fuel thermal input. The heat absorbed by air-cooling tube was measured to be around 54.27% of the fuel thermal input within the margin of measurement error of 6.44%. Therefore, the predicted and measured amounts are in a reasonable agreement. The predicted results also indicated that 97.4% of the heat transferred to the air-cooling tube was due to radiation, and 2.6% was due to convection. Furthermore, the calculation enthalpy of the chimney flue gas constitutes 9.78% of the fuel thermal input, while the actual value measured was 11.25%. Again, the agreement is acceptable. The predicted heat loss through the furnace walls accounts for 29.61% of the thermal input, compared with an actual measurement of 29.49%. Thus, these are also in a good agreement.

Table 2.4: Energy balance from measurements and from modeling data (reference temperature: 298 K)

<b>Energy [kW]</b>	<b>Characteristics</b>	<b>HiTAC prediction</b>	<b>CFD</b>	<b>HiTAC trial measured</b>
<b>Input</b>	1. Fuel power	184.04		182.0
	2. Combustion air sensible heat	84.12	(after preheated by the burner)	1.85 (before preheated by the burner)
	<b>Total</b>	<b>268.16</b>		<b>183.85</b>
<b>Output</b>	3. Heat taken away by the air-cooled tubes	95.09		99.78
	4. Heat of flue gas through burner	100.58		-
	5. Heat of exhaust after burner	16.46		9.57
	6. Sensible heat of flue gas through main chimney	17.99		20.69
	7. Heat loss from walls	51.27		48.13
	Radiation heat loss at inlets and outlets	3.23		-
	Uncounted loss	-		6.06
	<b>Total</b>	<b>267.85</b>		<b>183.85</b>

### 2.15.3.2 Furnace Wall Temperature

Furnace wall temperatures in the HiTAC test furnace were measured at various positions along the left-hand side wall of the test furnace (viewed from the burner side). Figure 2.2 presents a comparison of the temperature predictions and the measurements

showing a reasonable agreement, with maximum difference being about 10 °C with a range of error of 2.8%. These values obtained using a stationary thermocouple located on the furnace wall.

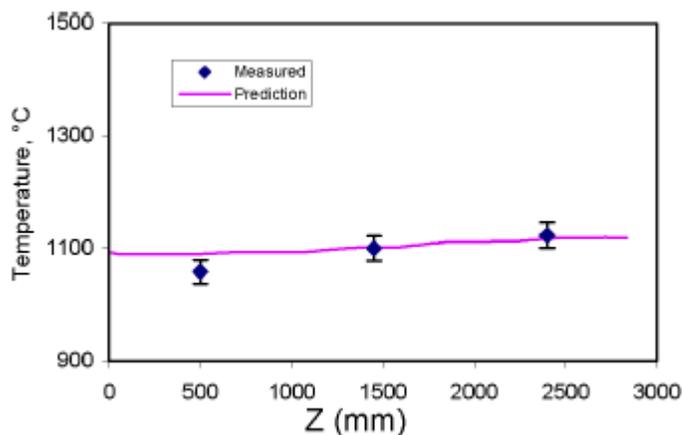


Figure 2.2: Wall temperature distribution along the side wall of the furnace at  $x = 0.8$  m, and  $y = -0.3$  m.

### 2.15.3.3 Gas Species

The uncertainties associated with the probe positions are  $\pm 10$  mm in the  $x$ - and  $z$ -directions, and  $\pm 2$  mm in the  $y$  direction. The uncertainty of  $O_2$  was 2.3%. The uncertainty of CO was 2.1%. These values only consider the instrument and calibration gas accuracies and do not consider any other error source such as probe effect on sample.

Figure 2.3 shows the measured and predicted concentrations of  $O_2$  at specific vertical distances from the burner face. The  $x$ -axis represents the vertical distance from the centerline of the burner.

Figure 2.3(a) shows that the lowest predicted concentrations of  $O_2$  occurred along the centerline of the burner at a distance of  $z = 0.3$  m from the burner face (wall).

This is expected, because the fuel jet's positioning on the burner axis results in a high concentration of fuel in this area. However, the actual oxygen concentration measured was much higher than predicted at this location. Possible reasons for this could be errors in measuring the location, the disturbing effect of the sucking probe had on the flue gas, and the assumption that the operation of burner achieved steady-state—the periodic operation of burner achieves better mixing.

A peak concentration of  $O_2$  occurred at 0.11 m from the firing centerline. This is approximately where the combustion air jets are located on the circumference of the burner face, so a high  $O_2$  concentration is quite credible. At a distance of about 0.2m and greater from the centerline of the burner, the concentration of  $O_2$  and  $CO_2$  were in approximate agreement with those expected for complete combustion of gasoil with 10% excess air.

The predicted concentrations of  $O_2$  follow similar trends to the measured values, exhibiting the same peak concentration location. Figure 2.3(b) shows that the predicted values of  $O_2$  concentration at 0.6m from the burner face exhibit similar trends to those shown in Figure 2.3(a), only more pronounced. Predicted peaks in  $O_2$  content of around 5% occur at 0.11m from the centerline of the burner, corresponding with the measured positions and values. These trends in predicted  $O_2$  values are still evident at even a greater distance—for example at 1.2m from the furnace face (see Figure 2.3(c))—albeit to a lesser extent. Although the measured and predicted peaks for  $O_2$  concentration were located at similar positions (0.15–0.2m from the centerline of the burner), the predicted value of  $O_2$  is higher than measured value. Besides the possible influence led by the sucking probe, there is a slight possibility that mixing and combustion in the model occurs at a marginally slower rate than might be inferred from the measured values.

At the furnace sides, the measured concentrations of  $O_2$  are approximately constant along the furnace depth and consistent with the expected values for complete combustion. The predicted contents of  $O_2$  agree with the measured ones.

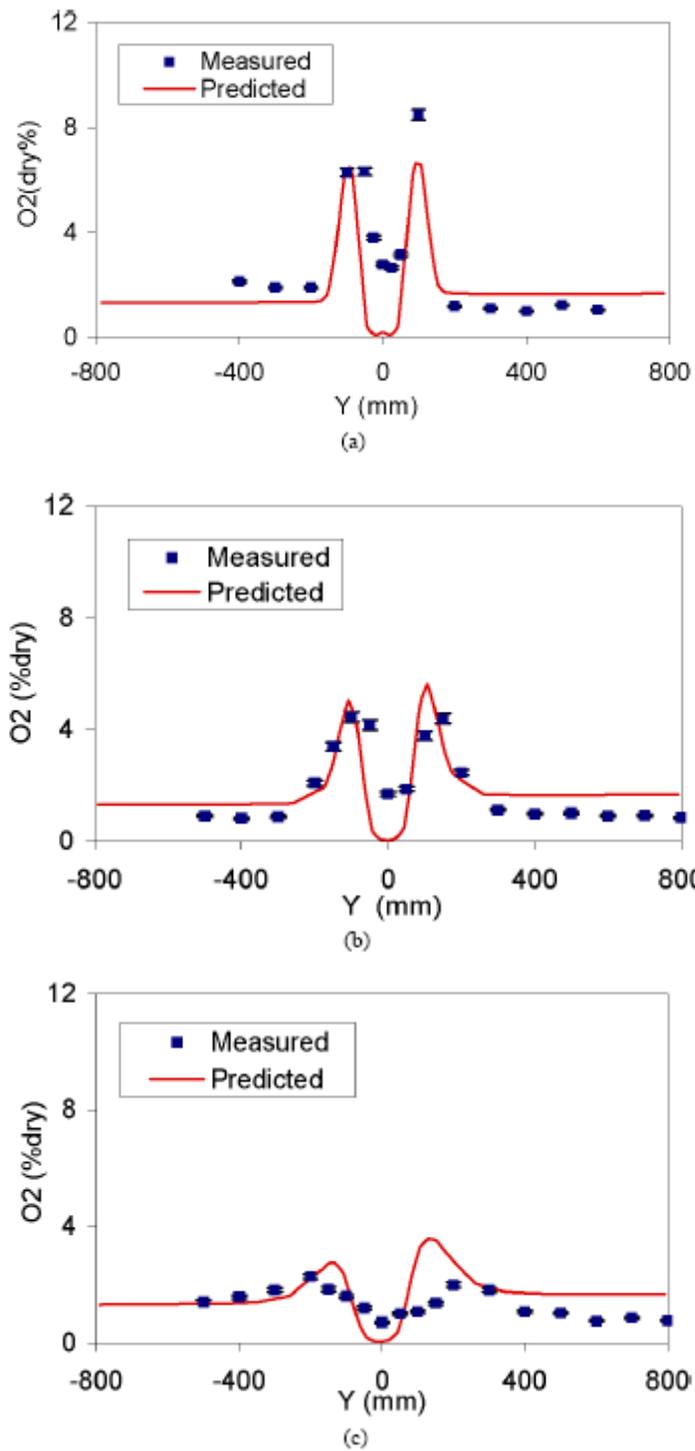


Figure 2.3: Predicted and measured O<sub>2</sub> profiles in the furnace: (a)  $x = 0, z = 0.3$  m, (b)  $x = 0, z = 0.6$  m, (c)  $x = 0, z = 1.2$  m.

Figure 2.4 reveals the values of the predicted and measured concentrations of CO at various distances from the face of the furnace. At 0.3m from the burner face shown in Figure 2.4(a), the predicted concentration of CO peaked at about 0.05m from the centerline. Meanwhile, two peaks are found. This coincides with the trend in the concentration of O<sub>2</sub> given above. The CO content rapidly decays with increasing distance from the centerline, and is negligible at around 0.1m. The measured concentration also peaks and minimizes at these positions. It seems that most of the chemical reaction (combustion) occurs in this zone. However, the peak CO concentrations of 13750 ppm is much higher than the predicted value of 4300 ppm.

At 0.6m from the burner face shown (Figure 2.4(b)), the predicted concentration of CO peaks at about 0.068m from the centerline, which is a little far away than the CO peaks at 0.3m from the burner face. This indicates that the flame is spread along furnace length direction. The CO content also rapidly decays with increasing distance from the centerline, and is negligible at around 0.15m. The measured concentration also peaks and minimized at these positions. These imply that the reaction zone enlarges with the distance from the burner. The peaks CO measured and predicted value are 20000 and 4800 ppm, respectively. At this location, the CO concentration reaches the maximum in the whole furnace hearth.

At 1.2m from the burner face shown in Figure 2.4(c), both the predicted and measured high CO concentrations appear in the region (-340m, 360m). Comparing with the CO concentrations at 0.6m from the burner face, this region further is increased. It can be seen that the reaction zone further enlarges. The similar trends (Figure 2.4(d)) are observed at section 2.15m from the burner face. Furthermore, near the sidewalls, both measured and predicted CO levels were very low and negligible and indicative of practically complete combustion.

Base on the above, a conclusion can be drawn that the chemical reaction zone is limited to the volume of the hypothetical cylinder determined by the air jets. Consequently it leads to a rather long HiTAC flame. In this trial case, the flame persists to whole furnace hearth. Additionally, the predicted locations of combustible gases, for

example the CO concentration, in furnace are in good agreement with the experimental values, what indicates that flame spread is good predicted.

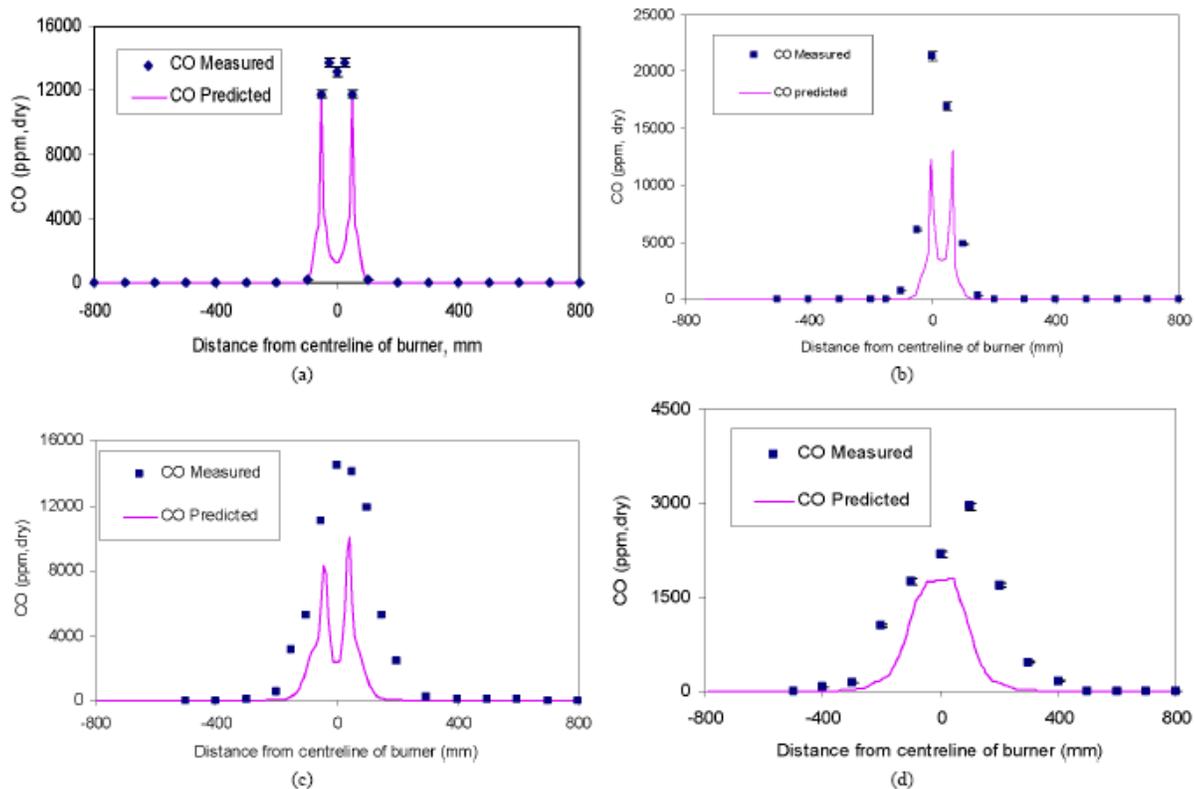


Figure 2.4: Predicted and measured CO profiles in the furnace: (a)  $x = 0, z = 0.3\text{m}$ , (b)  $x = 0, z = 0.6\text{m}$ , (c)  $x = 0, z = 1.2\text{m}$ , (d)  $x = 0, z = 2.15\text{m}$ .

## **CHAPTER 3**

### **METHODOLOGY**

#### **3.1 Introduction**

The objective of this chapter is to present the experimental study and numerical approaches for the performance of the pure propane combustion. Using numerical approach, the combustion chamber, gas burner and nozzle build up based on actual geometries. Geometric approximations, method to solve and others are also presented in this chapter. Pure propane gas will burn in combustion chamber using combustion laboratory unit C492. The experiment was running in several times. Only the best result will taken to proceed to the next stage. Data from experimental result were use to setting boundary condition in simulation. CFD's software, FLUENT 6.3, used in simulation process. Before doing the simulation the of the combustion laboratory unit C492 will design and mesh in GAMBIT software.

### 3.2 Overall of Research Methodology

The flowchart of research methodology in this study is shown in Figure 3.1. Numerical approach will be used to solve the two dimensional analysis of combustion chamber of C492 gas burner. The boundary condition of this analysis is taken from the experimental data.

This research started with searching and studying the recent research that was done by others researchers. All the research collected was analyzed and arrange in literature review. From the data in literature review, experimental work will run. The function of experimental work is to get data for boundary condition that will use in CFD modeling and simulation. The result from experiment and simulation will compare. If the percentage of differences data is small, the simulation is success. If not the CFD modeling will recheck and run simulation again.

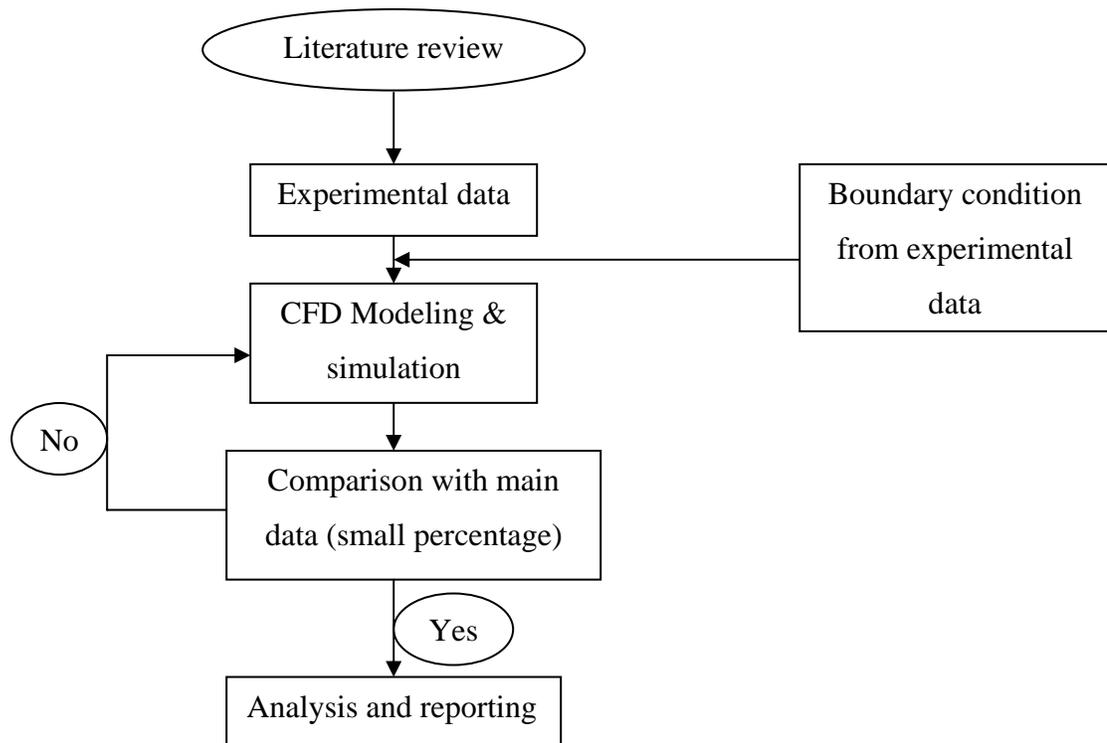


Figure 3.1: Flowchart of research methodology

### 3.3 Experimental Work

#### 3.3.1 Combustion Laboratory Unit C492

The experimental work for this research will use C492 gas burner. The height is 1560 mm, width is 800 mm, depth is 1800 mm, weight is 250 kg and maximum heat input is not exceeding 150 kW. Figure 3.2 show the picture of combustion laboratory unit C492 that been used for this experiment.



Figure 3.2: Picture of combustion laboratory unit C492

### 3.3.2 Gas Burner

The fuel for this research is pure propane gas. Connect to the  $\frac{3}{4}$  inch BSP inlet marked mains natural gas inlet at the rear of the frame. The gas pressure must be less than 50 mbar and ideally 12.5 to 20 mbar. Pressure in excess of 50 mbar will damage the gas meter unit. The maximum flow rate for pure propane gas inlet is not exceeding  $14\text{m}^3/\text{hr}$ . Figure 3.3 show the picture of C492 gas burner. Figure 3.4 show the picture of nozzle and air outlet flow. Figure 3.5 show the picture of adjustment place for air and fuel flow rate.



Figure 3.3: Picture of C492 Gas Burner



Figure 3.4: Picture of nozzle and air outlet



Figure 3.5: Picture of fuel and air adjustment

### 3.3.3 Flue Gas Analyzer

The C492 gas burner has an optional complex flue gas analyzer, designated C492D. This model includes O<sub>2</sub>, CO, NO and SO<sub>2</sub> sensors, with integral printout, and Windows™ software for recording and analyzing data away from the unit. It is used instead of the standard air analyzer supplied with the C492 gas burner.

Figure 3.6 show the system how flue gas analyzer works. Handset use to read the concentration of flue gas in exhaust. Then it transfers the data to gas analyzer. In gas analyzer the concentration will calculate and recorded. The data also can transfers to the computer using optional gas analyzer cable connection. In the computer the graph can be plot to show the flow of combustion process during experimental work. Then the data from the experiment can be print out and analyzed.

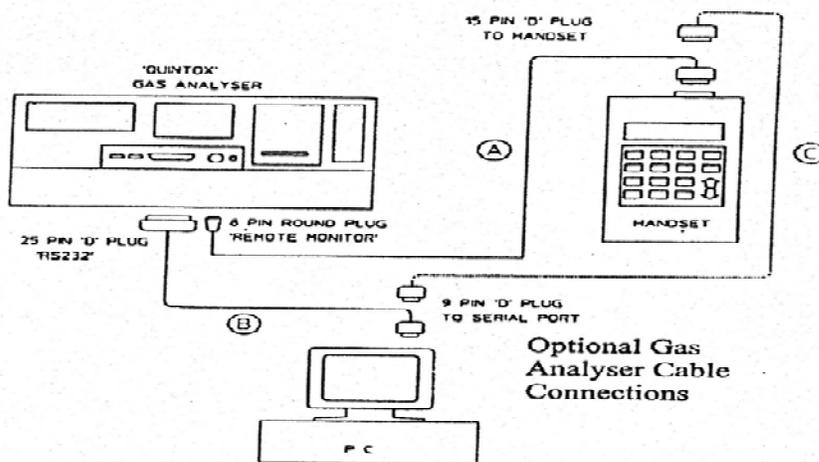


Figure 3.6: System of flue gas analyzer

### 3.4 CFD Modeling and Simulation

Fluent is a state of the art computer program for modeling fluid flow and heat transfer in complex geometries. It is capable to complete mesh flexibility, solving flow problem with unstructured meshes that can be generated the complex geometries.

Figure 3.7 shows the organizational structure of these components. Gambit design started with 2D geometry setup combustion unit C492. Then the design will mesh in 2D rectangle mesh. At the final step in Gambit, boundary condition will setting and export to Fluent for simulation. Figure 3.8 show the meshing geometry for the design.

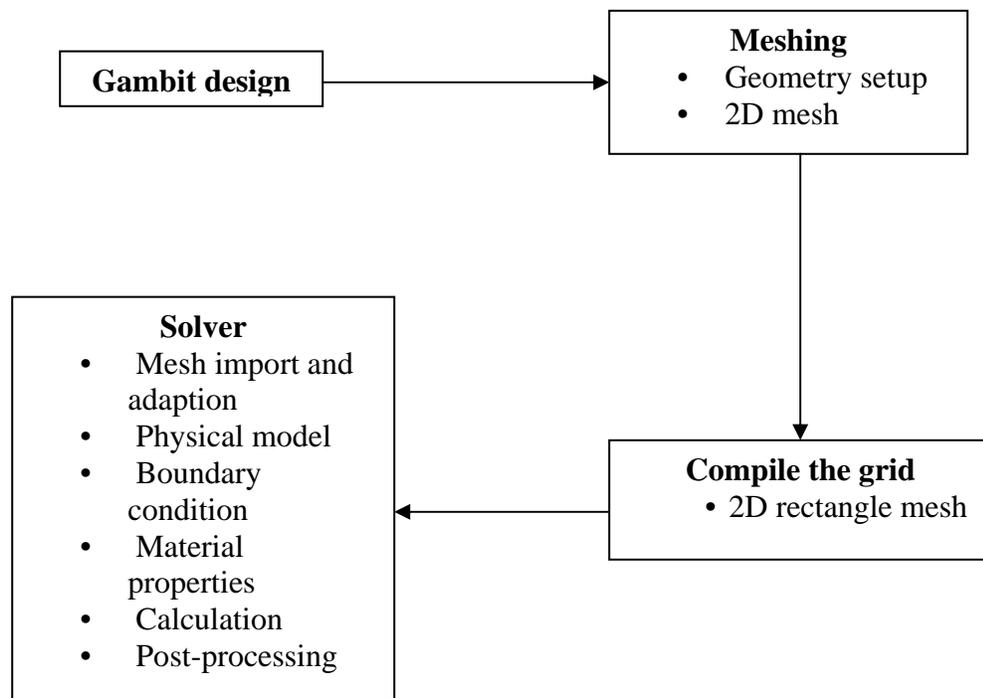


Figure 3.7: Program structure for Gambit

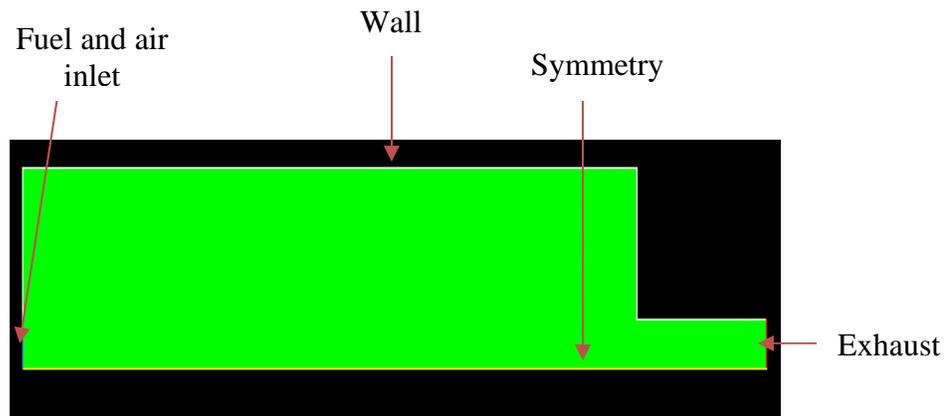


Figure 3.8: Meshing boundary in Gambit

### 3.4.1 Problem Solving Step

Problem solving steps using CFD analysis consist the problem identification, grid creation, solver execution and analysis the results. With a build-in post processing, it can automatic save on setting file data written in \*.dat and \*.cas file.

Figure 3.9 shows the detailed steps analysis of research. It starting with problem identification and pre-processing. Here the simulation is based on objective that wants to achieve. Then it divided to three parts that is defining a modeling goal, identify the domain to modeled and design and create grid. All this three parts is the main factors in solver execution. Setup the numerical model and compute the solution is the next step after solver execution. Transport species were defined and simulated. The result then analyzed and compare with the experimental data. If unsatisfactory, consider the model revisions, redesign and check grid again.

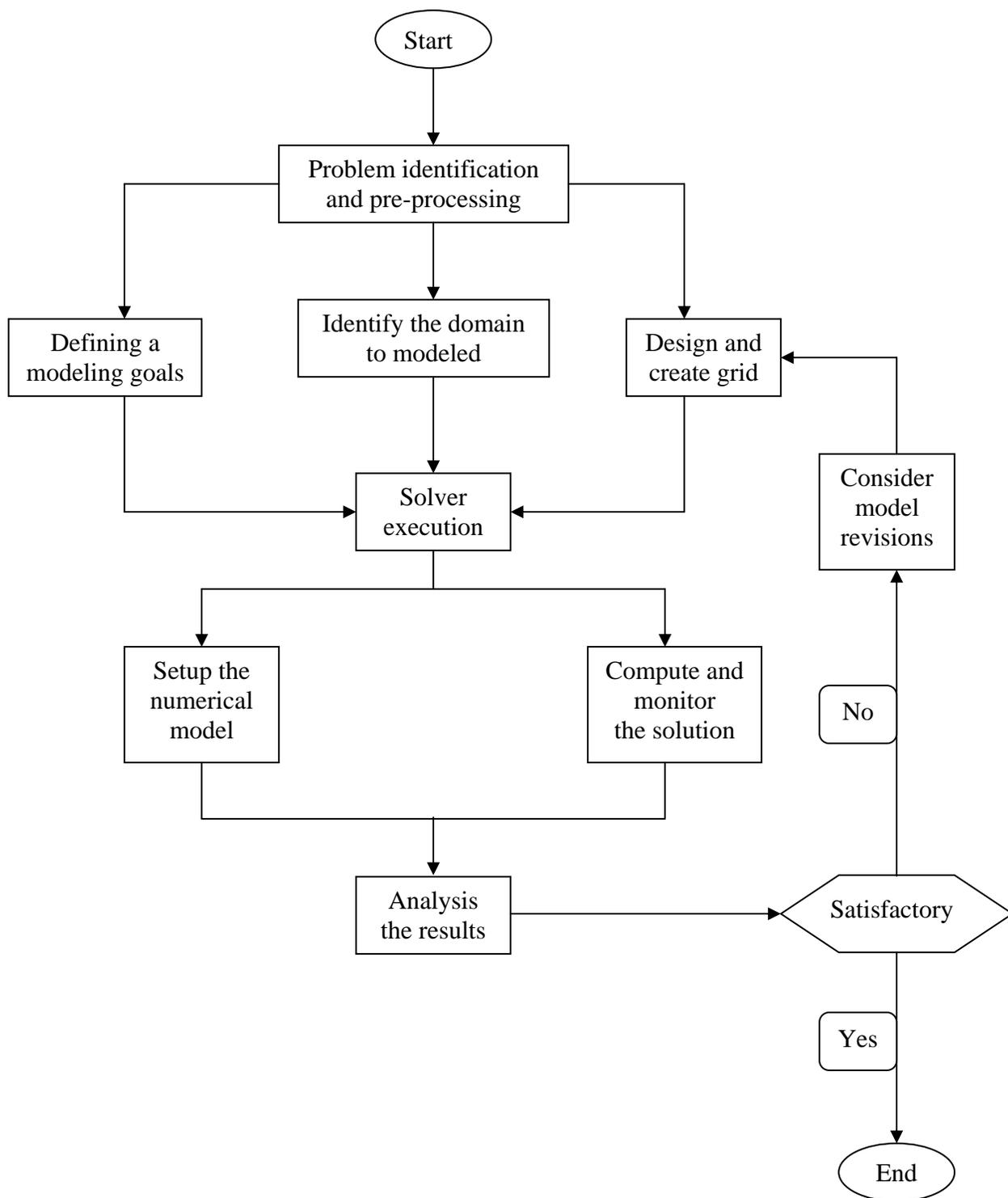


Figure 3.9: Step of CFD analysis

## **CHAPTER 4**

### **RESULT AND DISCUSSION**

#### **4.1 Introduction**

From the experimental work we may collected the data for flue gas, temperature inside the chamber, flame velocity and flame radiation characteristics. Several experiments were run and the result will take. All the data will record in one table. From the simulation part a study of contours was done for flame temperature, velocity vector, and mass fraction of  $O_2$ ,  $CO_2$ ,  $H_2O$  and  $C_3H_8$ . The data will analyze to compare the results from practical combustor and computer simulation. The value of percentage of differences will affect the objective of the research. In this research the lowest percentage is from average temperature in exhaust and the highest percentage is from mass fraction of  $O_2$ . The reason why this happen was done in discussion part. Comparison between experiment data and simulation data was recorded in Table 4.2.

## 4.2 Experimental Results

Experiment was run in three times. Average result were taken and use as boundary setting in simulation process. Table 4.1 shows the data collected from experimental work. In this experiment, air and fuel flow rate was set to 117.05 m<sup>3</sup>/hr and 3.79 m<sup>3</sup>/hr. All the data during combustion process were recorded in Table 4.1.

Table 4.1: Average data collected from experimental work

<b>Experiment characteristics</b>	<b>Average result</b>
Gas flow rate (m <sup>3</sup> /hr)	3.79
Air flow rate (m <sup>3</sup> /hr)	117.05
Gas flow rate (kg/hr)	6.82
Air flow rate (kg/hr)	136.95
Gas pressure (cmH <sub>2</sub> O)	11
Air inlet temperature t <sub>3</sub> (C )	21
Exhaust temperature t <sub>4</sub> ( C )	777
O <sub>2</sub> (%)	4.6
CO <sub>2</sub> (%)	10.7
CO (ppm)	12
NO (ppm)	2
H <sub>2</sub> (ppm)	542
Excess air (%)	28.7
Flame temperature (C )	1274
Flame length (cm)	64
Efficiency net (%)	63.9

### 4.3 The Simulation Results

Figure 4.1 show the temperature contours at constant  $C_p$ . The lowest temperature is at 300 K. While the highest temperature is at 3200 K. When combustion start the temperature is around 1300 K until 1800K. This is because the combustion is not complete yet. When the combustion was complete the temperature is around 2760 K until 3200 K.

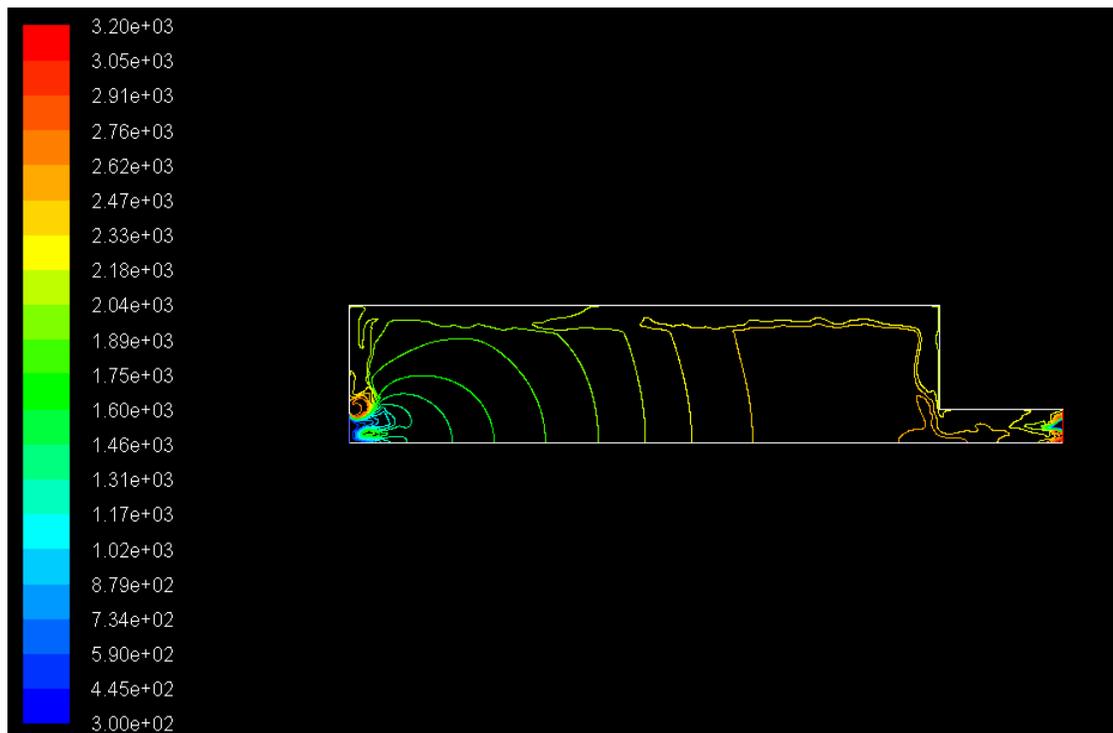


Figure 4.1: Temperature contours at constant  $C_p$ , K

Figure 4.2 show the temperature contours at variable  $C_p$ . The lowest temperature is 300 K and the highest temperature is 2260 K. In the early combustion the temperature is around 986 K. At the exhaust the temperature is mix from 590 K until 2260 K. Overall temperature along the chamber is around 1180 K until 1570 K.

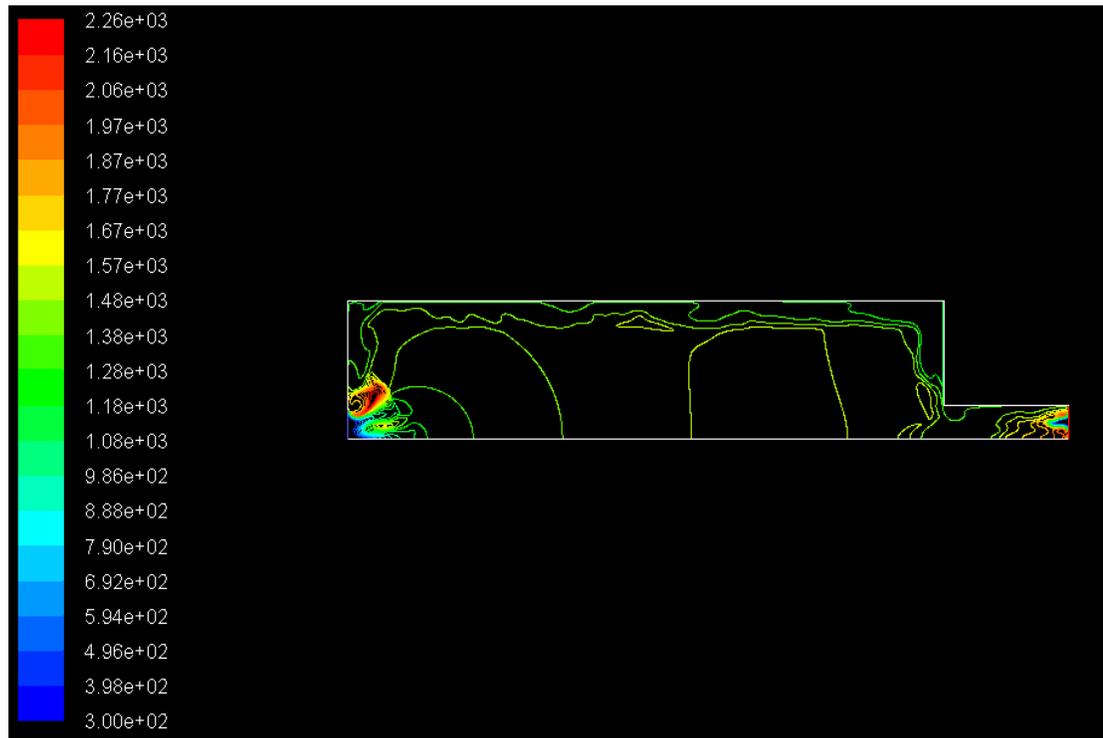


Figure 4.2: Temperature contours at variable  $C_p$ , K

Figure 4.3 show the contours of specific heat,  $C_p$ . The lowest specific heat is 1010 J/kg.K. The highest specific heat is 2310 J/kg.K. At the early combustion the  $C_p$  is around 1600 J/kg.K. Along the chamber, the  $C_p$  is increasing from 1790 J/kg.K to 1990 J/kg.K.

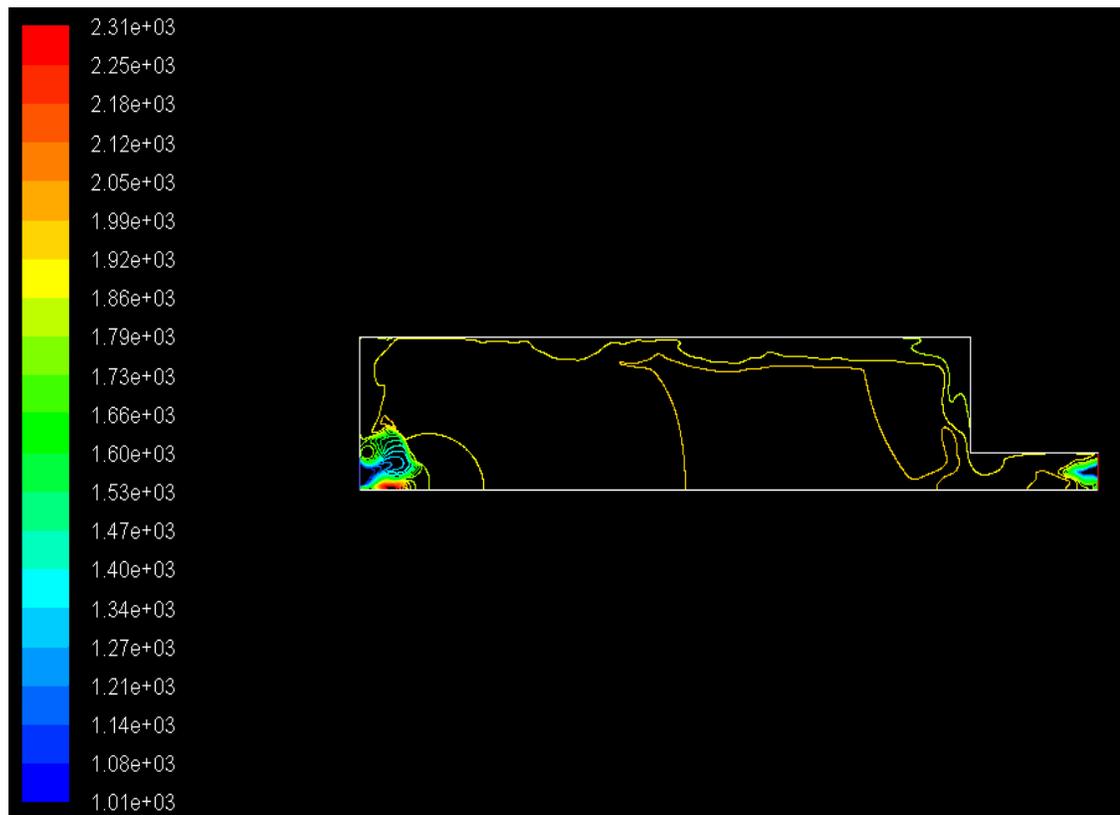


Figure 4.3: Contours of specific heat, J/kg.K

Figure 4.4 show the contours of velocity vector at variable  $C_p$ . The lowest velocity vector is 0.00129 m/s. The highest is 106 m/s. After the combustion, the velocity vector is around 10.6 m/s. When the flow going through the exhaust it increase to 63.3 m/s.

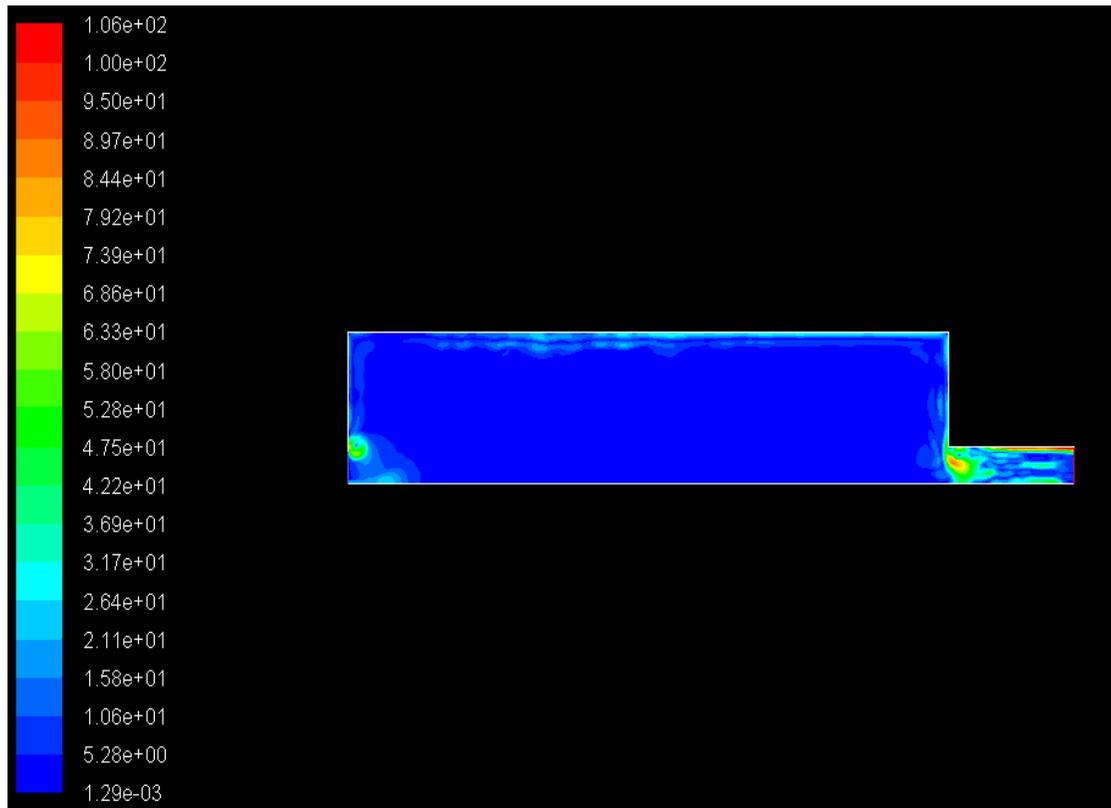


Figure 4.4 Velocity vector (m/s) at variable  $C_p$

Figure 4.5 show the stream function contours at variable  $C_p$ . The lowest value is 0.0000281 kg/s and the highest value is 0.0259kg/s. Along the chamber the value is around 0.0104 kg/s until o.0155 kg/s. The value is increasing above the air flow rate area from 0.168 kg/s until 0.022 kg/s.

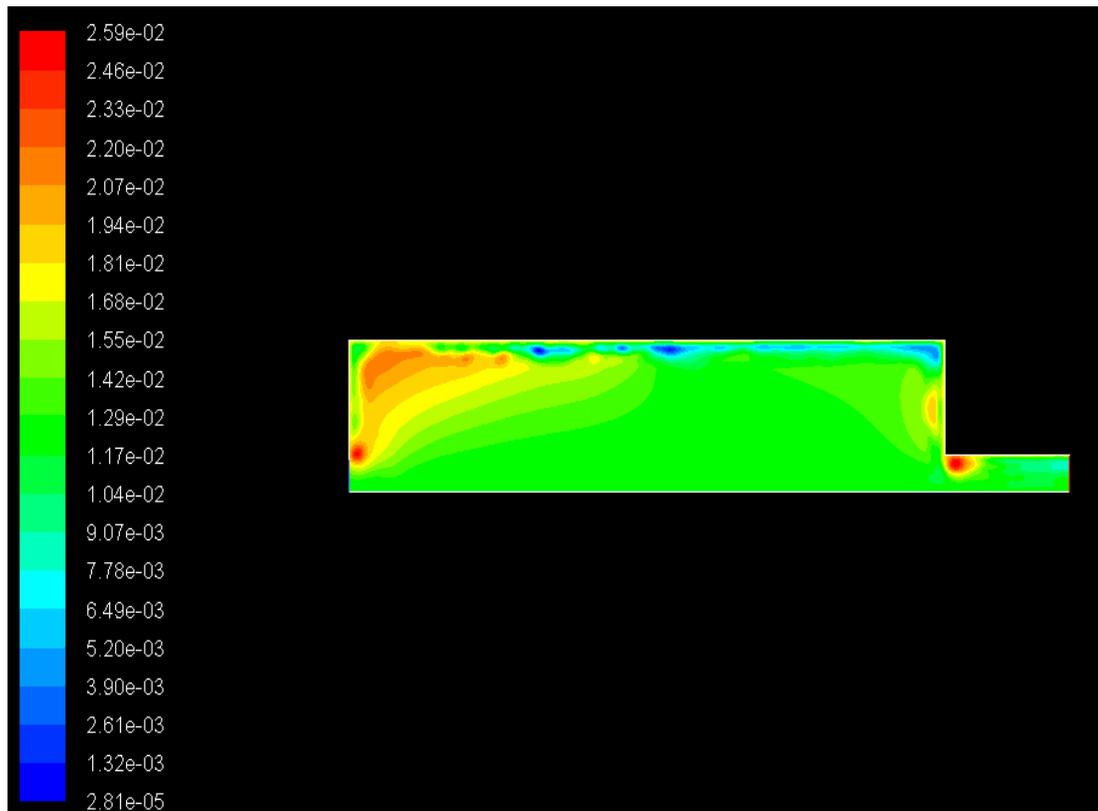


Figure 4.5: Stream function contours (kg/s) at variable  $C_p$

Figure 4.6 show the  $C_3H_8$  mass fraction. The lowest mass fraction is 0.00, after the combustion. The highest mass fraction is 1.00, at the fuel inlet. Along the chamber it show the mass fraction is around 0.25 until 0.30. The mass fraction at the exhaust is 0.00 because of complete combustion.

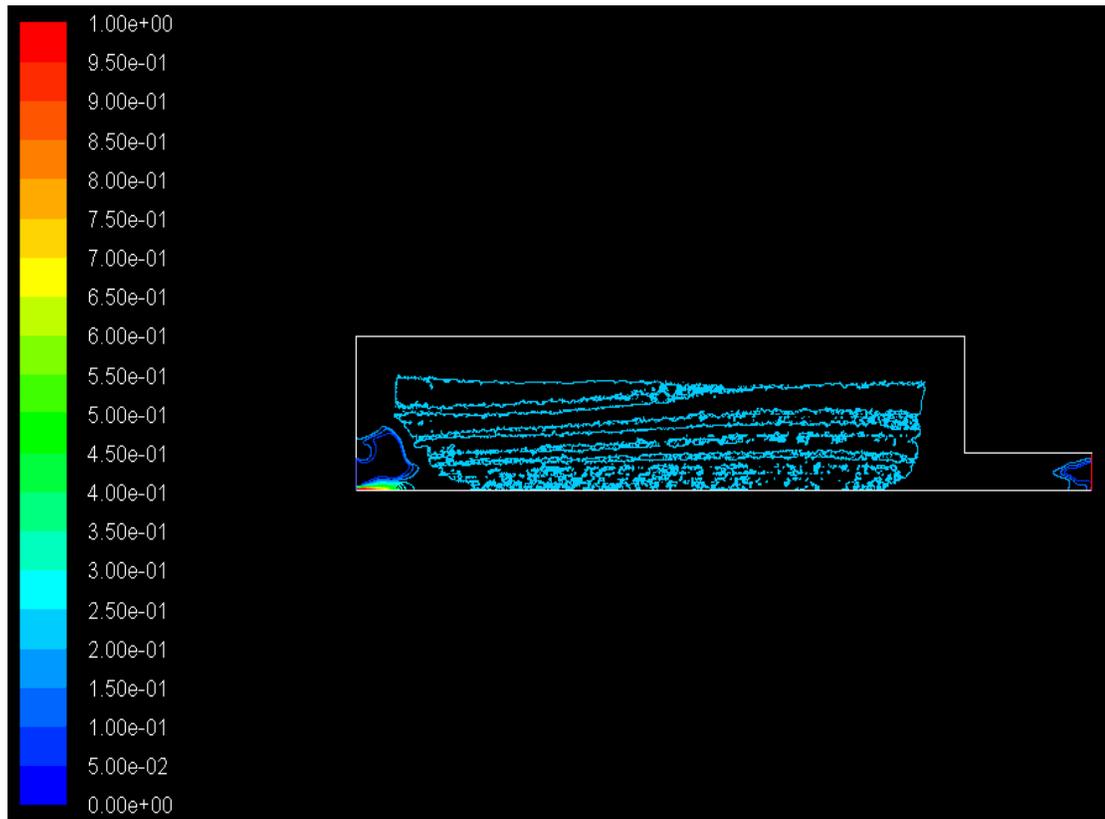


Figure 4.6:  $C_3H_8$  mass fraction

Figure 4.7 show the mass fraction for CO<sub>2</sub>. The lowest mass fraction is 0.00 and the highest mass fraction is 0.137. At early combustion process, less CO<sub>2</sub> produce. At the end of the combustion process, more CO<sub>2</sub> produce. Average mass fraction of CO<sub>2</sub> at the exhaust is 0.0823.

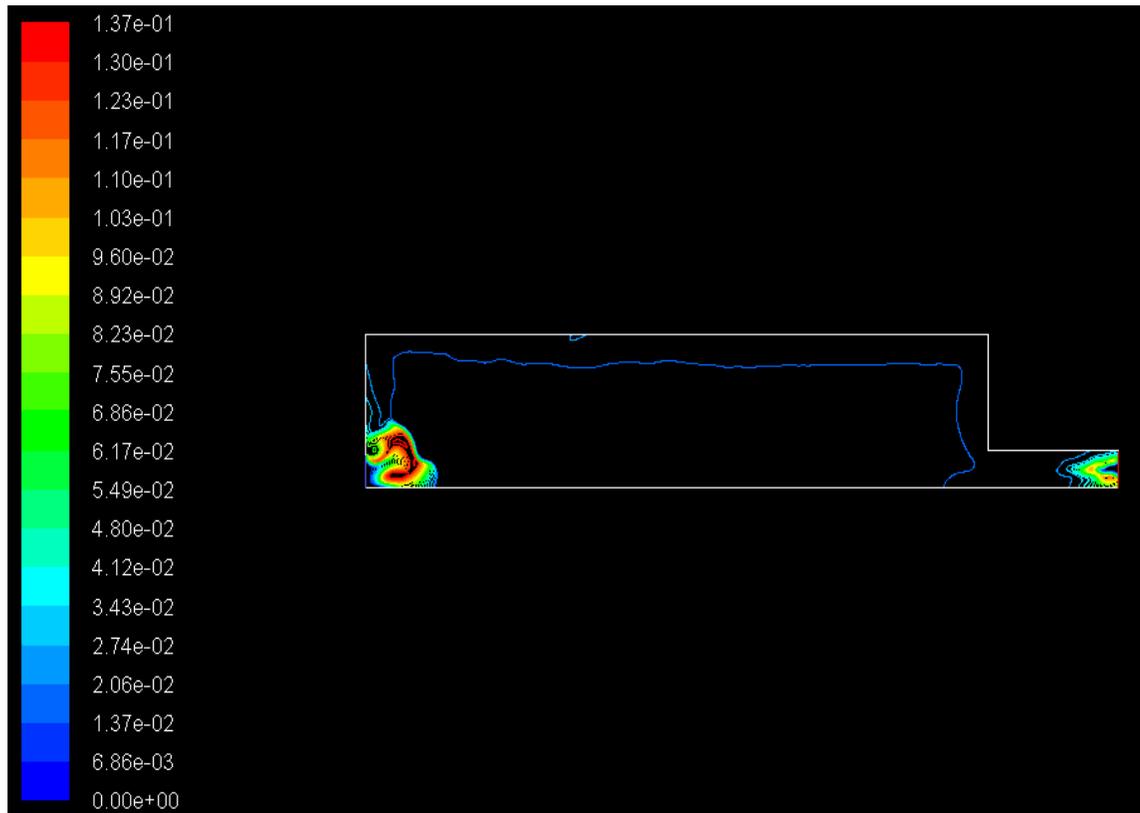


Figure 4.7: CO<sub>2</sub> mass fraction

Figure 4.8 show the mass fraction of H<sub>2</sub>O. The lowest value is 0.00 and the highest value is 0.075. At the early stage of combustion process less H<sub>2</sub>O produce. While the combustion going through the chamber more H<sub>2</sub>O produce. Average mass fraction of H<sub>2</sub>O at exhaust is about 0.055.

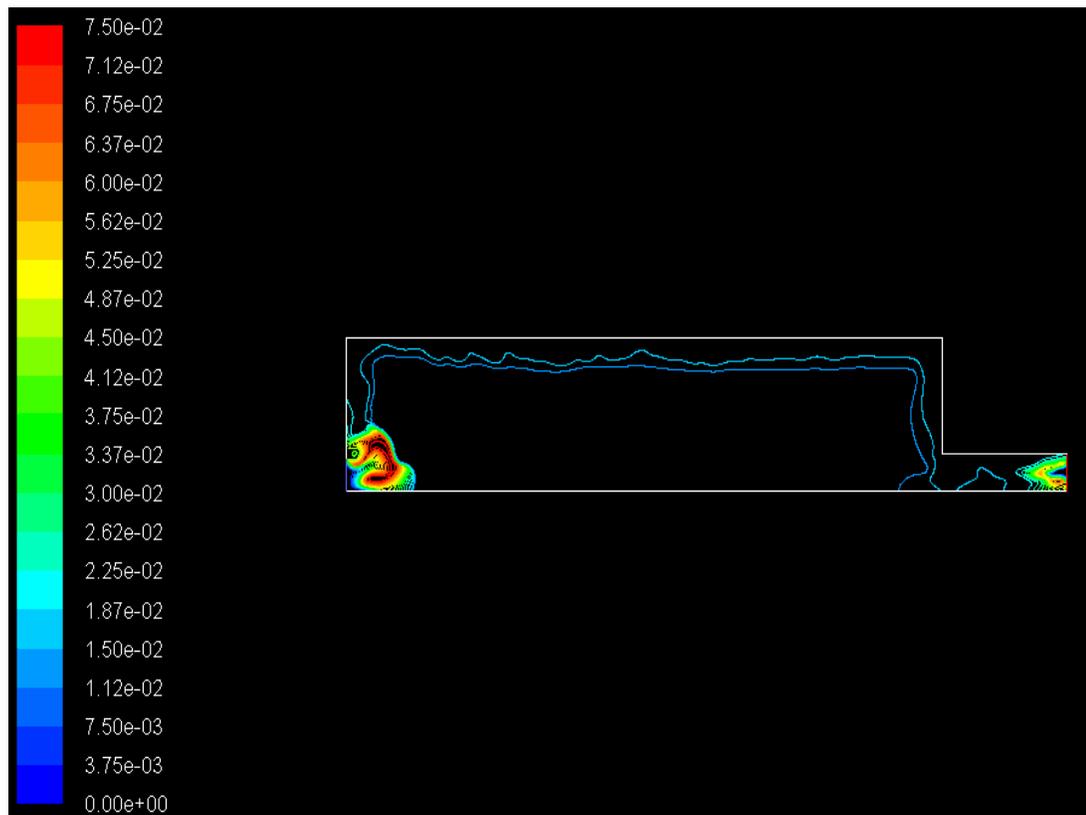


Figure 4.8: H<sub>2</sub>O mass fraction

#### 4.4 Comparison Data

In the end of the research, the data collected from experimental work will compare with the data collected from simulation process. The difference between these two data was present in percentage. Table 4.2 shows the comparison data and its percentage. From the table, exhaust temperature gives a smaller value of percentage compared to the other data. The highest percentage is for mass fraction of O<sub>2</sub> which is 41.92%. The reason for non-consistent percentage is because the efficiency of the equipment is much smaller than expected. From Table 4.1, it shows that the efficiency is only 63.9%. If the value is arranged 85% to 99%, maybe a better result can be achieved. Human errors also occur when running the experiment and simulation. First of all, the experimental set up must follow the right procedure. The timing must be balanced for each of the three experiments when taking the reading. Gas analyzer was used to take the reading for flue gas concentration. The efficiency of this analyzer will decrease when it is used more often in laboratory experiments. So that is because the percentage difference of concentration for some species in flue gas is too high in Table 4.2. In simulation process, the setting for boundary conditions is not accurate as the original design. Some data have to be changed to make the simulation much easier to run. To get an accurate result, the practical combustor model C492 has to be designed in three dimensions (3D). By the way, the result can be accepted because the value of percentage difference is around 10%.

Table 4.2: Comparison data between experimental work and simulation process.

Characteristics	Experimental data	Simulation data	Percentage difference, %
Exhaust temperature, K	1050	1139.6781	8.5
O <sub>2</sub> , %	0.046	0.065285072	41.92
CO <sub>2</sub> , %	0.107	0.126655266	18.36
CO, ppm	12	14.11261	17.61
NO, ppm	2	2.732109	36.61
H <sub>2</sub> , ppm	542	610.2134	12.59



## **CHAPTER 5**

### **CONCLUSION AND RECOMMENDATION**

#### **5.1 Introduction**

This work has addressed numerous facets of furnace and combustion of propane gas in experimental study and simulation approaches. Numerical study included the modeling of the two dimensional transient analysis on effects of boundary conditions. This chapter summarizes the important finding from the work carried out in this research. It also includes some suggestions for further work in each of the areas covered during this research.

## **5.2 Conclusions**

The aim of this thesis was to develop a CFD simulation to predict combustion performance for propane gas in term of emissions, flame temperature, velocity vectors and concentration of the combustion products, and validate with experimental data. This were achieved by critical investigation of existing methods and understand the concept of combustion process flow using combustion lab unit study applied new techniques of data collections for boundaries data. Previous and recent of numerous researchers still explore and study of this area using variety techniques to protect the poor fuel consumption and emission level.

### **5.2.1 CFD Modeling**

The transient analysis of dynamic mesh was successfully investigated with the CFD code, Fluent. The concept predicted of the CFD model validation has been defined in this thesis. The CFD model is used for the flow analysis two dimensional. The operating and boundary condition measured experimentally with the adjustment of gas flow rate and air flow rate. This research is significantly important to understand the characteristic of combustion process. This is important on designing new furnace in industrial work.

## **5.3 Recommendation for Future Research**

There is still scope for the further study to improve the accuracy of the prediction of the combustion process analysis. This section describes some of the possibilities for extending the work investigated in this study, based on the obtained

results and observations. This would greatly improve and produce new knowledge and confidence in this area to researcher. The first and foremost recommendation for the future work would be extended between fired at the various operating conditions such as:

- i) Further investigation is necessary on the experimental and simulation determination of parameters such operating pressure and temperature.
- ii) Visualizations results compared with experimental using laser application to measure velocity vector.
- iii) The present current methods can be advance investigated to extend its applicability to the multidisciplinary optimization.

## REFERENCES

- [1] R. Mancini, M. Weber, U. Boolettini, Predicting NO<sub>x</sub> emission of a burner operated in flameless oxidation mode, Proc. Combust. Isnt. 29 (2002).
- [2] Gas Turbine Combustion Second Edition, Authur H. Leferb
- [3] W. Blasiak, W. Yang, N. Rafidi, Physical properties of a high temperature flame of air and Propane on a regenerative burner, Combust Flame. 136 (2004)
- [4] G. Loffler,R. Sieber,M. Harasek, H. Hofbaur, R. Hauss and J. Landauf Institute of chemical engibeering, Viena University of Technology, Getreidemarkt , Austria.
- [5] G. Loffler,R. Sieber,M. Harasek, H. Hofbaur, R. Hauss and J. Landauf Institute of chemical engibeering, Viena University of Technology, Getreidemarkt , Austria.
- [6] Background Information Document For Industrial Boiler, EPA Contact No. EHSD 7136, Engineering Science. Washington DC, (1983)
- [7] Background Information Document For Small Steam Generating Units, US environmental ProtectionAgency, (1987).
- [8] A. Ka Gupta, S. Bolz, T. Hasegawa, Effect of air preheat temperature and oxygen concentrationon flame structure and emission, J, EnergyResuorc. Technol. 121 (1999)

- [9] D. L. Bauch, D. D. Drysdall, D. G. Horne, Evaluated Kinetic Data for High Temperature Reaction, (1973).
- [10] Peeters T. Phd Thesis, Delft Technical University, Netherlands, (1995).
- [11] Gheoghe Lazaroiu, Department of Power Plant, University Polytechnic of Bucharest, Romania.
- [12] T. Furuhashi, S. Tanno and T. Nakajima, Department of Chemical Engineering, Japan.
- [13] Patankar S V. Numerical Heat Transfer and Fluid Flow, (1980)
- [14] Weihong Yang and Blasiak, Department of Material Science and Engineering, Royal Institute of Technology, Sweden.

**APPENDIX A****A1 Safety Data Sheet for Propane**

Commercial Propane

**Shell Malaysia*****Safety Data Sheet***

Issued: September 24, 1996

SDS No. DMC04022

**Liquid Petroleum Gas**

## 1. IDENTIFICATION OF THE SUBSTANCE/PREPARATION AND COMPANY

<b>Product name:</b>	Shell Gas
<b>Product code:</b>	16666
<b>Product type:</b>	Liquefied petroleum gas
<b>Supplier:</b>	Shell Malaysia Trading Sdn. Bhd/ Shell Timur Sdn. Bhd.
<b>Address:</b>	Bangunan Shell, Damansara Heights, 50490 Kuala Lumpur
<b>Contact numbers:</b>	
<b>Telephone:</b>	03-251-2118

Telex: MA 31813  
 Fax: 03-251-2880

**Emergency telephone number:**

Toll free 1 800 88 3899

2. COMPOSITION/INFORMATION ON INGREDIENTS

**Synonyms:** Liquefied Petroleum Gas, LPG  
**Preparation description:** Complex mixture of hydrocarbons consisting predominantly of propane C3 and butane C4 hydrocarbons with low amount of others in the C1-C7 range. Low concentrations of sulphur, hydrogen sulphide and mercaptans may be present. It may also contain one or more of the following additives: odourants (usually ethyl mercaptan), anti-icing agents. 1,3-butadiene, classified as a Category 2 carcinogen, may be present at a concentration of less than 0.5 %(m/m).

**Dangerous components/constituents:**

Component name	CAS number	Content range	EC hazard	R phrases
Petroleum gases, liquefied	68476-85-7	>99 %(m/m)	F+	R12
1,3-butadiene	106-99-0	<0.5 %(m/m)	F+, Carc Cat 2	R12-45

Note: Dangerous Substances Directive, 67/548/EEC, Annex I numbers for the above substances are 649-202-00-6 and 601-013-00-X.

Contains the following substances for which exposure limits apply: liquefied petroleum gas, butane, 1,3-butadiene, hydrogen sulphide, ethyl mercaptan.

### 3. HAZARDS IDENTIFICATION

<b>Human health hazards:</b>	Prolonged exposure to vapour concentrations may affect the central nervous system. May cause frost burns due to low boiling point.
<b>Safety hazards:</b>	Extremely flammable liquefied gas. The vapour is heavier than air, spreads along the ground and distant ignition is possible.
<b>Environmental hazards:</b>	No specific hazards under normal use conditions.

### 4. FIRST AID MEASURES

<b>Symptoms and effects:</b>	Liquid may cause skin and eye burns. Prolonged exposure to vapour concentrations above the recommended occupational exposure standard may cause headache, dizziness, weakness, nausea, confusion, blurred vision, asphyxiation, cardiac irregularities, unconsciousness and even death.
<b>Protection of first aiders:</b>	Take appropriate steps to avoid fire, explosion and inhalation hazards.
<b>First Aid - Inhalation:</b>	Remove to fresh air. Keep warm and at rest. If the casualty is stuporous, some physical restraint may be necessary to prevent injury. If breathing but unconscious, place in the recovery position. If breathing has stopped, apply artificial respiration. If heartbeat absent give external cardiac compression.) Monitor breathing and pulse. OBTAIN MEDICAL ATTENTION IMMEDIATELY.
<b>First Aid - Skin:</b>	Drench affected parts with water. Remove contaminated clothing, rings, watches, etc., if possible, but do not attempt to do so if they are adhering to the skin. Do not attempt to reheat the affected parts rapidly - reheat slowly. Cover with a sterile dressing. Do not

apply ointments or powders. Note that contaminated clothing may be a fire hazard. Contaminated clothing should be soaked with water before being removed. It must be laundered before reuse.

**First Aid - Eye:**

DO NOT DELAY. Flush eye with copious quantities of water. Cover eye with a sterile dressing. OBTAIN MEDICAL ATTENTION IMMEDIATELY.

**First Aid - Ingestion:**

In the unlikely event of ingestion, obtain medical attention immediately.

**Advice to physicians:**

Treat symptomatically.

5. FIRE FIGHTING MEASURES

**Specific hazards:**

Hazardous combustion products may include: carbon monoxide, oxides of nitrogen, oxides of sulphur, unburnt hydrocarbons. The vapour is heavier than air, spreads along the ground and distant ignition is possible. Sustained fire attack on vessels may result in a Boiling Liquid Expanding Vapour Explosion (BLEVE).

**Extinguishing media:**

Shut off supply. If not possible and no risk to surroundings, let the fire burn itself out. Large fires should only be fought by properly trained fire fighters. Dry powder, carbon dioxide may be used for small fires. Water fog should be used to assist the approach to the source of the fire. All containers subject to fire or to radiant heat should be cooled by spraying with water.

**Unsuitable extinguishing media:**

Water in a jet. Use of Halon extinguishers should be avoided for environmental reasons.

**Other information:**

Keep adjacent containers cool by spraying with water. All storage areas should be provided with adequate fire fighting facilities.

## 6. ACCIDENTAL RELEASE MEASURES

<b>Personal precautions:</b>	Vapour can travel along the ground for considerable distances. Remove all possible sources of ignition in the surrounding area and evacuate all personnel. Shut off leaks, if possible without personal risk. Do not enter confined spaces. Ventilate contaminated area thoroughly. Do not breathe: vapour. Avoid contact with: skin, eyes and clothing. Take off immediately all contaminated clothing - but do not attempt to do so if clothing adhering to the skin. Contaminated clothing may be a fire hazard and therefore should be soaked with water before being removed.
<b>Personal protection:</b>	Wear: monogoggles, neoprene or nitrile rubber gloves, safety shoes or boots.
<b>Environmental precautions:</b>	No specific measures.
<b>Clean-up methods - small spillage:</b>	Allow to evaporate. Do not disperse liquid using water.
<b>Clean-up methods - large spillage:</b>	Attempt to disperse the vapour or to direct its flow to a safe location, for example by using water fog sprays. Otherwise treat as for small spillage.
<b>Other information:</b>	Test atmosphere for vapours to ensure safe working conditions before other personnel are allowed into the area. Local authorities should be advised if significant spillages cannot be contained. Observe all relevant local regulations.

## 7. HANDLING AND STORAGE

<b>Handling:</b>	This product is intended for use in closed systems only. Do not use in confined areas.
------------------	--

<b>Storage:</b>	<p>When using do not eat, drink or smoke. Do not breathe: vapour. Take precautionary measures against static discharges. Use cylinders in the upright position only - unless specially designed for use in other orientations. Store only in purpose designed pressure vessels or cylinders. Store outdoors or in adequately ventilated storerooms. Locate tanks away from heat and other sources of ignition. Do not store in the vicinity of cylinders containing compressed oxygen. All storage areas should be provided with adequate fire fighting facilities. Keep out of reach of children.</p>
<b>Product transfer:</b>	<p>Electrostatic charges may be generated during pumping. Ensure electrical continuity by bonding all equipment. Avoid contact with equipment in view of the risk of cold burns. Do not use compressed air for filling, discharging or handling.</p>
<b>Tank cleaning:</b>	<p>Cleaning, inspection and maintenance of storage tanks is a specialist operation which requires the implementation of strict procedures and precautions. These include issuing of work permits, gas-freeing of tanks, using a manned harness and lifelines and wearing air-supplied breathing apparatus. Prior to entry and whilst cleaning is underway, the atmosphere within the tank must be monitored using an oxygen meter and/or explosimeter.</p>
<b>Recommended materials:</b>	<p>For containers use: mild steel. For seals and gaskets, use: compressed asbestos fibre, or other materials specifically approved for use with this product. Spirally wound metal gaskets are also suitable.</p>
<b>Unsuitable materials:</b>	<p>With respect to metals, aluminium should not be used if there is a risk of caustic contamination of the product. Certain forms of cast iron are unsuitable. With respect to non-metallic materials, natural rubbers must</p>

**Other information:**

not be used. Nitrile rubbers and certain plastics may also be unsuitable, depending on the material specification and intended use. Ensure that all local regulations regarding handling and storage facilities are followed. Where large quantities of liquefied petroleum gas are stored, emergency and disaster plans must be developed in conjunction with local authorities.

## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

**Engineering control measures:** Use only in well ventilated areas. Provide adequate ventilation in storage areas.

**Occupational exposure standards:** ACGIH threshold limit values are given below. Lower exposure limits may apply locally.

Component name	Limit type	Value	Unit	Other information
Liquefied petroleum gas	TWA	1800	mg/m <sup>3</sup>	
Butane	TWA	1900	mg/m <sup>3</sup>	
1,3-butadiene	TWA	4.4	mg/m <sup>3</sup>	
Hydrogen sulphide	TWA	14	mg/m <sup>3</sup>	
Hydrogen sulphide	STEL	21	mg/m <sup>3</sup>	
Ethyl mercaptan	TWA	1.3	mg/m <sup>3</sup>	

Note: ACGIH - 'Threshold Limit Values for Chemical Substances and Physical Agents and Biological Exposure Indices', American Conference of Governmental Hygienists, Cincinnati, Ohio, 1996 edition.

**Respiratory protection:** Not normally required.

**Hand protection:** Wear neoprene or nitrile rubber gloves. Gloves must maintain flexibility down to the atmospheric boiling point of this product.

**Eye protection:** If splashes are likely to occur, wear: monogoggles, face shield.

**Body protection:** Safety shoes or boots - chemical resistant. If splashes are likely to occur, wear: overalls made of cotton or other natural fibres.

## 9. PHYSICAL AND CHEMICAL PROPERTIES

<b>Physical state:</b>	Liquefied gas
<b>Colour:</b>	Colourless
<b>Odour:</b>	Distinctive and unpleasant if stenching, odourless if unstenched
<b>Boiling point:</b>	circa - 20°C
<b>Vapour pressure:</b>	circa 5.8 bar/ga at 37.8°C
<b>Density:</b>	circa 560 kg/m <sup>3</sup> at 15°C
<b>Vapour density (air=1):</b>	circa 1.5 at 15°C
<b>Flash point:</b>	-104°C
<b>Flammability limit - lower:</b>	2.2 %(V/V)
<b>Flammability limit - upper:</b>	10 %(V/V)
<b>Auto-ignition temperature:</b>	> 450°C
<b>Explosive properties:</b>	In use, may form flammable/explosive vapour- air mixture
<b>Oxidizing properties:</b>	Not applicable
<b>Solubility in water:</b>	Data not available
<b>n-octanol/water partition coefficient:</b>	log P <sub>ow</sub> = 2.3 (estimated value)
<b>Evaporation rate:</b>	Data not available

## 10. STABILITY/REACTIVITY

<b>Stability:</b>	Stable.
<b>Conditions to avoid:</b>	Heat, flames and sparks.
<b>Materials to avoid:</b>	Strong oxidizing agents.
<b>Hazardous decomposition products:</b>	None known.

## 11. TOXICOLOGICAL INFORMATION

<b>Basis for assessment:</b>	Toxicological data have not been determined specifically for this product. Information given is based on data on the components and the toxicology of similar products.
<b>Acute toxicity - oral:</b>	Data not available.
<b>Acute toxicity - dermal:</b>	Data not available.
<b>Acute toxicity - inhalation:</b>	LC <sub>50</sub> >5 mg/l (Gas).
<b>Eye irritation:</b>	Not irritating. Liquid causes cold burns.
<b>Skin irritation:</b>	Not irritating. Liquid causes cold burns.
<b>Respiratory irritation:</b>	Not irritating (Gas).
<b>Skin sensitization:</b>	Not expected to be a skin sensitizer.
<b>Carcinogenicity:</b>	This product has not been evaluated in long-term chronic exposure tests. May contain 1, 3-butadiene, classified as a Category 2 carcinogen at a concentration of less than 0.1% (m/m). Other components are not known to be associated with carcinogenic effects.
<b>Mutagenicity:</b>	Not considered to be a mutagenic hazard (Gas).
<b>Human effects:</b>	See Section 4 for information regarding acute effects to humans.

## 12. ECOLOGICAL INFORMATION

<b>Basis for assessment:</b>	Ecotoxicological data have not been determined specifically for this product. Information given is based on data on the components and the toxicology of similar
------------------------------	--

	products.
<b>Mobility:</b>	Evaporates extremely rapidly from water or soil surfaces. Disperses rapidly in air.
<b>Persistence/degradability:</b>	Oxidizes rapidly by photochemical reactions in air.
<b>Bioaccumulation:</b>	Does not bioaccumulate.
<b>Ecotoxicity:</b>	Low acute toxicity to mammals.
<b>Sewage treatment:</b>	Not applicable.
<b>Other information:</b>	In view of the high rate of loss from solution, the product is unlikely to pose a significant hazard to aquatic life.

### 13. DISPOSAL CONSIDERATIONS

<b>Precautions:</b>	See Section 8.
<b>Product disposal:</b>	Given the nature and uses of this product, the need for disposal seldom arises. If necessary, dispose by controlled combustion in purpose-designed equipment. If this is not possible, contact the supplier.
<b>Container disposal:</b>	Return part-used or empty cylinders to the supplier.
<b>Local legislation:</b>	Environmental Quality Act

### 14. TRANSPORT INFORMATION

<b>UN Number:</b>	1965
<b>UN Class/Packing Group:</b>	2.1, Packing Group not applicable
<b>UN Proper Shipping Name:</b>	Hydrocarbon Gas Mixture, Liquefied, n.o.s. (Propane Mixture)
<b>UN Number (sea transport, IMO):</b>	1965
<b>IMO Class/Packing Group:</b>	2.1, Packing Group not applicable
<b>IMO Symbol:</b>	Flammable Gas
<b>IMO Marine Pollutant:</b>	No
<b>IMO Proper Shipping Name:</b>	Hydrocarbon Gas Mixture, Liquefied, n.o.s. (Propane Mixture)
<b>ADR/RID Class/Item:</b>	2, 4° (b)

<b>ADR/RID Symbol:</b>	Flammable Gas Shunt With Care (RID only)
<b>ADR/RID Kemler Number:</b>	23-1965
<b>ADR/RID Proper Shipping Name:</b>	Mixture C (Trade name: propane mixture)
<b>ADNR Class/Item:</b>	
<b>UN Number (air transport, ICAO):</b>	1965
<b>IATA/ICAO Class/Packing Group:</b>	2.1, Packing Group not applicable
<b>IATA/ICAO Symbol:</b>	Flammable Gas
<b>IATA/ICAO Proper Shipping Name:</b>	Hydrocarbon Gas Mixtures, Liquefied, n.o.s. (Propane Mixture)
<b>Local regulations:</b>	
<b>Other information:</b>	UN Number 1965 is an AEGPL recommendation. Other numbers may be required to be used locally. Transport of this product on passenger aircraft is forbidden.

## 15. REGULATORY INFORMATION

<b>EC Label name:</b>	Contains propane
<b>EC Classification:</b>	Extremely Flammable
<b>EC Symbols:</b>	F+
<b>EC Risk Phrases:</b>	R12 Extremely flammable
<b>EC Safety Phrases:</b>	S2 Keep out of the reach of children.
	S9 Keep container in a well-ventilated place.
	S16 Keep away from sources of ignition - No Smoking.
<b>EINECS (EC):</b>	All components listed
<b>National legislation:</b>	
<b>Other information:</b>	Mobile gas cylinders containing butane, propane or liquid petroleum gas are currently exempt from the labelling provisions of European Commission Directive 67/548/EEC.

## 16. OTHER INFORMATION

<b>Uses and restrictions:</b>	Fuel for use in suitably designed domestic and industrial combustion equipment, domestic cooking appliances and motor vehicles. Also used as an aerosol propellant and a feedstock for the petrochemical industry. This product must not be used in applications other than the above without first seeking the advice of the supplier. Abuse involving repeated and prolonged exposures to high concentrations of vapour ('sniffing') may cause death by either asphyxiation or cardiac arrest. Abuse involving direct ingestion of the liquefied gas may cause death by freezing the larynx and causing the lungs to fill with fluid - an effect similar to drowning.
<b>Technical contact point:</b>	OG BUSINESS
<b>Technical contact number:</b>	03-251-2118
<b>Telephone:</b>	MA 31813
<b>Telex:</b>	
<b>Fax:</b>	03-251-2880
<b>SDS history:</b>	Edition number: 3 First issued: June 18, 1993 Previous revision: April 15, 1996 Revised: September 24, 1996
<b>Revisions highlighted:</b>	Section 2: List of dangerous components added. Section 3 and 7: Editorial changes. Sections 6 and 8: Revised personal protection. Section 12: Estimated ecotoxicity data deleted. Changes indicated by vertical bar to left of text.
<b>SDS distribution:</b>	This document contains important information

to ensure the safe storage, handling and use of this product. The information in this document should be brought to the attention of the person in your organisation responsible for advising on safety matters.

**Other information:**

(To be provided by the supplier)

**References:**

Useful references include the following:

The Institute of Petroleum, London, 'Model Code of Safe Practice', Part 9, current edition.

The Liquefied Petroleum Gas Association Codes of Practice, LPGA.

CONCAWE, Brussels, 'Liquefied petroleum gas'. Product dossier No 92/102, 1992.

UK Health and Safety Executive, 'The Storage of LPG at Fixed Installations', Health and Safety Series Booklet HS(G)34, current edition.

UK Health and Safety Executive, 'The Keeping of LPG in cylinders and Similar Containers', Guidance Note CS4, current edition.

National Fire Protection Association, 'Standard for the Storage and Handling of Liquefied Petroleum Gases', NFPA 58

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not be construed as guaranteeing any specific property of the product.

## APPENDIX B

### B1 Experimental Data

Test characteristics	Test no. 1	Test no. 2	Test no. 3	Average value
Gas flow rate (m <sup>3</sup> /hr)	3.78	3.79	3.80	3.79
Air flow rate (m <sup>3</sup> /hr)	117.25	117.00	116.90	117.05
Gas flow rate (kg/hr)	6.96	6.80	6.70	6.82
Air flow rate (kg/hr)	137.10	136.80	136.95	136.95
Gas pressure (cmH <sub>2</sub> O)	11.6	10.9	10.5	11.0
Air inlet temperature t <sub>3</sub> (C)	20	21	22	21
Exhaust temperature t <sub>4</sub> (C)	778	777	776	777
O <sub>2</sub> (%)	4.7	4.6	4.5	4.6
CO <sub>2</sub> (%)	11	10.5	10.6	10.7
CO (ppm)	12.6	11.9	11.5	12
NO (ppm)	2	2	2	2

H2 (ppm)	542	543	541	542
Excess air (%)	28.4	28.9	28.8	28.7
Flame temperature (C )	1277	1270	1275	1274
Flame length (cm)	69	63	60	64
Efficiency net (%)	63.9	63.8	64.0	63.9