



**MODELLING OF HIGH EFFICIENCY MULTI-FUEL
TWO-STROKE GAS ENGINE SYSTEMS**

By

Farzad Shokrollahihassanbarough

A thesis submitted to
The University of Birmingham
For the degree of
DOCTOR OF PHILOSOPHY

School of Mechanical Engineering
The University of Birmingham
Edgbaston, Birmingham, UK

June 2018

UNIVERSITY OF
BIRMINGHAM

University of Birmingham Research Archive

e-theses repository

This unpublished thesis/dissertation is copyright of the author and/or third parties. The intellectual property rights of the author or third parties in respect of this work are as defined by The Copyright Designs and Patents Act 1988 or as modified by any successor legislation.

Any use made of information contained in this thesis/dissertation must be in accordance with that legislation and must be properly acknowledged. Further distribution or reproduction in any format is prohibited without the permission of the copyright holder.

Abstract

In order to study the knock threshold gaseous fuels, a rapid compression machine (RCM) has been used. As natural gas contains mostly methane as well as small proportions of various hydrocarbons with different weights, this work focuses on obtaining the influences of blending separately various proportions of ethane, propane, butane and finally n-pentane into methane. These fuels were selected to investigate the effects of the high and low methane number (MN) mixtures on the combustion phenomenon of real reciprocating engines.

The idea behind this machine is to better understand different phenomena associated with the operation of internal combustion engines. The evolution of the RCMs and the development of new machines capable of increased control over experimental conditions are essential to the refinement of combustion modelling processes.

An experimental study into the variation of the peak pressure and compression ratio was conducted on the aforementioned mixtures. As the mixture contains a higher proportion of methane, higher driving pressure is required to achieve the knock threshold operating condition. The peak pressure and compression ratio reduce as the methane content in the mixture reduces by blending heavier hydrocarbons; however, the rate of reduction slows down for methane-ethane, methane-propane and methane-

butane mixtures. As pentane is mixed into the methane, the peak pressure and compression ratio decline rapidly and never slow down.

A further investigation into the ignition delay, EOC pressure and temperature has been conducted. The ignition delay of the mixtures varies between 0.6 ms and 0.9 ms at knock threshold operating points, with λ 1.2; except the ignition delay time of methane-pentane mixture which soars rapidly from 1.1 ms to 2 ms. The EOC pressure and temperature decline gradually for the lower proportions of the methane content in the mixture; however, there is a huge drop in the mixture of 8% pentane with 92% methane. Later in the work, the methane number of the mixtures based on the peak pressure and compression ratio have been presented. It identifies that the MN and either Pmax or CR are proportional together, except when the methane is blended with high proportions of ethane in the mixture. A high content of ethane leads to drop the mixture resistance, since the MN calculator is not able to calculate it accurately.

A 1-D engine simulation model has been created in the AVL BOOST to calculate the heat release rate and mass fraction burnt. Special attention has been given to valve timing and piston motion definitions to simulate the RCM in the BOOST platform, as it is not a complete reciprocating engine and the piston stays at its position during the intake and exhaust processes.

Dedication

To my lovely parents Mohammad Ali and Fahimeh

The only sister Fariba and always beloved brother

Fariborz

I dedicate this thesis

With

Love and Respect

Acknowledgment

The completion of this work owes a lot to the contribution and support of so many people in my professional and personal life. This is where I show my gratitude and acknowledge their support which is certainly immeasurable in words.

And foremost, I would like to thank my lead supervisor, **Professor Mirosław L. Wyszynski**, for the eternally guidance, advice and help all through the years of the project. I enjoyed and gained useful experiences during tutoring the master and bachelor students and being teaching assistance for Biofuel and advance thermal courses within these years. I also have had great experience during my secondment at Wartsila in Finland.

I am also eternally grateful of second supervisor, **Professor Athanasios Tsolakis** for his advice and help during the project, especially when I needed some data from the engines laboratory. None of this work would be at all possible without the brilliant help of the barrage of technicians at fuel laboratory at Wartsila Oy (Finland) during my secondment: **Per Lofholm, Juna Leino, Juha-Pekke Sundell**.

I would like to express my deepest gratitude to **Dr Hessam Jahangiri, Dr Soheil Zera'ati, Dr Aydin Sabouri** and **Dr Ali Alqahtani** for their noble and friendly advice. My sincere thanks also go to **Mr. Omid Doustdar** for both technical and emotional supports.

At the end I would appreciate my family, especially my parents (the most important ones in my life). There are no words to express their limitless support, thank you for love and supports given to me over all of these years. Thanks also my brother and sister for endless supports and limitless loves.

This project has partially received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 691232 - Knocky - H2020-MSCA-RISE-2015/H2020-MSCA-RISE-2015.

This thesis was proofread for conventions of language, spelling and grammar by “Janet’s Proofreading Service”.

Table of Contents

Abstract	I
Dedication.....	III
Acknowledgment	IV
Table of Contents.....	VI
List of Figures	XII
List of Tables.....	XIX
List of Abbreviations.....	XX
Chapter 1 – INTRODUCTION.....	1
1.1 Introduction.....	2
1.2 Research Outline.....	2
1.3 Aim of the Study.....	3
1.4 Objectives and Approaches	4
1.5 Thesis Outline.....	5
1.5.1 Chapter 2- Review of Literature	5
1.5.2 Chapter 3- Experimental Setup and Techniques.....	6
1.5.3 Chapter 4- Feasibility of Methane-propane Mixtures’ Combustion Characteristics as a Reference Curve.....	6
1.5.4 Chapter 5- Study of Combustion Characteristics of Methane Blending by Ethane and Butane in an RCM.....	7

1.5.5 Chapter 6- Study of Combustion Characteristics of Blending Pentane in Methane by Using an RCM	7
1.5.6 Chapter 7- Conclusion, and Recommendations for Future Work.....	7
GRAPHICAL ABSTRACT.....	8
Chapter 2 – REVIEW OF LITERATURE	9
2.1 Introduction.....	10
2.2 Fuel Reactivity Investigation Methods.....	12
2.2.1 Shock Tube	13
2.2.2 Flow Reactors	16
2.2.3 Rapid Compression Machine (RCM)	18
2.2.3.1 Overview of the Rapid Compression Machines.....	18
2.2.3.2 Evolution of the Rapid Compression Machines.....	25
2.2.3.3 Chemical Kinetic Studies	28
2.3 Methane Number	32
2.4 Knock Intensity.....	34
2.5 AVL Simulation Overview.....	35
2.5.1 AVL BOOST Review	35
Chapter 3 – EXPERIMENTAL AND SIMULATION SET-UP	39
3.1 Introduction.....	40
3.2 RCM Experiments’ Set-up	41
3.2.1 RCM Specifications	41
3.2.2 Control System, Data Acquisition and Processing	44

3.3 Novel Aspects of RCM.....	45
3.4 Fuel Properties and Fuel Preparation.....	46
3.4.1 Fuel Properties	46
3.4.1.1 Methane	47
3.4.1.2 Ethane	47
3.4.1.3 Propane	48
3.4.1.4 Butane.....	48
3.4.1.5 N-pentane	48
3.4.2. Fuel Preparation	49
3.5 Piston Motion and Volume and Compression Ratio in the RCM	52
3.6 Air and Fuel Induction Methods.....	54
3.6.1 Non-premixed Air-fuel Injection	55
3.6.2 Premixed Mode Premixed Air-fuel Mixing in the Reactor.....	55
3.7 RCM Simulation Setup.....	56
3.7.1 RCM Combustion Model in AVL BOOST	56
3.7.1.1 Predefined Heat Release Method (Wiebe Function).....	58
3.7.1.2 User Defined Heat Release Method (ROHR)	60
3.7.2 Thermodynamic Analysis	64
3.7.3 AVL BOOST Combustion Model Calibration and Validation.....	66
3.8 Experimental Test Procedure.....	68
Chapter 4 - FEASIBILITY OF METHANE-PROPANE MIXTURES'	
COMBUSTION CHARACTERISTICS	70

4.1 Introduction.....	71
4.2 Tests Fuels	73
4.3 Modifications Made to the RCM during the Research.....	74
4.3.1 Combustion Cylinder and Chamber Heating Modification	74
4.3.2 Driving Pressure Accuracy Improvement.....	77
4.3.3 Valve and Check Valve Modification.....	77
4.3.4 Piston Damping Modification.....	78
4.4 Challenges and Limitation Related to the RCM's Performance	78
4.4.1 Ideal and Non-ideal RCM Operation	79
4.4.2 Core Gas.....	80
4.4.3 Effects of Heat Loss on RCM Operation	81
4.5 Test Condition and Test Methods.....	84
4.6 Lambda Investigation based on the Methane-Propane Mixture	85
4.7 Variable Spark Timing	88
4.8 Simulation Assumptions.....	95
4.8.1 Basic Model	95
4.8.2 Inlet and Exhaust.....	96
4.8.3 In-cylinder Modelling	97
4.9 Results.....	99
4.9.1 Simulation and Experimental Results	99
4.9.2 Knock Intensity Results	103

4.9.3 Optimized Methane-Propane Reference Curve	106
4.9.3.1 Pressure Methane-Propane Reference Curve	106
4.9.3.2 Methane Number Reference Curves	111
4.10 Conclusion	114
 Chapter 5 – STUDY OF COMBUSTION CHARACTERISTICS OF	
METHANE BLENDING WITH ETHANE AND BUTANE IN AN RCM.....	
5.1 Introduction.....	117
5.2 Tested Fuels and Fuel Properties	118
5.3 Test Conditions and Test Methods	119
5.4 Experiment Conditions	120
5.5 Results and Discussion	121
5.5.1 Methane-ethane Mixtures	121
5.5.2 Methane-butane Mixtures	129
5.5.3 Pressure Methane-ethane and Methane-butane Reference Curves	136
5.5.4 Compression Ratio Methane-ethane and Methane-butane Reference Curves	138
5.5.5 Methane Number Reference Curves	140
5.6 Conclusion	143
 CHAPTER 6 – STUDY OF COMBUSTION CHARACTERISTICS OF	
BLENDING N-PENTANE IN METHANE BY USING AN RCM.....	
6.1 Introduction.....	145
6.2 Tested Fuels and Fuel Properties	146

6.3 Experimental Methods.....	149
6.4 Results and Discussion	153
6.4.1 Methane-pentane Reference Curve	164
6.4.2 Methane Number Reference Curves	166
6.5 Conclusion	168
CHAPTER 7 – CONCLUSION AND FUTURE WORKS.....	170
7.1 Conclusion	171
7.2 Recommendations for Future Works.....	176
List of Publications.....	178
References	179
APPENDIX A	195

List of Figures

Figure 2-1 Schematic of shock tube operation (Quinn and Kontis 2013).....	13
Figure 2-2 Wave system in the shock tube and typical non-reactive pressure measurements showing testing time (Campbell, Wang et al. 2015)	14
Figure 2-3 Pressure history and CH-band emission for Decane, 5.0MPa, 885 K, stoichiometric (Campbell, Wang et al. 2015).....	15
Figure 2-4 Schematic of flow reactor (Beerer, McDonnell et al. 2009)	16
Figure 2-5 ignition delay definition using laser and light output in flow reactor (Beerer, McDonnell et al. 2009).....	17
Figure 2-6 n-dodecane ignition delay times over wide temperature conditions in an RCM and shock tubes (Allen 2012).....	19
Figure 2-7 Schematic of RCM operation (Mittal and Sung 2007).....	21
Figure 2-8 Typical pressure trace in the RCM showing ignition delay time definition (Materego 2015).....	23
Figure 2-9 Typical operational boundaries of shock tube, flow reactor and RCM for iso-octane (Materego 2015).....	24
Figure 2-10 summary tested conditions in prior investigations published in this literature for different fuels (Materego 2015)	26
Figure 2-11 The graphical overview of the literature on natural gas mixtures for the different targeted pressures and temperatures (Ramalingam, Zhang et al. 2017).....	31
Figure 2-12 interface of the EN 16726 MN Calculation.....	33
Figure 3-1 Rapid Compression Machine (RCM) at Wartsila's Fuel Laboratory	42
Figure 3-2 Rapid Compression Machine (RCM) in Wartsila's Fuel Laboratory	42
Figure 3-3 Interface of the RCM program to control the operation.....	44
Figure 3-4 Stainless steel gas fuel mixing reactor.....	50
Figure 3-5 Displacement measurement instruments in rapid compression machine (RCM) by an incremental displacement component.....	52

Figure 3-6 Stroke sensor signal in displacement measurement in RCM during compression and expansion processes	53
Figure 3-7 Piston motion of the RCM with respect to an real engine piston motion	53
Figure 3-8 Models used in the RCM to produce swirl in the combustion chamber..	54
Figure 3-9 AVL BOOST simulation model	57
Figure 3-10 Key regions required by ROHR as flame development angle ($\Delta\theta_d$), rapid burning rate ($\Delta\theta_b$), shown as mass fraction burnt curve (Heywood 1988).....	60
Figure 3-11 An example of general pressure trace and ROHR and combustion duration from RCM results at knock combustion.....	61
Figure 3-12 AVL BOOST calibration algorithm	67
Figure 4-1 Trace heating cable system spinning through the outer surface of the RCM cylinder.....	75
Figure 4-2 First test of temperature behavior of the pre-heating system in RCM, setting points of 110 °C and 75°C, without a trace heating cable.....	76
Figure 4-3 Temperature test behaviour of pre-heating system in the RCM, only with a trace heating	76
Figure 4-4 Temperature stabilizing tests of pre-heating system in RCM with setting points of 93°C and 80°C, with initial trace heating.....	76
Figure 4-5 Piston motion creates roll up vortex during compression in lower section and containment of boundary layer through a crevice (upper section) through proper design (Sung and Curran 2014).....	82
Figure 4-6 Comparison of predicted temperature fields at 10.4ms from the end of compression for N ₂ gas using creviced and non-creviced piston heads (Materego 2015)	83
Figure 4-7 Effects of slow and fast flow rate and lean-to-rich mixtures on the peak pressure and ARR.....	85
Figure 4-8 Effects of slow and fast flow rate and lean-to-rich mixtures on the ignition delay time and ARR	86
Figure 4-9 An example of a typical pressure trace of the mixture filling the chamber with a fast flow rate and lambda of 0.81, 1.2 and motored pressure.....	87

Figure 4-10 (a) Piston position (b) calculated compression ratio: of the RCM tests with a spark timing constant of 155 mm aBDC, with blending different propane proportions in the methane.	88
Figure 4-11 Influences of the variable spark timing on ignition delay of the mixture of methane 50% and ethane 50%.....	89
Figure 4-12 An example of the influences of the variable spark timing on the peak pressure since the spark varies from 1 mm bTDC to 20 mm bTDC with the mixture of methane 85% and propane 15%	90
Figure 4-13 An example of influences of the variable spark timing on the peak pressure trace with different driving pressure of 20.5 bar and 22.2 bar in the mixture of 50% methane and 50% ethane; (SC: self-Combustion)	91
Figure 4-14 Detailed initial conditions of the mixture containing 50% methane and 50% ethane for variable spark timings.	92
Figure 4-15 An example of detailed pressure trace (pressure rise due to compression, spark ignition and main combustion) of mixture including 50% methane and 50% ethane.....	93
Figure 4-16 Examples of pressure trace when the spark timing is varied from 2.6 mm bTDC to 20 mm bTDC for the mixture of 50% methane and 50% ethane.....	94
Figure 4-17 A view of the RCM model created in AVL BOOST, identifying the sections of the model (intake and exhaust ducts and cylinder)	95
Figure 4-18 Valve timing profile which is used in the AVL BOOST platform to model the RCM induction and exhaust processes.....	96
Figure 4-19 Piston movement and volume of the cylinder in the RCM, after the piston starts moving rapidly for the mixture containing pure methane	98
Figure 4-20 Approaching the knock threshold operating condition of the mixtures containing: a. pure methane; b. methane 90% and propane 10%; c. methane 80% and 20% propane; and d. methane 70% and 30%.....	100
Figure 4-21 Ignition delay time for the methane-propane mixtures and temperature of the mixtures at the EOC process	101
Figure 4-22 Comparison of the experimental and simulation investigation of the pressure trace and volume of the chamber in the RCM, since the Wiebe mode is used in the combustion model	102

Figure 4-23 Comparison of the ROHR Experimental and simulation investigation for different mixtures of the methane and propane.....	102
Figure 4-24 Procedure used to identify the knocking intensity of the methane-propane mixtures with different driving pressure	103
Figure 4-25 a. In-cylinder pressure, b. spectrum of pulsation and c. knock intensity for pure methane; d. In-cylinder pressure, e. spectrum of pulsation and f. knock intensity for 90% methane mixed in 10% propane	104
Figure 4-26 a. In-cylinder pressure, b. spectrum of pulsation and c. knock intensity for 80% methane plus 20% propane; d. In-cylinder pressure, e. spectrum of pulsation and f. knock intensity for 70% methane plus 30% propane.....	105
Figure 4-27 Summarised peak pressure measurement of the methane-propane mixtures for different methods used to achieve the final smooth reference curve.....	107
Figure 4-28 Summarised compression ratio measured from the methane-propane mixtures for different methods used to achieve the final smooth reference curve..	109
Figure 4-29 Summarized measured peak pressure and calculated MN for the methane-propane mixture tested in the RCM	112
Figure 4-30 Summarized measured compression ratio and calculated MN for the methane-propane mixture tested in the RCM.....	113
Figure 5-1 Approaching to the threshold operating condition of the mixtures containing: a. 98% methane plus 2% ethane; b. 85% methane plus 15% ethane; c. 50% methane plus 50% ethane; and d. pure ethane.....	122
Figure 5-2 Repeatability tests of pressure trace for the mixtures containing of: a. 98% methane and 2% ethane; b. 85% methane and 15% ethane; c. 50% methane and 50% ethane; d. pure ethane	123
Figure 5-3 Detailed pressure (caused by compression, ignition and chemical reaction) of mixtures containing: 98% methane, 2% ethane; 85% methane 15% ethane; 50% methane 50%, ethane and pure ethane	124
Figure 5-4 Peak pressure of the methane with different ethane proportions, since compression ratio increases at knock threshold operating condition	125
Figure 5-5 EOC temperature of the mixtures containing: 98% methane plus 2% ethane; 85% methane plus 15% ethane; 50% methane plus 50% ethane; and pure ethane.	126
Figure 5-6 EOC Pressure for the mixtures containing: 98% methane plus 2% ethane; 85% methane plus 15% ethane; 50% methane plus 50% ethane; and pure ethane.	127

Figure 5-7 Ignition delay of the mixture containing of different proportions of methane and ethane with respect to compression ratio.....	128
Figure 5-8 Rate of heat release for different proportions of methane-ethane mixtures	128
Figure 5-9 Approaching to the threshold operating condition of the mixtures containing: a. methane 99% and butane 1%, b. Methane 97% and butane 3% c. methane 95% and butane 5% d. methane 90% and butane 10%.....	130
Figure 5-10 Repeatability tests of pressure trace for the mixture containing: a. methane 99% and butane 1%; b. methane 97% and butane 3% c. methane 95% and butane 5% d. Methane 90% and butane 10%.....	131
Figure 5-11 Influences of driving pressure on EOC temperature for mixtures containing 99% methane plus 1% butane; 97% methane plus 3% butane; 95% plus methane 5% butane; and 90% methane plus 10% butane	133
Figure 5-12 Influences of driving pressure on EOC pressure for mixtures containing 99% methane plus 1% butane; 97% methane plus 3% butane; 95% plus methane 5% butane; and 90% methane plus 10% butane	134
Figure 5-13 Influences of compression ratio on the peak pressure of the mixtures containing 99% methane plus 1% butane; 97% methane plus 3% butane; 95% methane plus 5% butane; and 90% methane plus 10% butane	135
Figure 5-14 Rate of heat release for different proportions of methane-butane mixtures	136
Figure 5-15 Summary of peak pressure for different proportions of methane-ethane and methane-butane mixtures.....	137
Figure 5-16 Summary of compression ratio for different proportions of methane-ethane and methane-butane mixtures	139
Figure 5-17 Methane Number calculated by two methods (WMN, EN 16726) for methane-ethane and methane-butane W.R.T peak pressure.....	141
Figure 5-18 Summarized calculated compression ratio and calculated MN (WMN, EN 16726) for the methane-ethane and methane-butane mixtures tested in the RCM .	142
Figure 6-1 Mixing tank with valve equipped to inject the liquid n-pentane into the mixing during the process	147
Figure 6-2 N-pentane bottle and syringes for injection to the mixing reactor	147

Figure 6-3 Influence of the higher content of the pentane mixture in the RCM, piston hits the BDC	152
Figure 6-4 Study of the mixture containing 99% methane plus 1% n-pentane: a. approaching to the knock threshold operating condition by adjusting the driving pressure; b. piston motion closed to TDC with adjusting the driving pressure; c. pressure repeatability investigation at knock threshold condition; d. stroke repeatability investigation at knock threshold condition.....	153
Figure 6-5 Study of the mixture containing 98% methane plus 2% n-pentane:.....	154
Figure 6-6 Study of the mixture containing 96% methane plus 4% n-pentane: a. approaching to the knock threshold operating condition by adjusting the driving pressure; b. piston motion closed to TDC with adjusting the driving pressure; c. pressure repeatability investigation at knock threshold condition; d. stroke repeatability investigation at knock threshold condition.....	155
Figure 6-7 Study the mixture containing of 97% methane plus 3% n-pentane; a. approaching to the knock threshold operating condition by adjusting the driving pressure b. piston motion closed to TDC with adjusting the driving pressure c. pressure repeatability investigation at knock threshold condition d. stroke repeatability investigation at knock threshold condition.....	156
Figure 6-8 Study the mixture containing of 92% methane plus 8% n-pentane;.....	157
Figure 6-9 Influences of driving pressure on the compression ratio variation for different mixtures of methane-pentane, approaching to the threshold operating conditions	158
Figure 6-10 Influences of the blending of pentane into methane on ignition delay and temperature for different mixtures of methane and pentane	159
Figure 6-11 influences of the compression ratio on the peak pressure	160
Figure 6-12 influences of driving pressure on the EOC stage for different methane-pentane mixtures, approaching to threshold operating condition.....	161
Figure 6-13 influences of driving pressure on the EOC stage for different methane-pentane mixtures, approaching to threshold operating condition.....	162
Figure 6-14 pressure analysis of different proportions of pentane blended into methane	163
Figure 6-15 Summary of peak pressure and compression ratio of different proportions of methane plus n-pentane mixtures.....	165

Figure 6-16 WMN and EN16726 methane number with respect to the peak pressure data measured in the RCM	166
Figure 6-17 WMN and EN16726 methane number with respect to the compression ratio data measured in the RCM.....	167
Figure 7-1 Summarised reference curve for all tested mixtures in chapters 4, 5 and 6 with respect to Pmax	174
Figure 7-2 Summarised reference curve for all tested mixtures in chapters 4, 5 and 6 with respect to WMN	175

List of Tables

Table 2.1 AVL BOOST elements' trees (Version 2010)	36
Table 3.1 Specification of the RCM in the Wartsila Fuel Laboratory	43
Table 3.2 properties of the gaseous fuels tested in this work with RCM.....	47
Table 4.1 Properties of the gaseous fuels tested in this work with the RCM.....	73
Table 5.1 Properties of the gaseous fuels tested in this work with the RCM.....	118
Table 5.2 Properties of the gaseous fuels tested in this work with the RCM.....	119
Table 5.3 Peak pressure and compression ratio errors occurring during the repeatability test	124
Table 5.4 Calculated errors for the mixture at TDC for pressure trace and compression ratio.....	132
Table 6.1 Properties of n-pentane which was mixed with methane in different proportions.....	146
Table 6.2 Properties of the methane and n-pentane with different proportions	148
Table 6.3 Comparison of the methods used to adjust the methane-n-pentane mixtures	150

List of Abbreviations

AFR	Air-Fuel Ratio
ARR	Accuracy, Repeatability and Reproductively
aTDC	after Top Dead Centre
ARR	Accuracy, Repeatability, Reproducibility
bTDC	before Top Dead Centre
BDC	Bottom Dead Centre
CI	Compression Ignition
CO	Carbone Monoxide
CR	Compression Ratio
DKM	Detailed Kinetic Model
EOC	End of Compression
FS	Fast Feeding
GC/MS	Gas Chromatography/Mass Spectrometry
HC	Unburned Hydrocarbon
IC	Internal Combustion
IDT	Ignition Delay Time
LHV	Low Heat Value
MFB	Mass Fraction Burnt

MN	Methane Number
NTC	Negative Temperature Coefficient
PLIF	Planar laser induced fluorescence
PM	Particulate Matter
RCM	Rapid Compression Machine
ROHR	Rate of Heat Release
SC	Self-Combustion
SF	Slow Feeding
SI	Spark Ignition
SOC	Start of Combustion
t_{50}	Compression Time
TDC	Top Dead Centre
WMN	Wartsila Methane Number

Chapter 1 – INTRODUCTION

1.1 Introduction

The aim of this chapter is to give a brief review of motivation and background of the PhD research investigation accomplished by the author. A portion of this study was devoted to investigate the precise method(s) for testing different gaseous mixtures, so that they will be used as reference data for testing new unknown gases in the rapid compression machine (RCM). The RCM is a technical combustion device which has traditionally been used for investigating fuel ignition kinetics in a well-characterized, zero-dimensional system. The RCM test environment seeks to validate the global behaviour of different mixtures; since the engine is isolated at a prescribed condition (e.g. temperature, pressure, reactant concentration). By considering the objectives of the study, it seems practical to review the available data in the literature to find out the possibility of generating different reference curves according to tested mixtures in real engines.

1.2 Research Outline

The research presented in this thesis was carried out by the author at the fuel laboratory in Vassa (Finland) with the help and support from the Wartsila technicians. The research was mainly conducted to investigate the effects of the various gaseous fuels blended into methane (the highest methane number fuel) on the combustion characteristics, since the RCM is operated at knock threshold operating condition.

The research is described and discussed over three chapters. The first chapter covers the investigation of various mixtures of methane and propane, to accomplish

the best method which can be used for future studies. Then the effects of the propane blended into the methane on the combustion characteristics have been studied. The investigation for this chapter also contains of temperature investigation, lambda adjustment, spark timing, peak pressure and compression ratio and ROHR.

In the next chapter, first various proportions of ethane were blended into the pure methane with the method concluded as defined in Chapter 4. Then, different volumes of butane were mixed into the different pure methane volumes. Here, in this chapter, the effects of (separately) adding ethane and butane on the pure methane were obtained.

In the final chapter, the n-pentane was blended into the pure methane. As n-pentane at room temperature is in liquid form, so it should be individually injected into the mixing reactor. Different methods were investigated to replace the previously used methods; however, two valves were installed between the driving tanks. This helped avoid the piston hitting the bottom of the cylinder after combustion. Then the influences of mixing different proportions of n-pentane in the pure methane were studied.

1.3 Aim of the Study

The influences of the separate blending of different fuels into the pure methane will be studied. Blending heavier hydrocarbon fuel into the methane was conducted to

investigate the possibility of producing different reference curves; so that these curves can be used to specify the unknown fuels, which have not been tested in real engines.

1.4 Objectives and Approaches

The main objective of this research was to study the impact of blending various fuels into pure methane using the RCM, in pursuance of making different reference curves. These curves can specify unknown, either high or low, methane number fuels. A mixing reactor was used to blend the fuels. The pressure also was measured using a Kistler piezoelectric transducer.

The following areas were investigated throughout the author's PhD study:

- The study of the temperature distribution on the RCM combustion chamber
- The effects of flow rate and lambda on the combustion repeatability of the RCM
- The effect of advancing spark timing on the combustion operated by methane-propane
- The effect of blending various proportions of propane into the pure methane on the combustion characteristics of the mixtures operated in the RCM
- The effect of blending (separately) various proportions of ethane and butane into the pure methane on the combustion characteristics of the mixtures operated in the RCM
- The effect of blending various proportions of n-pentane into the pure methane on the combustion characteristics of the mixtures operated in the RCM

The novel idea investigated in this thesis includes:

- Modelling the gaseous mixtures in the RCM, mixtures of gaseous fuels (methane, ethane, propane, butane, n-pentane)
- Investigation of the gaseous blends in the RCM (methane, ethane, butane) mixing the n-pentane and converting it into the vaporised phase and then mixing with the pure methane.
- Installing a spark plug in the head of the cylinder, instead of only compressing the mixture.

1.5 Thesis Outline

The presented work consists of seven chapters for the study of the effect of blending heavier gaseous fuels with methane and investigating the knock threshold operating conditions of those mixtures by using rapid compression machine (RCM). Each chapter of the work is briefly described in following pages:

1.5.1 Chapter 2- Review of Literature

This chapter reviews the literature that is pertinent to this investigation and the literature already published on the topic of combustion characteristics of various fuels tested in the RCM is represented in this chapter. An introduction to the new possible gaseous mixtures for internal combustion engines and especially spark ignition engines is also included in this chapter; and furthermore, achievements of researchers on the study of combustion characteristics of fuels in the RCM are declared.

1.5.2 Chapter 3- Experimental Setup and Techniques

The detailed information concerning the RCM and instrumentation set-up, as well as the detailed information of the data acquisition and recording systems was given in this chapter.

The calculated parameters with respect to the real engine with which the parameters were used, were introduced in this chapter. Finally, the detailed RCM assumptions created in the AVL BOOST with different assumptions (fuel mixtures) are presented.

1.5.3 Chapter 4- Feasibility of Methane-propane Mixtures'

Combustion Characteristics as a Reference Curve

This chapter provides the effects of increasing propane proportions from 0% to 50% in the pure methane; as well as investigating the combustion characteristics of the various proportions of the methane and propane mixtures. As the various mixtures are tested, different driving pressures can be achieved. In the first part, the effects of advancing and retarding spark timing was investigated. In the next part, combustion characteristics of the mixtures have been obtained.

1.5.4 Chapter 5- Study of Combustion Characteristics of Methane Blending by Ethane and Butane in an RCM

In this chapter, two fuels (ethane and butane) were mixed into the pure methane. One is a lighter and one is heavier hydrocarbon fuel, in comparison with the propane used in Chapter 4. This chapter provides the detailed combustion characteristics of the mixtures affected by blending heavier fuels into the pure methane. Finally, the energy released by the mixtures during the combustion was calculated in this chapter.

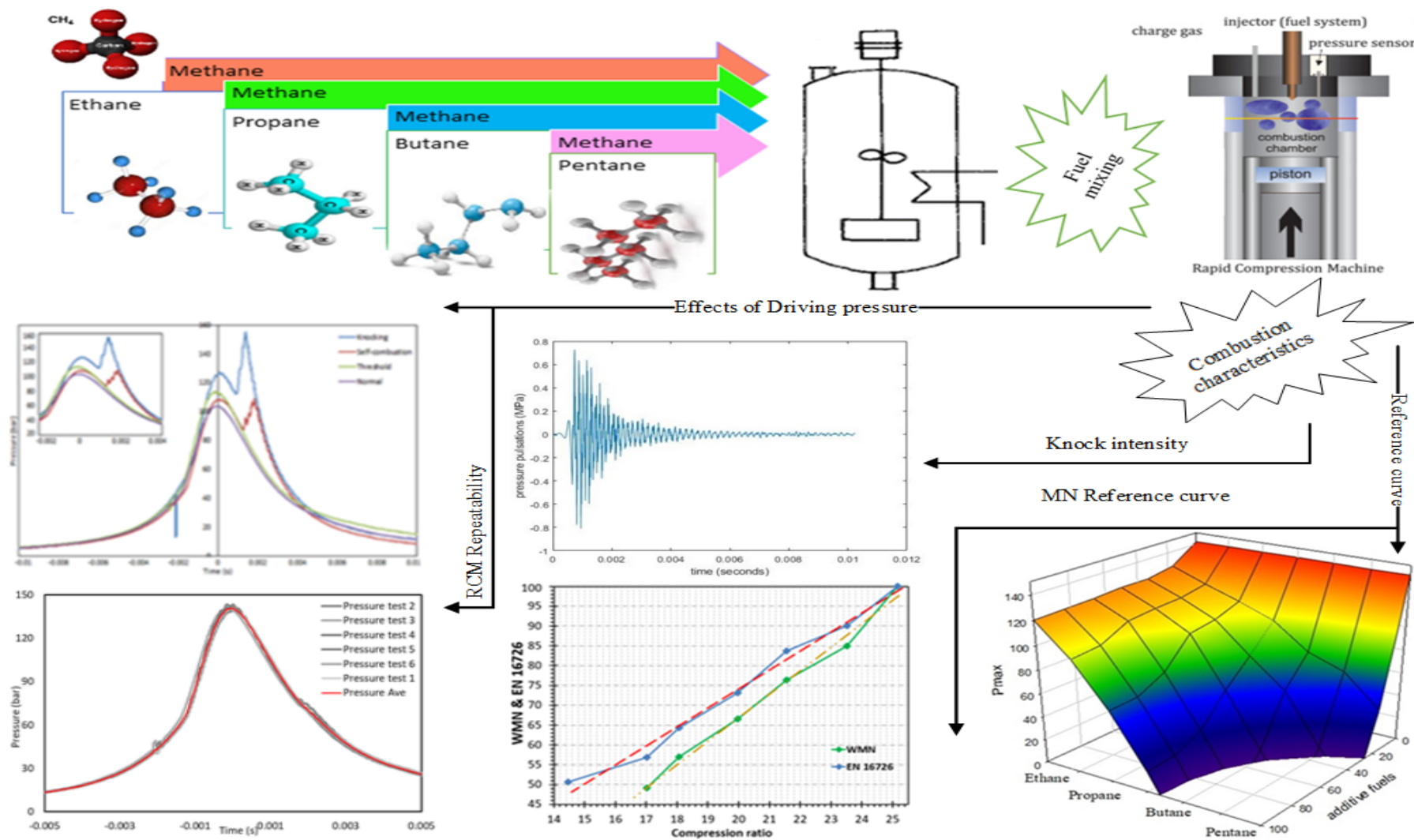
1.5.5 Chapter 6- Study of Combustion Characteristics of Blending Pentane in Methane by Using an RCM

In chapter six, the combustion behaviour of various mixtures of n-pentane and methane was investigated. To provide the mixture, a new technique was used to inject the liquid n-pentane into the mixing tank. Moreover, new methods were investigated to run the RCM based on the n-pentane and methane mixtures. Finally, the mixtures were tested to study the effects of various proportions of the n-pentane and methane mixtures.

1.5.6 Chapter 7- Conclusion, and Recommendations for Future Work

This chapter reviews the research carried out in this investigation and provides the key conclusions of this thesis. Recommendations for future work are then given.

GRAPHICAL ABSTRACT



Chapter 2 – REVIEW OF LITERATURE

2.1 Introduction

The transportation sector has been for many decades the second main consumer of the energy in the world after the industrial sector. Around 27% of the world's total energy consumption is from transportation (Allcott and Wozny 2014, Sieminski 2014); and furthermore, it is increasing by the rate of 1.1% annually according to the Energy Information Administration journal (EIA 2013). The transportation sector is the biggest global consumer of liquid fuels and contributes around 65% of the total growth in the global consumption of liquid fuels (EIA 2013). Petroleum liquid fuels have a higher energy content based on both their volume and mass. They are capable of performing well, available and easy to handle at an affordable price; thus, they predominate in comparison with other fuels (Libert, Spector et al. 2007). Besides, the highly industrialised infrastructure of oil production, transportation and distribution have been developed, and rising global demand as well as political instabilities, especially in the Middle East have stimulated price fluctuations for many years. On the other hand, with an increasing number of fuel suppliers, this will continue to lower prices in the upcoming years. However, the recent political issues regarding US leaving from the international agreements, have caused them to start gradually rising (Conti, Holtberg et al. 2016).

Although the increasing trend of conventional liquid fuels is expected to continue in all sectors, these are one of the main contributors to global warming of the earth; thus, gaseous fuels have been considered by researchers recent years due to their energy content and lower emissions. Global warming, smog formation and acid rain are devastating effects from conventional liquid fuels. According to the consequences

of using these fuels, strict regulations have been introduced throughout the world, to achieve higher engine efficiency, with new, cleaner and sustainable fuels.

Gaseous fuels have been studied recently to investigate their behaviour with different mixtures. These studies help to mimic the results which might occur in real engines based on the fuels' physical and chemical characteristics (Muradov and Veziroğlu 2008).

One of the key basic fuel combustion characteristics which plays an important role in combustion efficiency is auto-ignition. Auto-ignition is an instantaneous exothermic heat release of the fuel, without any influences from external sources after a delay time. Pressure, temperature and mixture concentration can affect the auto-ignition. Thus, the generation of the gaseous fuels is a very attractive proposition; under different conditions it provides a challenge for the new generation fuels and engines (Liu, Zhang et al. 2014, Mitakos 2014, Bradley, Lawes et al. 2015, Nam, Lim et al. 2017).

The knocking phenomenon in SI engines originates from the condition of the end gas which is ignited without external sources, accompanied with a rapid rise and oscillatory pressures which might be very detrimental to the engine. The compression ratio is limited in SI engines by the knocking combustion, limiting fuel efficiency and CO₂ emissions' reduction. Auto-ignition usually occurs at hotspots because of the inhomogeneity of temperature and composition distribution (Heywood 1988,

Bradley, Lawes et al. 2015, Ferguson and Kirkpatrick 2015, Mansfield, Wooldridge et al. 2015). Auto-ignition is characterised using the ignition delay time, which is the time passed from ignition to the onset of the main combustion phase. In general, ignition delay times of non-aromatic hydrocarbons decrease exponentially as the temperature increases. This is true for higher and lower temperature ranges; however, a negative temperature coefficient (NTC) occurs at intermediate temperatures. Accordingly, ignition delay times which are measured during the tests, are characterised for a homogeneous mixture at a given temperature and pressure (Griffiths, Halford-Maw et al. 1993, Pfahl, Fieweger et al. 1996, Griffiths, Halford-Maw et al. 1997, Gersen, Mokhov et al. 2010).

Close to the auto-ignition region, combustion occurs in two stages; after an initial delay, heat is released in a first stage which is known as “cool flame”, it is followed by the main heat release. According to the studies released by Mittal in 2007, aromatic hydrocarbons do not demonstrate NTC behaviour, nor the two-stage ignition phenomenon (Mittal and Sung 2007).

2.2 Fuel Reactivity Investigation Methods

The ignition delay time from the experimental measurements have been used to investigate the auto-ignition behaviour of the fuels. The time during which most of the heat release occurs is called the excitation time and it is of high importance (Lutz, Kee et al. 1989). Ignition delay time is in the range of milliseconds; while the excitation

time is in microseconds and makes the measurements very difficult. Therefore, the excitation time is calculated by using chemical kinetic models.

Ignition delay time measurements in the either real engines or turbines would be extremely difficult to take due to the continually changing conditions and the complex flow fields. Therefore, a relatively simple device was used to investigate the ignition delay time measurements under simpler controllable conditions. For low pressure investigations, constant volume vessels, combustion bombs, and flow reactors have all been used; however, the RCM and shock tubes are suitable for high pressure engines (Materego 2015). Thus, these devices have been introduced as following sections.

2.2.1 Shock Tube

Shock tubes have been used for almost 120 years. The idea of the shock tube first arose from deflagration-detonation transition detection within the flame propagation in tubes by French physicists F. Mallard, H. Le Chatelier, M. Berthelot, and P. Vieille (Fomin 2010). A shock tube allows the study of the high temperature combustion process, since the temperature and pressure can be changed over wide

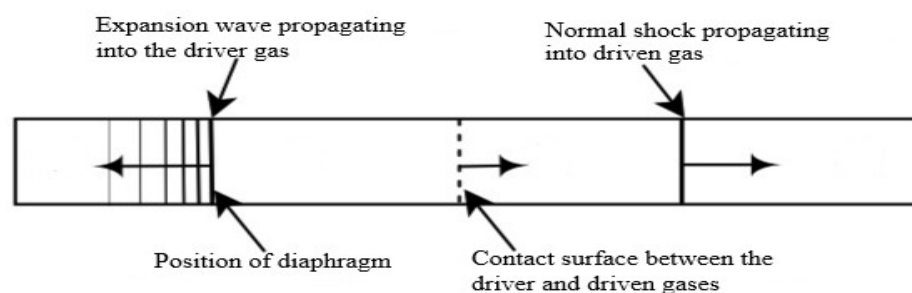


Figure 2-1 Schematic of shock tube operation (Quinn and Kontis 2013)

range. Although the first model of the shock tube was constructed by Vieille in 1899 (Vieille 1899), the British scientists, Payman and Shepherd generally stimulated it in 1937. They continued to design a high pressure “pure” shock tube in which it was initiated by splitting a diaphragm separating gases into high and low pressures sections (Payman and Shepherd 1946). Since then shock tubes have been developed including optical tubes to visualize and record the process inside the shock tube (Pfahl, Fieweger et al. 1996), and now they are employed for studying auto-ignition at high pressure and temperatures (Materego 2015).

A typical shock tube device has been depicted in Figure 2.1. In general, a shock tube has a closed tube which is separated into two sections by a diaphragm, with substantially different pressures. Diaphragms are usually made from cellophane, aluminium, copper or steel, depending on the shock pressure and temperature required (Campbell, Wang et al. 2015)

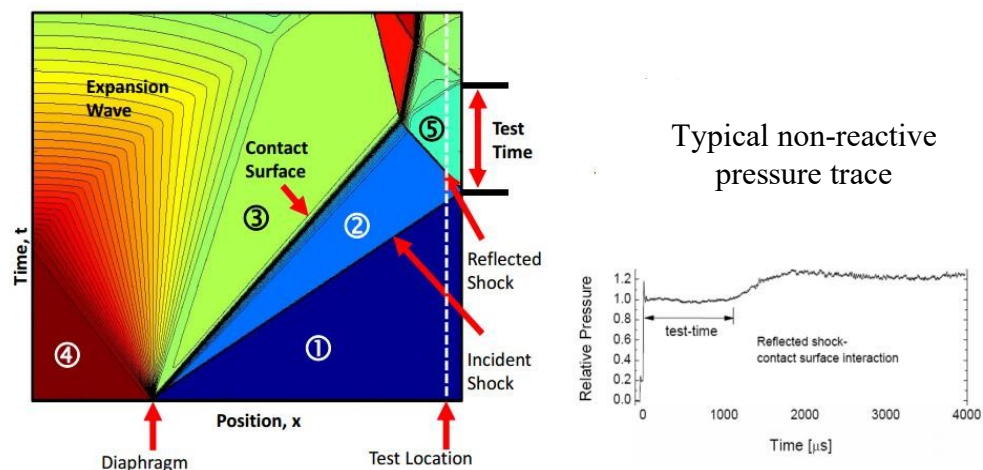


Figure 2-2 Wave system in the shock tube and typical non-reactive pressure measurements showing testing time (Campbell, Wang et al. 2015)

Shock wave theory has been used to investigate the ignition delay in shock tubes. When the diaphragm is broken, it acts as a separator of low and high-pressure sections; thus, the shock wave is generated. First the wave propagates through the low-pressure section and instantaneously compresses the test mixture. The distance created by the incident's shock and the contact surface shows the upper limit of the test time, which can be achieved by the shock tubes, as shown in Figure 2.2. Shock tubes are used to measure the ignition delay up to 1-3 ms (Huang, Hill et al. 2004). However, the new generation of shock tubes, which includes extending the driver section, are able to measure longer ignition delay times. To be more precise, 55 ms has been achieved by the Princeton group (Campbell, Wang et al. 2015).

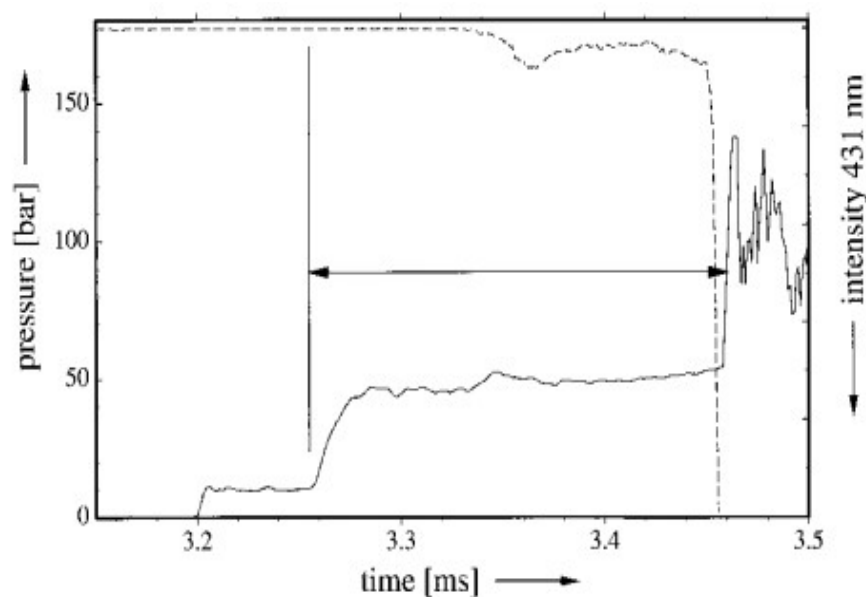


Figure 2-3 Pressure history and CH-band emission for Decane, 5.0MPa, 885 K, stoichiometric (Campbell, Wang et al. 2015)

In Figure 2.3, ignition delay time measurements are usually derived from the measured pressure traces within the test section and detection of CH-radical band emissions (Pfahl, Fieweger et al. 1996). Shock tubes mostly are recommended to be

used for measuring a relatively short ignition delay time due to their limitations, as mentioned previously. Shock tubes are capable of compressing the mixture suddenly using incident and reflected shocks, leading to a reduction in the influences associated with the compression process. Recently, shock tubes have been developed by using an aerosol, which it is equipped to modify the end wall section to permit filling it with an aerosol mixture (Davidson, Haylett et al. 2008). Vapour-phase ignition delay times of low vapour pressure fuels, without the need for a heated shock tube and separate mixing chamber have been enabled by this development conducted by the Stanford group.

2.2.2 Flow Reactors

As shown in Figure 2.4, flow reactors are cylindrical tubes like shock tubes which have hot turbulent air flow within them. Fuel is instantaneously injected into the stream of hot air at the throat of the high velocity nozzle, leading to downstream mixing. The tube needs to be surrounded by the heater to ensure uniform temperature. Since the fuel and air are mixed, auto-ignition occurs and it is observed by means of light emissions or a sudden temperature rise of at least 50 K (Petersen, Kalitan et al. 2007).

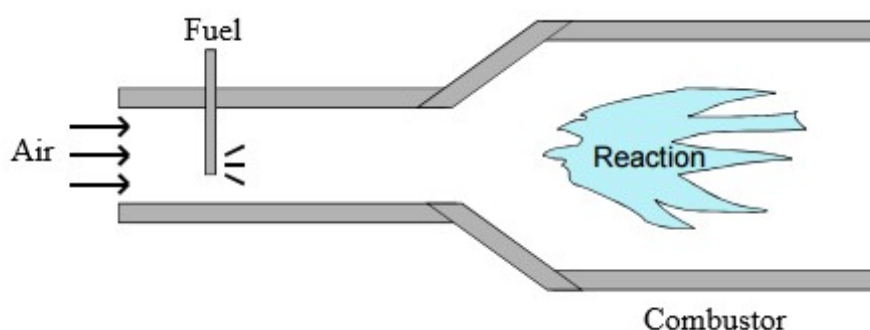


Figure 2-4 Schematic of flow reactor (Beerer, McDonell et al. 2009)

A laser detection system is usually used to detect the time interval between the fuel/air mixing to the ignition point and the initial point of the fuel/air mixing. It is known as the ignition delay time as shown in Figure 2.4 (Petersen, Kalitan et al. 2007).

Longer ignition delay times usually in excess of 100 ms, are measured by the flow reactors; it is due to the difficulties associated with perturbations in the mixing region. They mostly operate in the pressure range between 0.1 MPa and 3 MPa and the maximum temperature of 1000 K (Petersen, Kalitan et al. 2007, Beerer, McDonnell et al. 2009)

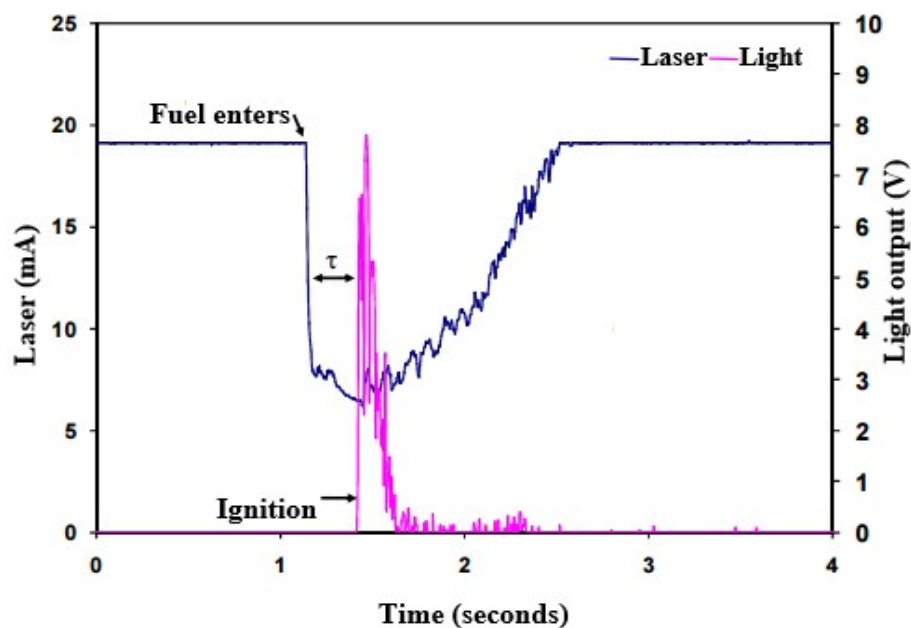


Figure 2-5 ignition delay definition using laser and light output in flow reactor (Beerer, McDonnell et al. 2009)

2.2.3 Rapid Compression Machine (RCM)

As described above, an RCM is an excellent tool used for studying auto-ignition under highly repeatable, well-characterized and controlled conditions. The RCMs are used to directly measure ignition delay times, as well as perform optical diagnostic tests, collect speciation data and study methods for controlling other auto-ignition phenomena. The RCM simulates a single compression stroke of an internal combustion engine by rapidly compressing a piston into a cylinder containing a reactive fuel/air mixture. These RCMs are typically designed to operate with compression times of 20 to 50 ms, creating an environment with compressed pressures of up to 100 bar and temperatures between 600 K and 1000 K.

2.2.3.1 Overview of the Rapid Compression Machines

The historical development of the rapid compression machine (RCM) dates back to 1906. The auto-ignition temperature of fuels was studied by using the RCM (Falk 1906, Falk 1907). The RCM was reviewed by Affleck and Thomas; they were driven by the momentum transfer of falling weights or through the use of a flywheel-driven crank. However, the novel RCMs' mechanics are basically different and pneumatically-driven and hydraulically-stopped systems have been replaced (Affleck and Thomas 1968, Beeley, Griffiths et al. 1980, Lee and Hochgreb 1998, Kitsopanidis and Cheng 2006). At the University of Michigan, the free sabot piston design was ceased since the interference fit between the bore and piston at the end of the stroke was formed (Donovan, He et al. 2004). Furthermore, the RCMs with designed cam pistons was put out of use at the University of Science and Technology at Lille design

(Ribaucour, Minetti et al. 1992). With the new designs, the RCMs are capable of achieving higher compression ratios and reducing the compression period. Donovan and Mittal have conducted several studies on the RCM existence (Donovan, He et al. 2004, Mittal 2006).

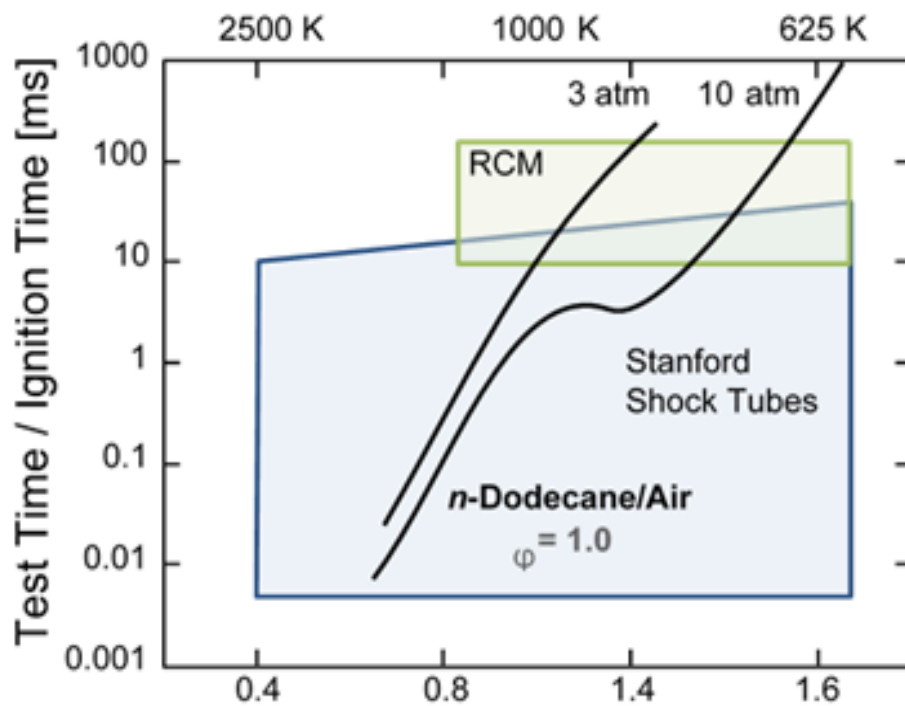


Figure 2-6 n-dodecane ignition delay times over wide temperature conditions in an RCM and shock tubes (Allen 2012)

According to Casey Allen (Allen 2012), it is not useful to simulate 3D fluid mechanics models due to the fact that most of the RCM designs minimize the fluid motion. This approach helps the researcher to use “zero-dimensional” tools. Several studies have evaluated the practicability of this approach by characterizing the origin of the RCM test environment (Allen 2012).

Temperature and concentration field characterizations in the RCM during the compression and early stages of reaction were investigated by using schlieren photography, chemiluminescent imaging and planar laser induced fluorescence (PLIF) (Griffiths, MacNamara et al. 2002). The post-compression was focused in their work to identify the inhomogeneity temperature distribution introduced by the gas, as well as characterizing the influences of these interactions with the auto-ignition chemistry and spatial development of ignition within the chamber during the RCM test. Moreover, Griffiths et al. reviewed prior studies about the existence of a roll-up vortex and investigations of the nature of the gas core in “zero-dimensional” tools. The face of the piston is surrounded by the cool boundary layer gases at the end of the compression stage and then they penetrate into the core gas region at 2 ms. During the gas phase oxidation processes, “zero-dimensional” codes can be reasonably accurate for prediction of the ignition delay time if the fuel and conditions of the tests are not in a negative temperature coefficient behaviour region. In the positive low-temperature dependence oxidation regime, if the heat release of the oxidation is well-characterized, then more precise predictions are expected due to the fact that reference temperature obtained for the adiabatic core characterizes the experiments and drives the reaction chemistry. For a moderate-temperature region, the NTC is more prone to occur (Figure 2.6). In this case, the early stages of reaction occur most rapidly in the cooler core. The main hot ignition event occurs in the cooler cores due to the temperature conditions.

Temperature inhomogeneity is minimized as the reactions rises, which may seem to be desirable; however, reactive intermediates are also generated during these stages which make the cooler core more sensitive to subsequent phases of reaction. A

creviced piston was removed at the University of Leeds to investigate the Griffiths et al. claim. Vortex formation is suppressed by the absence of a creviced piston, as well as supporting the longevity and uniformity of the adiabatic core. Casey Allen concluded that the interpretation of the regimes which drive the ignition process is valid for any RCM system where thermal stratification exists; however, he determined that general understanding about the timescales for core deterioration may not be applicable to RCM designs with creviced pistons (Allen 2012).

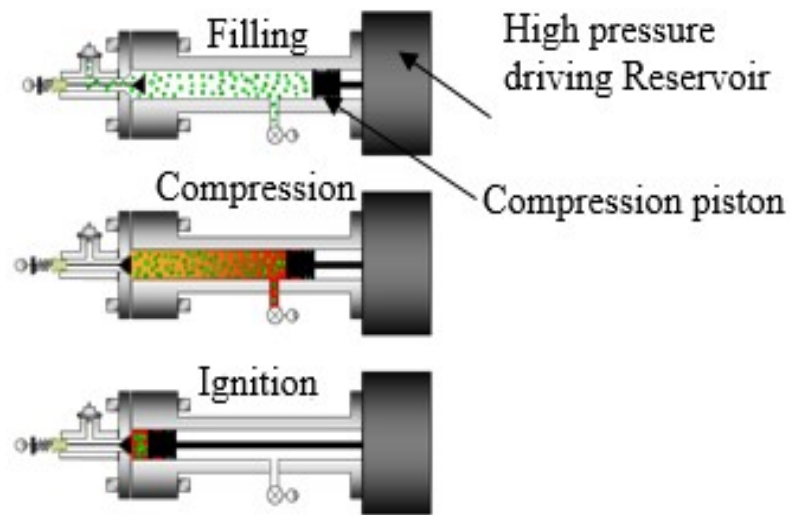


Figure 2-7 Schematic of RCM operation (Mittal and Sung 2007)

Temperature characterization of the core gas region within the compression and after compression for a flat piston was implemented by Mittal and Sung (2006). Although according to their study, it was concluded that as the hot and cool gases are mixed, a zero-dimensional environment with the flat piston was not suitable, the creviced piston significantly augmented the volume of the adiabatic core region. Based on the observations, core clearance volume is affected by test conditions and lower pressure leads to faster deterioration. Finally, it has been determined that a post

compression period up to 100 ms of RCM can be modelled as zero-dimensional since a creviced piston is used.

To achieve fully understanding of the reaction conditions an accurate study of heat loss from the RCM is needed, because only accepting the presence of an adiabatic gas core does not eradicate the other issues about the RCM's reaction quality. Understanding the accurate amount of heat loss is necessary, otherwise zero-dimensional modelling will not be reliable. Heat loss for each unique test used to be obtained in regards to the experimental means (Tanaka, Ayala et al. 2003, Mittal and Sung 2007); the requirements to do so are mentioned in the research of Würmel et al.(2007). Würmel focused on fuel ignition delay on diluent gas composition and hence mixture thermos-physical properties (*i.e.*, specific heat, thermal conductivities).

As shown in Figure 2.7, the RCM is a single compression device, where compression is achieved by a simple piston-cylinder configuration. The piston is driven by highly compressed air supplied from the bottles at the driven section and chemical reactions occur at the experimental section. The compression process should be instantaneous; otherwise the chemical reaction will start during the compression process. The RCMs have the capability to sustain the pressure and temperature after compression for around 120 ms, compared to that of 55 ms in the shock tubes (Mittal and Sung 2007).

In most RCMs, the ignition delay time is obtained from the recorded pressure. It is defined as the duration between the end of compression and the maximum pressure rise rate point (dp/dt) (Westbrook, Curran et al. 1998, Mittal, Chaos et al. 2008, Gersen, Mokhov et al. 2010) as shown in Figure 2.8. There is also another definition to obtain the ignition delay time, which is the time interval from the end of compression to the time when the pressure achieves 20% or 50% of the maximum pressure rise (Tanaka, Ayala et al. 2003, Mittal and Sung 2007, Ihara, Tanaka et al. 2009). The aforementioned methods reach the same results due to the very rapid rise in pressure during ignition. The typical regions in which the ignition delay time can be obtained by using the specified device are shown in Figure 2.8.

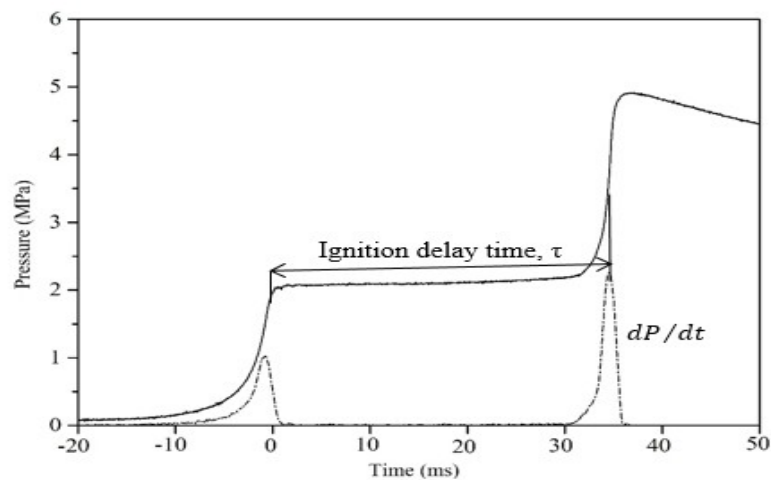


Figure 2-8 Typical pressure trace in the RCM showing ignition delay time definition (Materego 2015)

Figure 2.9 represents the ignition delay curve of i-octane comparison from the reduced mechanism of (Pepiot-Desjardins and Pitsch 2008); an equivalence ratio of 0.6 and a pressure of 2.0 MPa (Grogan, Goldsborough et al. 2015). Data from an RCM consists of the pressure in the combustion chamber measured over the course of an experiment. A typical pressure trace for a non-reactive and reactive experiment is

given in Figure 2.8. The dashed line is the data for a non-reactive experiment, which shows an increase in pressure due to compression and a gradual pressure drop over the post-compression period. This pressure drop is primarily attributed to heat loss to the surrounding boundaries, although seal leakages can contribute as well. The solid line is the pressure trace for a reactive experiment. The compressed pressure, P_c , (i.e. the pressure at the end of compression) is the same for both experiments. Heat release due to ignition causes a second spike in pressure in the reactive experiment.

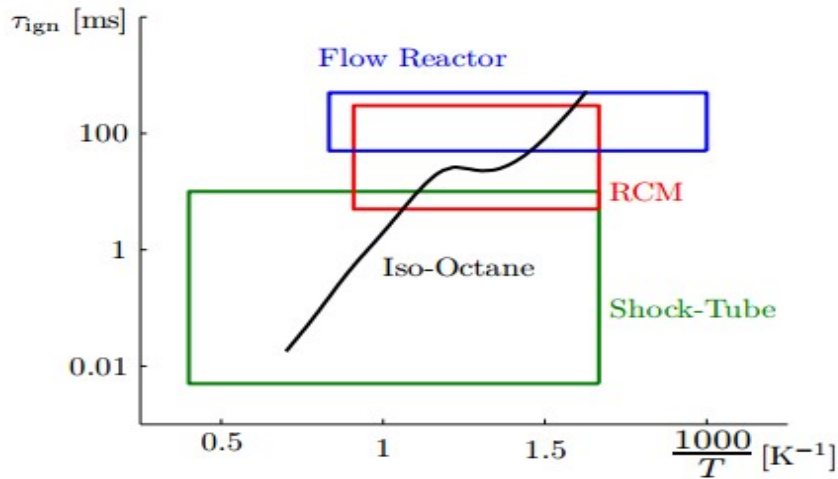


Figure 2-9 Typical operational boundaries of shock tube, flow reactor and RCM for iso-octane (Materego 2015)

Ignition delay times are calculated as the time from the pressure inflection point, indicating where the piston has reached top dead centre (TDC), to the time at which ignition occurs (see Figure 2.8). First-stage ignition is represented by τ_1 and the total ignition delay time by τ .

Temperature is challenging to measure directly in RCMs because the response times of temperature reading instruments (*i.e.*, resistance temperature devices (RTD) or thermocouples) do not allow the change in temperature to be recorded in real time.

Therefore, the compressed temperature is estimated by using isentropic relations. Nonreactive pressure traces are used under the adiabatic core assumption to approximate heat loss by using an “effective volume” approach, e.g. (Tanaka, Ayala et al. 2003, Sung and Curran 2014) and can allow for the temperature over the course of the experiment to be approximated. Accurately determining the temperature within the combustion chamber at TDC is of utmost importance in properly characterizing a fuel. Ignition delay times are reported as a function of the compressed temperature (T_c) *i.e.* the temperature at the end of compression.

In summary, an ideal RCM facility must have the capability to test with fast compression times over a range of compression ratios while collecting pressure data and providing optical access and gas sampling as well. A more detailed overview of the use of RCMs for chemical ignition studies is given by (Sung and Curran 2014).

2.2.3.2 Evolution of the Rapid Compression Machines

Some RCMs have been redesigned to offer more control over experimental conditions. The idea behind these machines is to better understand different phenomena associated with the operation of internal combustion engines. While these are also fundamental reactors, the data obtained from them incorporate more of the transport processes that are present in engines.

One such machine is the University of British Columbia's, rapid intake and compression machine (RICM), which can account for the flow field introduced by induction in an internal combustion engine prior to the compression stroke (Dohring 1986).

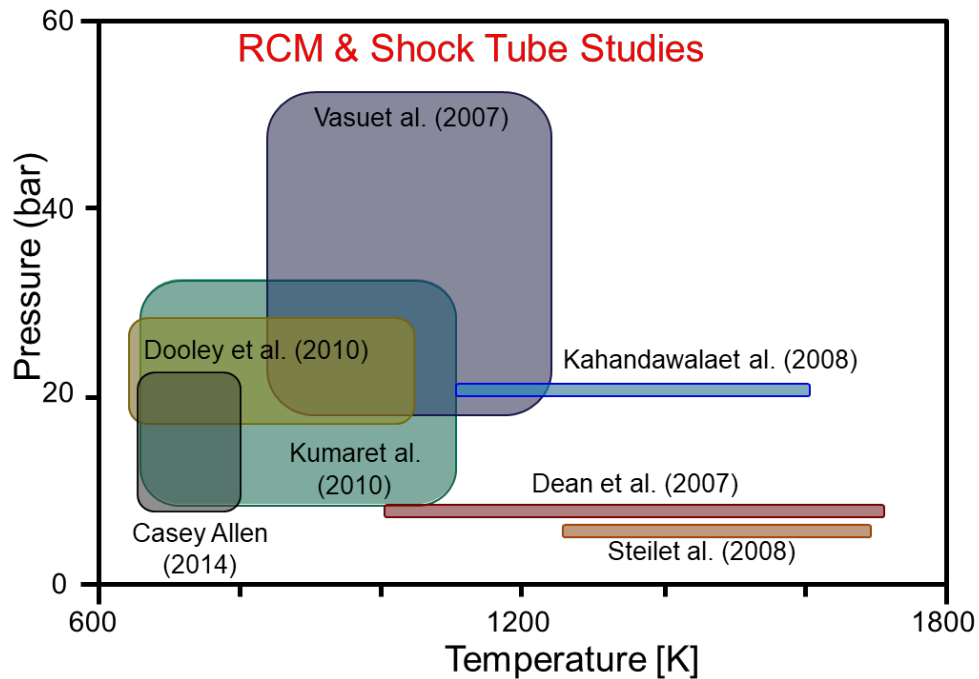


Figure 2-10 summary tested conditions in prior investigations published in this literature for different fuels (Materego 2015)

Another machine is the rapid intake, compression and expansion machine (RICEM) at the Korea Advanced Institute of Science and Technology, which has adapted a traditional RCM with a gas supply system and expansion that can be used to account for the fluid mechanics associated with the induction and power stroke in an internal combustion engine (Cho, Jeong et al. 2010).

The rapid compression expansion machine (RCEM) at the Tokyo Institute of Technology can simulate intake, compression, expansion and exhaust strokes of a single-cylinder engine using hydraulic actuation (Kobori and Kamimoto 1995). This machine uses a spool valve operating mechanism which allows for either intake and compression or compression and exhaust to be tested.

Another unique RCEM design exists at Pohang University of Science and Technology (Park, Huh et al. 2000); It operates like a single-cylinder internal combustion engine with a crankshaft that rotates at a constant speed. This machine is capable of simulating a four-cycle internal combustion engine while also suppressing most of the turbulence present in the combustion chamber.

Overall, the evolution of RCMs and the development of new machines capable of increased control over experimental conditions are essential to the refinement of combustion modelling processes. The field of chemical kinetics relies heavily on data collected from these machines for validation purposes.

The summary of the regions of the works conducted by different researchers illustrated in Figure 2.9. In this study, the RCM is equipped with a spark plug, to ignite the mixture close to the EOC process. It was used to ignite the mixture to simulate the same conditions of the real spark ignition engines in the RCM. Therefore, according to the mixtures used in this study, the pressure varies widely when it reaches to around

to 142 bar for pure methane used as fuel, and pressure declines to approximately 80 bar when 8% n-pentane was blended into 92% methane.

2.2.3.3 Chemical Kinetic Studies

Detailed kinetic models (DKMs) describe the dynamic evolution of a chemically reactive system. These models contain pertinent chemical species and elementary reaction pathways for describing and modelling fuel oxidation. Ignition delay time measurements, speciation data and optical diagnostics are directly used to improve the capabilities of chemical kinetic modelling by providing reliable experimental data that characterize combustion processes. On a global level, ignition delay times are used to validate these chemical kinetic models. Poor agreement between experimentally determined ignition delay time measurements and numerical model results require further refinement of the mechanism and an evaluation of specific elementary reactions. Highly refined DKMs are useful when incorporated into simulations of low complexity, *i.e.* zero-dimensional models, or even highly complex three-dimensional computational fluid dynamic (CFD) simulations; they provide reliable, predictive modelling used for the advancement of transportation, power generation and manufacturing technologies.

Experimental facilities used to collect data to validate DKMs often encounter issues due to uncertainty in measurements; poor characterization of experimental conditions; and realities that are challenging to directly measure or understand. A rapid compression machine (RCM) is one such device. The RCMs are fundamental reactors

which are used to recreate internal combustion engine conditions in a clean, controlled environment. For RCM data to be useful, it is essential to create a thermodynamically well-defined environment to accurately characterize an experiment. Under ideal conditions, ignition delay measurements could be performed in a quiescent, homogeneous gas phase mixture that is instantaneously compressed to a repeatable, specified reaction condition; whereupon the environment would remain isothermal and isobaric until ignition occurs. This ideality cannot be reproduced in practice, especially where low-temperature (600 K – 900 K) kinetics are being investigated.

In the literature, there are discrepancies among data obtained from different RCM facilities for the different fuels under similar test conditions (Minetti, Carlier et al. 1996, Würmel and Simmie 2005, Mehl, Curran et al. 2009). These discrepancies are primarily attributed to “facility-dependent” effects such as heat loss to surrounding boundaries, seal leakages, chemical phenomena, or the presence of complex aerodynamics (Minetti, Carlier et al. 1996, Sung and Curran 2014). Inconsistencies in the experimental test setup and operation offer a trivial explanation as well. For kineticists, discrepancies in experimental data introduce challenges in selecting proper validation data, as well as in reducing model uncertainties.

Further, a lack of understanding of heat loss effects can greatly influence the interpretation of data obtained from RCMs. Numerical modelling of an assumed “zero-dimensional” system is a valid approach to estimate the temperature trace for an experiment and much work has been done to illustrate this (Mittal and Sung 2007, Mittal, Raju et al. 2010, Mittal and Chomier 2014). Heat loss is included in the 0-D

model in one of two ways. One method adds a heat loss term into the energy equation; the other is through adding an effective volumetric expansion. Both of these methods are tuned to match experimental data (*i.e.* agreement among pressure drops). However, it is believed that simplifying assumptions used in these analyses limit the ability to accurately represent the physical conditions present in experimentation (Mittal, Raju et al. 2008, Chaos and Dryer 2010, Mittal, Raju et al. 2010, Goldsborough, Banyon et al. 2012). In general, a lack of characterization of heat loss present in RCM experiments and inconsistencies in defining experimental conditions lead to an increase in uncertainty in experimental measurements; thus, increasing the uncertainty associated with the model validation.

Oxidation of CH_4 and $\text{CH}_4/\text{C}_2\text{H}_6$ mixtures was studied at pressures relevant to knocking in large bore gas engines by using the RCM at EOC temperatures ranging between 885 K and 940 K, at a compressed gas pressure of 105, 125, 150 and 160 bar and at varying equivalence ratios of 0.417, 0.526 and 1. This study described the methods and limitations of performing high-pressure magnitude experiments in RCMs; and furthermore, the modelling and validation of the kinetic mechanism against experimental data. The reaction rate constant for H-atom abstraction from CH_4 by HO_2 radical was optimized in order to achieve better agreement with the new data. The modifications have a result on accurate prediction of IDTs (Ramalingam, Zhang et al. 2017).

In Tanoue et al's study (2017), the influences of pre-chamber combustion characteristics were investigated to improve the efficiency of cogeneration natural gas

engines. The effects of a torch flame were generated by a pre-chamber to investigate its effects on main combustion. It concluded that the ignition plug position is far from the nozzle exit of the pre-chamber; unburned gas is injected before burned gas and that the burned gas spreads all over the unburned, resulting in a steeper rise in the heat release rate. However, if the ignition plug position is in the vicinity of the nozzle exit, the combustion gas is ejected during the total injection period, resulting in a gradual rise in that heat release rate(Tanoue, Kimura et al. 2017).

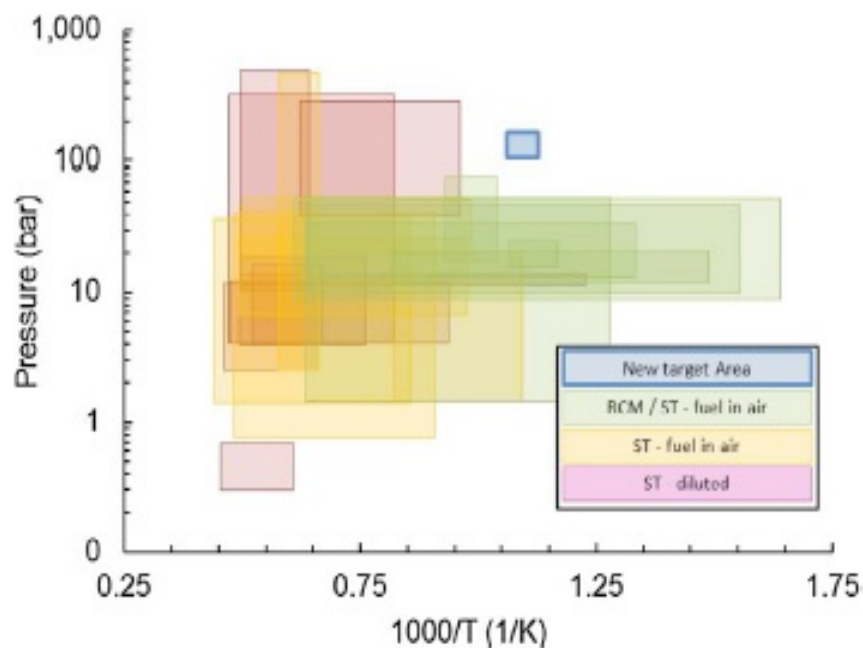


Figure 2-11 The graphical overview of the literature on natural gas mixtures for the different targeted pressures and temperatures (Ramalingam, Zhang et al. 2017)

The influences of initial temperature and fuel properties on knocking conditions were studied by Tanoue. He found that unburned fuel mass fraction and temperature

didn't directly affect knock intensity; however, initial temperature and fuel properties affect the knocking occurrence. Besides, with higher initial temperature knocking occurs earlier, while it does not affect the timing of knock occurrence (Tanoue, Jimoto et al. 2017).

Liu et al. studied the effects of H₂ and CO on CH₄ ignition and flame propagation at fuel rich and stoichiometric conditions relevant to an EGR system. The tests were done over a range of temperatures ($T = 860\text{-}1080\text{ K}$), with equivalent ratio of $\phi = 1\text{-}1.5$ at $p = 20\text{ bar}$. According to results, adding H₂ in CH₄, had little effect on ignition delay time at low temperature; but H₂ promotes IDTs significantly at high temperatures. Moreover, CO had little effect on IDT in all conditions (Liu, Song et al. 2018).

2.3 Methane Number

One of the major difficulties when testing fuels for knock resistance is the measurement and quantification of knock. In the ASTM knock rating methods for gasoline, unknown fuels are directly compared to reference blends. It is more difficult to test the gaseous fuels due to their ignition properties.

Therefore, an indirect method needs to be taken into account to calculate the MN (Leiker, K et al. 1972, Schaub and Hubbard 1985, Heywood 1988, Ryan, Callahan et al. 1993). A map of reference fuel MN versus compression ratio at light knock was created and termed the “MN guide line”. Then, an unknown fuel was tested in the

engine and the compression ratio required to produce light knock was compared to the MN guide line; thereby producing an MN (Malenshek and Olsen 2009). These investigations all were done by the Cooperative Fuel Research (CFR) engine. There are plenty of published works dedicated to gaseous fuel knock testing; however, more precise investigations on MN are still required, since the mixtures have different proportions of fuels. In this study, two different methane number algorithms are used; these algorithms were developed by the Wartsila and European standard.

Methane Number Calculation

Input

Gas composition Volume-%

CO2.....Carbon dioxide.....[%]	.000
N2.....Nitrogen.....[%]	.000
O2.....Oxygen.....[%]	.000
H2.....Hydrogen.....[%]	.000
CO.....Carbon monoxide.....[%]	.000
CH4.....Methane.....[%]	83.900
C2H4.....Ethylene.....[%]	.000
C2H6.....Ethane.....[%]	8.000
C3H6.....Propylene.....[%]	.000
C3H8.....Propane.....[%]	3.000
C4H6.....Butadiene.....[%]	.000
C4H8.....Butene.....[%]	.000
C4H10.....Butane.....[%]	2.000
C5H12.....Pentane.....[%]	3.100
C6+.....Hexanes+.....[%]	.000
H2S.....Hydrogen sulphide.....[%]	.000
H2O.....Water vapour.....[%]	.000
Total [%]	100.000

MWM
Energy. Efficiency. Environment.

mn-Version : 2.0.1

Clear

Calculate

Help

Exit

Output

MWM
Methane Number [-] 47 ?
mzdll-Version: 2.0.1

Figure 2-12 interface of the EN 16726 MN Calculation

2.4 Knock Intensity

Knock intensity can be clearly quantified either by:

- The spectral data of the original pressure signal; or
- The filtered pressure data.

From the Fig. 4.10, it can be seen that when the knock occurs, the pressure oscillation is composed of several resonant frequencies which they can be affected by the auto-ignitions. The auto-ignitions participating in the oscillations depend on the end-gas initial condition. The resonant frequencies are explained in more detail in (Hudson, 2001). To filter the pressure oscillations in order to get useful information, it is necessary to know what the major frequency components are. Therefore, the spectral data of the pressure oscillations are considered. The spectral data can be the results of either a discrete or a fast Fourier transform. The useful frequencies in the pressure oscillation signals should be determined to get much information on the frequency axis. The observation that the useful pressure oscillation frequencies when knock occurs are between 6 and 25 kHz, is consistent with results from other researchers (Hudson, 2001). A manuscript of determination of the most useful pressure frequency when knock occurs and the intensity of the knocks have been expressed in Appendix A.

Oscillations significantly different in shape and peak are these resulting from fuel auto-ignition, which might occur at the end phase of controlled combustion. Such oscillations can reach several hundreds kPa or even more (Szwaja,2011). High pressure oscillations come from methane-propane mixture auto-ignition at the end

combustion phase are followed by oscillations caused by combustion instabilities. Intensity of these types of oscillations can be expressed by their maximal peak pressure (PP) at the individual combustion events. Thus, PP_i is defined with the equation (Naber, Blough, 2006; Szwaja, 2011).

$$PP_i = \max[|HFPO_i(t)|] \quad \text{Equation 2.1}$$

Following this definition, the mean knock intensity can be expressed as the mean intensity denoted as the PP, which is identified by the equation:

$$PP = \frac{1}{n} \sum_{i=1}^n PP_i \quad \text{Equation 2.2}$$

where:

n – number of combustion events,

i – single combustion event.

2.5 AVL Simulation Overview

2.5.1 AVL BOOST Review

Many categories have been created by the AVL company, to develop models and simulation of engines. The AVL package contains different simulation platforms such as FIRE, CRUISE and BOOST. The AVL BOOST is capable of simulating and modelling an entire engine which includes the combustion and emission analysis. In this study, the BOOST platform is used for the investigations and which is applied for

the thermodynamics' analysis. A graphical user interface, an interactive pre-processor, an interactive post processor for fast analysis of the results and comparison with experimental data, extensive interactive context, efficient simulation, and animated display of pressure profiles have been proposed in the BOOST platform (Version 2010).

As BOOST is a powerful tool to model the engine's performance analysis, it can be applied for a wide range of tasks, various engine concept comparisons, optimizing the engine geometry (inlet, exhaust, valves etc. with respect to power, torque and fuel consumption), valve timing and cam profile adjustment, supercharge and turbocharging systems, orifice noise optimization and evaluation of engine performance (Version 2010).

Table 2.1 AVL BOOST elements' trees (Version 2010)

Element	Symbol	Specification
Engine	E ()	Engine element
System Boundary	SB ()	Provides the conditions of the calculation model to a user-definable ambient.
Measuring Point	MP (X)	Access to allow data and gas conditions over crank angle at a certain location in a pipe.
Element	Symbol	Specification

Monitor	MNT ()	Is used to produce transient results in the results folder and in online monitoring for an arbitrary number
Plenum	PL ()	An element in which spatial pressure and temperature differences are not considered.
Cylinder	C ()	Cylinder element
Restriction	R ()	Consider a distinct pressure loss at a certain location in the piping system.
Throttle	T ()	Controls the air flow in a pipe as a function of the throttle angle.
Junction	J ()	Used to connect three or more pipes. In the case of three pipes, a refined junction model may be used. This considers geometric information such as the area ratio of the connected pipes and the angles between the pipes. In other cases a simple constant pressure model is available.
Pipe	numbers	Pipes to connect different features

AVL BOOST proposes several features which are summarised in Table 2.1:

- Pipes and junctions
- Perforated pipes
- Flow restrictions

- System boundaries
- Plenums and crankcases
- Air cleaners and air cooler
- Turbocharging and supercharging: single and multiple entry turbines, variable geometry turbines, power turbine
- Combustion model: wiebe function, two-zone wiebe for NO_x, experimental burn rate input, constant pressure, constant volume
- Control functions: BOOST internal engine control unit, PID controller

Different analyses of the calculation results in various modes have been created in the AVL BOOST; such as message analysis, transient analysis, traces analysis, series analysis and acoustic analysis. The average results for each cycle calculated versus cycle number or time are given in the transient analysis. The trace graphs are shown with respect to crank angle, which can be also exported as different files such as text, Word and Excel (Version 2010, Alqahtani, Shokrollahihassanbarough et al. 2015).

Chapter 3 – EXPERIMENTAL AND SIMULATION SET-UP

3.1 Introduction

The test equipment used throughout this study is described in this chapter. This includes the details of the test bench and instrumentation, as well as the details of the models created in AVL BOOST. The RCM control methodology, data acquisition systems and analysis methods are described in the following subcategories.

The RCM test facilities have been developed by the Wartsila Fuel Laboratory at Vaasa in Finland, founded by the European Union under the “Knocky project” grant. The maintenance and development of the facilities during the investigation was the responsibility of the author. Developing the engine test cell facility involved modifying the RCM test bench performance, while the fuel mixing was developed. Regarding the maintenance of the facilities, this included repairing small parts such as checking valves, sealing, O-rings, heating system, etc. when they failed more than fifteen sets of reference curves were created, which it means more than 6000 tests for a period of six months.

Overall, this chapter provides an overview of the current test facility, the RCM cell modifications, experimental and simulation setups.

3.2 RCM Experiments' Set-up

The RCM is known as an experimental device to simulate a single compression stroke of internal combustion engines (ICEs). It also is used for chemical kinetic studies (Sung and Curran 2014, Desantes, Lopez et al. 2017). It is an alternative for both shock tubes and flow reactors to investigate the low-intermediate temperature auto-ignition chemistry at ideal operating conditions (Darcy, Nakamura et al. 2014, Nakamura, Darcy et al. 2014, Alexandrino, Alzueta et al. 2018).

The enormous flexibility of the RCM allows the researchers to reach close to the thermodynamic conditions of real engines by analysing influences in mixture formations, vaporization, ignition, flame propagation and combustion (Han, Deng et al. 2017, Liu, Song et al. 2018). It offers a wide range of operating conditions, with very low vibration during operation.

3.2.1 RCM Specifications

The present RCM is fabricated as a flexible device which incorporates the key features of various existing RCMs and allows a wide range of experimental conditions. Figure 3.1 shows the RCM used during this research. It is a single horizontal piston machine which is pneumatically driven by compressed air and damped hydraulically. This technique is extensively used by existing RCMs (Mittal 2006, Lee, Vranckx et al. 2012) due to its proven ability. The Wartsila's RCM has dimensions of about 2.6 m in length and 1.2 m in height with a width of 0.6 m. A compression ratio can be achieved between 5 and 30, attained by varying the compression stroke between 120 mm and 250 mm. It is possible to change the stroke by adjusting the number of removable

components, leading to vary the hydraulic chamber and consequently initial volume before compression (Mittal and Sung 2006, Lee, Vranckx et al. 2012).

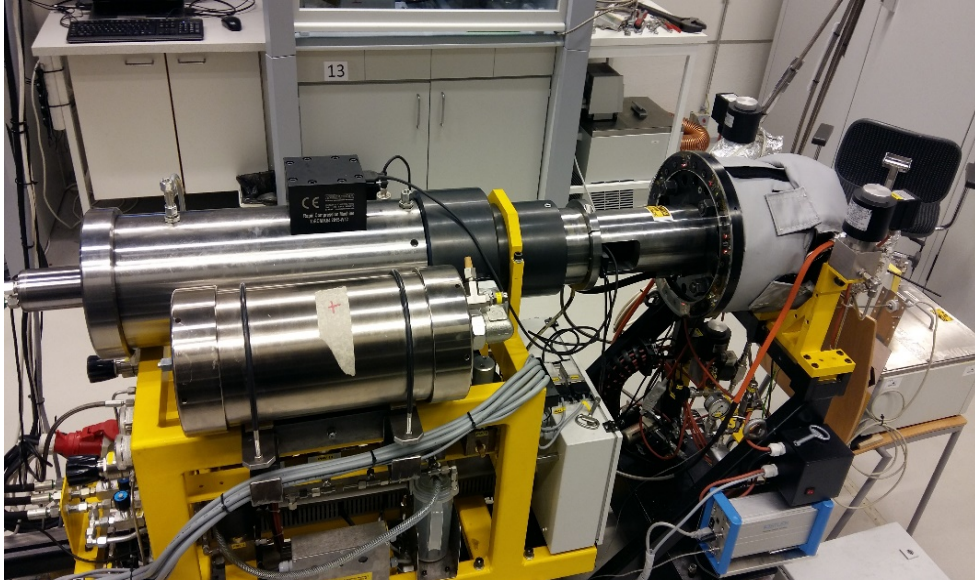


Figure 3-1 Rapid Compression Machine (RCM) at Wartsila's Fuel Laboratory

The Wartsila RCM was designed and fabricated based on two functional parts: “experimental section” and “driven section”, shown in Figure 3.2 and identified as an interior sectional view. The experimental section contains the cylinder head, cylinder wall and piston with the combustion bowl. The driven section combines the stroke drive, mass balance and stroke setting as a modified stroke.



Figure 3-2 Rapid Compression Machine (RCM) in Wartsila's Fuel Laboratory

From a functionality point of view, the driving air chamber pushes the piston towards top dead centre (TDC). The hydraulic chamber has two functions. At the commencement point, high oil pressure holds the piston at the starting position. Then at the end of the procedure, it acts as a damper to decelerate the pistons and to prevent system vibration and damage. The RCM test components can be varied and thereby, the gas temperature and pressure. The test section is equipped with a pressure transducer port, a thermocouple port, optical ports (portable), and gas inlet and outlet ports, according to the data released by Testem Company in Germany.

Table 3.1 Specification of the RCM in the Wartsila Fuel Laboratory

Bore	B = 84 mm
Stroke	S = 120-250 mm
Compression ratio	CR = 5-30
Driving pressure	Up to 80 bar
Piston bowl	$d_{\text{bowl}} = 42$ mm bowl depth = 4 mm
Cylinder pressure	P _{max} up to 250 bar
Cylinder head	Flexible, pre-chamber, 1.5 cm ³
Pressure detection	Piezoelectric transducer 0-300 bar
Heating	Distributed heating system throughout the cylinder and cylinder head at 80°C-120°C
Ignition system	Spark plug, @ Pre-chamber
Fuel	i) Methane/propane mixture ii) Methane/ethane mixture iii) Methane/butane mixture iv) Methane/n-pentane mixture

To maintain the uniform state conditions for an extended period of time in the centre or core region of the test section, the piston design has vital influence for the

RCM. Also, a creviced piston design is adopted, which it is common among most of the RCMs. More optimized designs significantly improve the accuracy of measuring knock occurrence conditions.

3.2.2 Control System, Data Acquisition and Processing

A computer was managed to control the RCM. The pressure, piston position, wall temperature, etc. are considered as measuring signs and they were registered simultaneously by a data acquisition system (National Instrument 6259) and integrated in the interface. A pressure transducer (piezoelectric Kistler-5018) was fitted in the RCM cylinder head to measure the in-cylinder pressure directly from each combustion

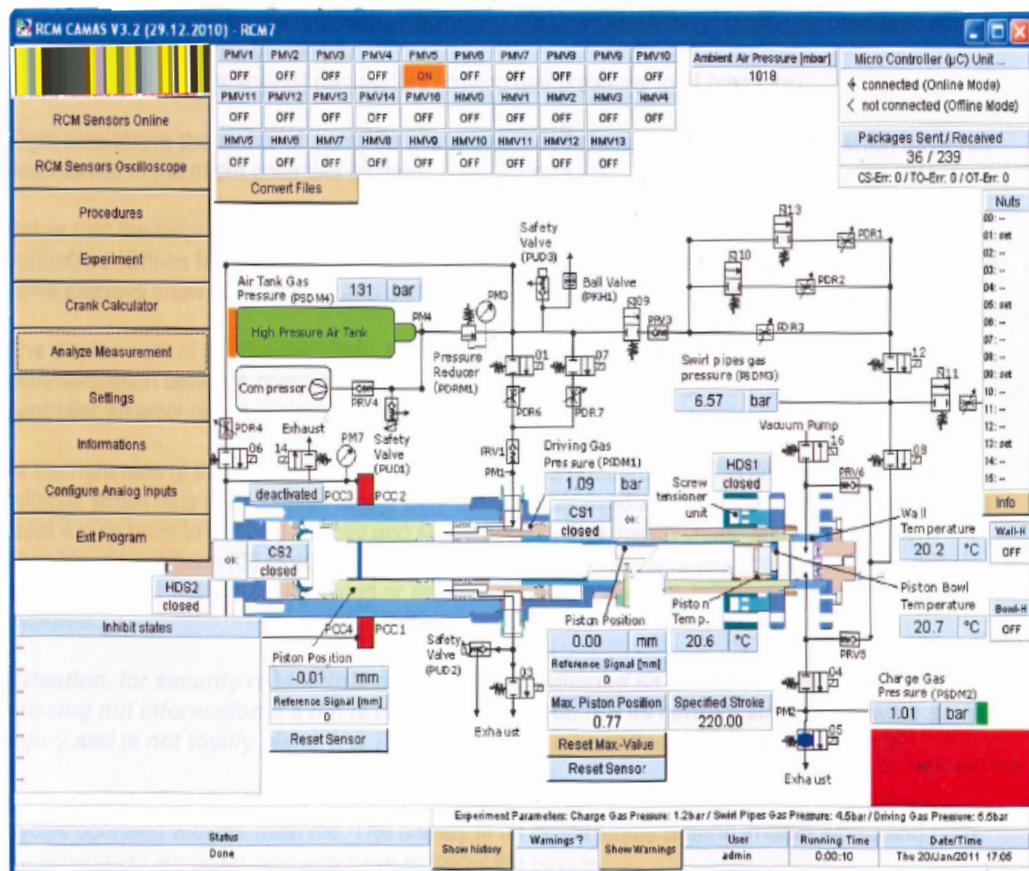


Figure 3-3 Interface of the RCM program to control the operation

process. The pressure signals were amplified and then converted into digital signals by the data-acquisition processing device. The initial temperatures of the RCM were measured by two sensors mounted in the piston wall and piston bowl. The data acquisition was triggered simultaneously with the opening of the solenoid for the fast-acting valve. The interface of the program controller has been shown in Figure 3.3.

3.3 Novel Aspects of RCM

It has been proposed to investigate the gaseous combustion characteristics while different gaseous fuels blended into together. The foundation of the RCM modifications and ARR investigations are based on the premixed methane-propane mixtures; however, several modifications to the RCM have been developed whereby the gaseous mixtures are heated up to a certain temperature as it is loaded.

The RCM starts operation at a vacuum condition, it is essential to mount a check valve behind the valves in both air and fuel pipelines. It helps in reducing the leaks and it enables the RCM operation to be more reliable and closer to the correct lambda.

The heating elements should be mounted across the cylinder wall, to provide a uniform and homogeneous temperature across the interior chamber walls, otherwise the mixtures are affected by any local hot spots (Heywood 1988). The temperature profile of the combustion chamber was examined by using a thermocouple at different

locations and different time intervals. The temperature investigations will be presented in section 4.4.1.

Most studies on the RCMs were focused on the ignition delay time of the liquefied fossil fuels. Thus, they were compressed at certain pressures with different air/fuel mixtures, to assess the ignition delay time. Here, in this work, first gaseous mixtures are studied to figure out a reference curve like that used in the liquid form. Moreover, a spark plug is equipped to ignite the mixture as well as the driving pressure varying, instead of changing the λ .

3.4 Fuel Properties and Fuel Preparation

3.4.1 Fuel Properties

Linear and branched chain alkanes, or paraffin, constitute a major portion of most modern fuels, including natural gas and petroleum-based fuels, and there is a long history of their being studied using RCMs. Here, methane, ethane, propane, butane and n-pentane mixtures were investigated, first to improve the RCM performance. The methane/propane mixtures have been investigated to achieve high accuracy and repeatability, as well as producing a reference curve according to the results released from the methane/propane tests. The other mixtures have been studied since the methane was chosen as the base fuel to mix with the other fuels. The properties of the fuels used in this investigation are shown in Table 3.2.

Table 3.2 properties of the gaseous fuels tested in this work with RCM

Fuel	LHV (MJ/nm ³)	Density (kg/nm ³)	Air-Fuel ratio @ stoichiometric (nm ³ /nm ³)
Methane	35.88	0.71	9.52
Ethane	64.36	1.32	16.66
Propane	93.18	2.02	23.8
Butane	114.375	2.5	30.94
Pentane*	30423.6	626	38.08

* Liquid form

3.4.1.1 Methane

Methane is the primary constituent of natural gas and its ignition chemistry is important for a range of conventional and advanced combustion strategies. Methane is a very unreactive fuel, in part due to the high activation energy required for abstraction of H-atoms and also because of the relatively low reactivity of the methyl radicals formed; which can, for example, undergo self-combination producing stable ethane molecules. Hence it is difficult to study methane auto-ignition at the lower temperature (600-1000 K) conditions typically encountered in RCMs, and high pressures must be utilized and a narrow range of temperatures covered.

3.4.1.2 Ethane

Ethane as a second largest component of natural gas, expected (Gersen, Mokhov et al. 2011) involving carbon chains longer than methane. Ethane is more reactive than methane (Goldsborough, Hochgreb et al. 2017).

3.4.1.3 Propane

Propane is the smallest alkane. It is a significant component of ‘wet’ natural gas, as well as petroleum. It is a gas at standard temperature and pressure, but compressible to a transportable liquid. It is one of a group of liquefied petroleum gases (LPG) (Goldsborough et al. 2017).

3.4.1.4 Butane

Butane is a component of “wet” natural gas and as well as a component of petroleum, and it is a primary constituent of refined LPG. Furthermore, it is used as a blending agent for gasoline in cold weather environments due to its relatively high vapour pressure. (Goldsborough, Hochgreb et al. 2017).

3.4.1.5 N-pentane

N-pentane is an intermediate/heavy component of ‘wet’ natural gas and is also present as a lighter component within petroleum feed-stocks. It is often used as a primary constituent to denature ethanol that is produced for E85 flexible fuel. Since its octane rating is lower than that of gasoline, it can be blended with high fractions of ethanol, which has a research octane number (RON) of 109, and thus can achieve an octane rating which is suitable for modern gasoline engines (Goldsborough, Hochgreb et al. 2017).

3.4.2. Fuel Preparation

Test mixtures were prepared in a 10-liter stainless steel mixing reactor and was used to charge the RCM chamber at the specified pressures. Figure 3.4 shows the gas mixing system as well as a 10-litre auxiliary reactor that can be used for low calorific mixtures which increase the number of tests. Before starting the gas mixture preparation procedure, the chamber and pipes should be vacuumed, thus the combustion chamber is only filled by the mixture. A WELCH pump was used to vacuum the gas reactor and the gas pipelines, around 20 mbar. After that, the (outlet) valve of the mixing bottle should be closed. Subsequently, the gas pipelines are again vacuumed and then the specified fuels are added into the bottle to be mixed. A compressor-mixing valve is mounted in the reactor in which the test mixtures are prepared and allowed to mix together to ensure homogeneity of the mixture. A detailed explanation of the mixture preparations has been expressed in several published works (Shiga, Ozone et al. 2002, Di, He et al. 2014, Nakamura, Darcy et al. 2014, Goldsborough, Hochgreb et al. 2017, Tanoue, Jimoto et al. 2017).

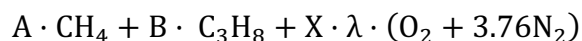
Before filling the combustion chamber, poppet and solenoid valves are opened, and the whole system is vacuumed to the pressure of 20 mbar. The combustion chamber is filled with the gas mixture to the desired pressure, by opening the bottle that contains the test mixture. The poppet valve is then closed and the mixture is ready for compression. After each test, the exhaust gases in the chamber are evacuated to the outside, to be ready for the next test. The solenoid valve in the gas-filling line is equipped for safety purposes, and electrically connected such that when the solenoid valve is used as a trigger the fast-acting valve is open, the solenoid in the gas-filling

line is always closed. This prevents flame propagation back to the gas-mixture bottle when the poppet valve is not properly closed.



Figure 3-4 Stainless steel gas fuel mixing reactor

All test gases used in this study have purity greater than 99.5%. The composition ratios of the gas mixtures are calculated from the measured partial pressures of the individual gases, as summarized in Table 3.3.



Where A and B express volumetric proportions of methane and propane, respectively; X indicates the number of moles of oxygen per mole of fuel in different mixtures and air is assumed to consist of $(\text{O}_2 + 3.76\text{N}_2)$. Nevertheless, lambda (λ) will be expressed in each section, as it has been varied in chapters 4, 5 and 6. Partial pressure and Dalton's law were applied to investigate the filling amount of the mixtures. The mixtures were assumed to behave as ideal gas since they are not close to very low

temperatures and around 1 atm; furthermore, gases do not take up extra volume and they do not have intermolecular reaction.

In this study, the fuel doses of most of the tests have been set for approximately 5 kJ and in a few cases, they are set at 3.5 kJ, where the new methods and techniques have been investigated for specific mixtures. These fuel doses have been proposed by the Wartsila engine technology team, thus the energies were correlated with the real Wartsila results.

$$P_{\text{total}} = P_{\text{air}} + P_{\text{fuel}} \quad \text{Equation 3.1}$$

According to the ideal gas law, from the air and fuel in the chamber,

$$P \cdot V = n_{\text{mole}} \cdot R \cdot T \quad \text{Equation 3.2}$$

As the temperature and universal gas constant are the same, we have the following equation

$$\frac{n_{\text{air}}}{n_{\text{fuel}}} = \frac{P_{\text{air}}}{P_{\text{fuel}}} \quad \text{Equation 3.3}$$

$$n_{\text{fuel}} = \frac{P \cdot V}{R \cdot T} \quad \text{Equation 3.4}$$

both fuel and final charged pressure can be investigated.

3.5 Piston Motion and Volume and Compression Ratio in the RCM

Displacement measurement in the RCM is carried out by an incremental displacement sensor on the magnetic principle; where the resolution of the sensor is 0.05 mm. The initial points (zero point at the bottom dead centre-BDC) before each shot and after air-fuel add, driving pressure charging processes must be calibrated to calculate the exact displacement of the piston during each test. The elasticity of the machine should be taken into account, so that there is a small variant in the maximum piston position, as it occurs in real engine. This small inaccuracy can be neglected since the test conditions remain the same, so the corresponding changes in length are not changed.



Figure 3-5 Displacement measurement instruments in rapid compression machine (RCM) by an incremental displacement component

The peak pressure remains almost continuous for the constant driving pressure; thus, the maximum piston stroke can be obtained by calculating the difference to the maximum piston stroke, the relative displacement with respect to the top dead centre (TDC) with an accuracy of ± 0.05 mm.

According to the configuration of the RCM represented earlier in Table 3.1, section 3.2.1, the volume of the RCM chamber is calculated as the following:

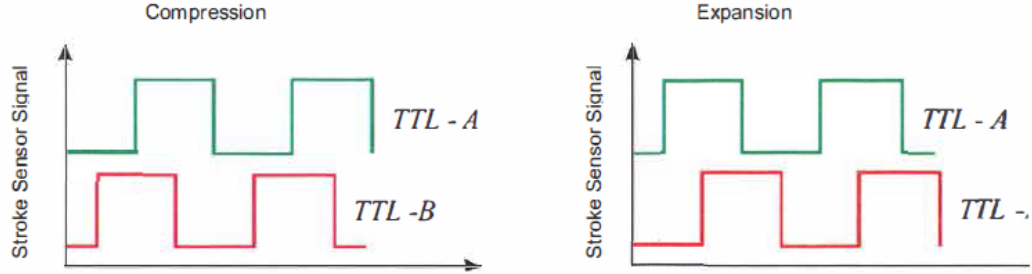


Figure 3-6 Stroke sensor signal in displacement measurement in RCM during compression and expansion processes

$$\text{Volume}_{\text{chamber}} = \text{Volume}_{\text{bowl}} + \text{Volume}_{\text{piston @TDC}} \quad \text{Equation 3.5}$$

The volume of the piston bowl (constant) is calculated as:

$$\text{Volume}_{\text{bowl}} = \pi \left(\frac{(\text{piston bowl diameter})^2}{4} \right) \cdot \text{bowl height} \quad \text{Equation 3.6}$$

The volume of the chamber (variable) is calculated as:

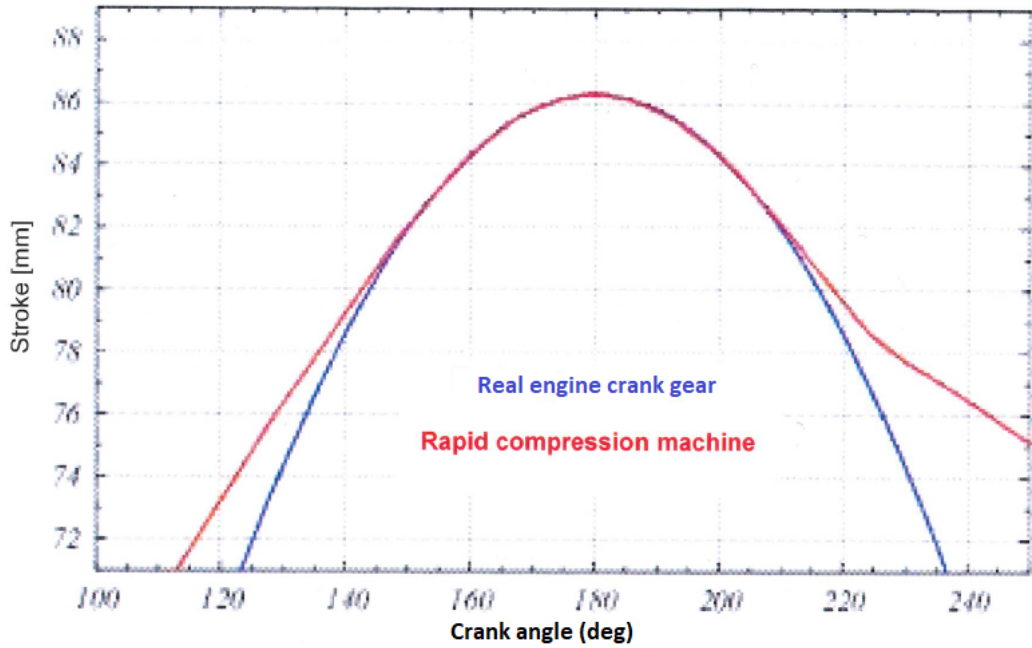


Figure 3-7 Piston motion of the RCM with respect to an real engine piston motion

$$\text{Volume}_{\text{piston @TDC}} = \pi \cdot \left(\frac{(\text{piston bowl diameter})^2}{4} \cdot (\text{Stroke} - \text{Max. piston position}) \right)$$

Equation 3.7

3.6 Air and Fuel Induction Methods

The fuel mixture was blended in the mixing reactor under the same condition. There are two methods to feed the fuel mixtures in the chamber in this study. Air and fuel are fed into the chamber by separate vessels, so that first fuel is induced into the chamber and when the pressure is achieved to the set point, the air is fed into the RCM chamber to reach the final partial pressure; these pressures are controlled by a pressure sensor equipped almost at a 0.5 m distance to the chamber.

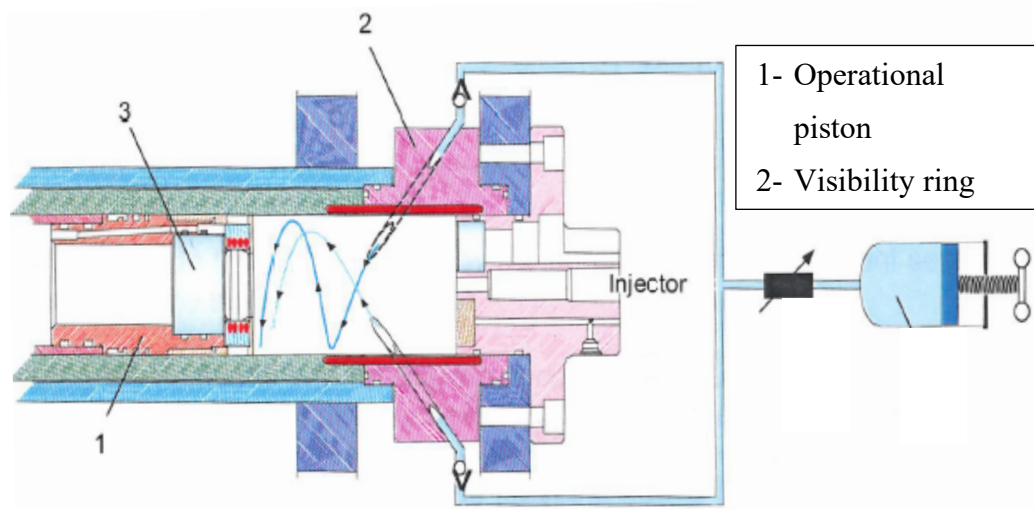


Figure 3-8 Models used in the RCM to produce swirl in the combustion chamber

Secondly, the air also can be blended in the mixing reactor as the mixture is prepared. It helps to improve the homogeneity of the mixture and air, achieving better and repeatable results.

Figure 3.8 is a standard mode of producing swirl. Two different channels are mounted tangentially to define the amount of air and fuel blowing into the chamber, leading to produce swirl just before the compression phase starts.

3.6.1 Non-premixed Air-fuel Injection

In this method, the fuel blend and air are mixed inside of the RCM chamber. To make sure that we test precisely the correct mixtures, it is necessary to flush the pipelines with the new mixture; thus, the previous mixtures tested in the RCM, do not affect the investigations of the new mixture. The fuel pipelines are then filled with the new mixture. First, the fuel fills the chamber up to a certain pressure, then the fuel valve is closed. As the chamber is vacuumed, the mixture occupies the chamber throughout. Then the air valve is opened. The air fills to the specified pressure and then the air valve is closed. This conventional method is not capable of mixing air and fuel as homogeneously as the premixed method.

3.6.2 Premixed Mode Premixed Air-fuel Mixing in the Reactor

It is aimed to have as homogenous an air-fuel mixture as possible. The air and the mixture were combined to improve the homogeneity causing more reliable combustion results.

3.7 RCM Simulation Setup

The first step of the experimental procedure is to prepare a desired composition of the combustible mixture through the partial pressure of each component. After that, by supplying compressed air from the bottle, the driving cylinder connected to the cam can move forward in a straight line. The rod on the cam pushes the piston towards TDC and thereby compresses the mixture in the combustion chamber. The time at which the mixture in the pre-chamber is ignited can therefore be controlled by the ignition plug. Once combustion is complete, the chamber is vented and flushed with air to remove any condensed water vapour and cool the RCM chamber to the initial adjusted temperature of the experiment.

3.7.1 RCM Combustion Model in AVL BOOST

An AVL BOOST model was created to simulate the in-cylinder conditions recorded in the experiments, in order to calculate the average in-cylinder pressure and heat release of the mixtures. The model was then calibrated and verified using different cases, to ensure the model was accurate enough for the engine conditions tested in this investigation (Version 2010). Figure 3.9 shows the AVL BOOST model used in this study.

Different groups of simulation packages such as BOOST, CRUISE and FIRE have been released to the market. The AVL BOOST package has been used in this study; which is applied to carry out thermodynamics' analysis. This platform is simulation software developed for the wide range of different types of engines.

It is capable of simulating an engine cycle including the combustion and emissions. The graphical user interface, an interactive pre-processor and post-processor are offered for fast analysis of the results and comparison with the experimental data. Moreover, it offers interactive context, efficient simulation; and an animated display of pressure profiles.

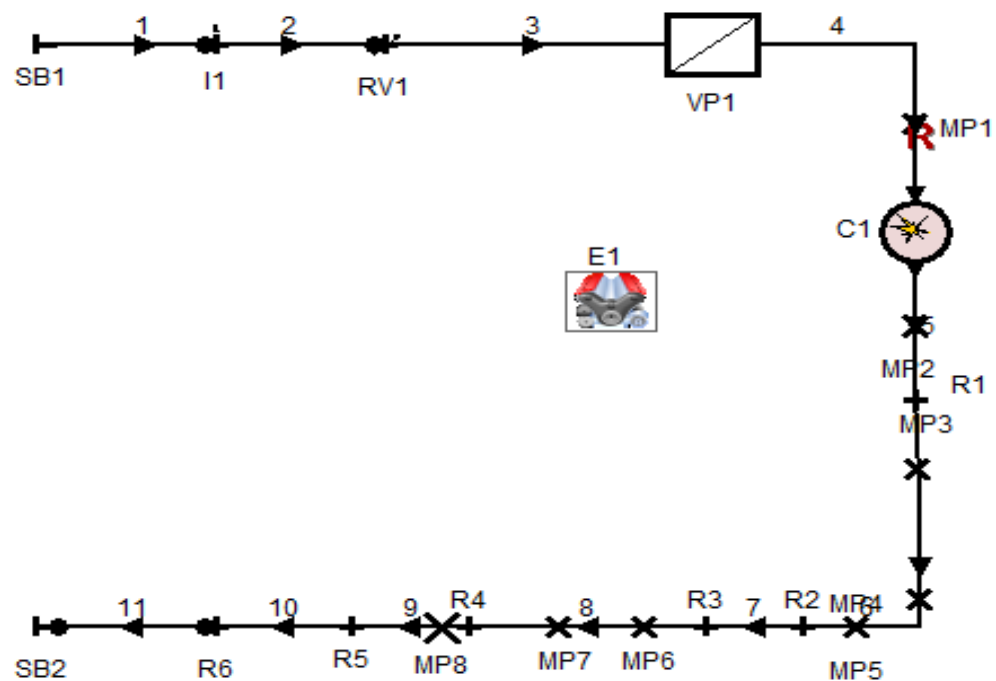


Figure 3-9 AVL BOOST simulation model

The following steps were taken into account in order to create the RCM model in BOOST:

1. Intake and exhaust systems and components were measured
2. Engine geometry such as the bore, stroke and port diameters were measured

3. The information was then used to construct the AVL BOOST model geometry
4. Relative piston motion was calculated for each individual test
5. Adjustment of the RCM speed in RPM with the Wartsila's real engine
6. Valve timing was chosen from the real engine with almost the same configurations for the RCM

3.7.1.1 Predefined Heat Release Method (Wiebe Function)

The Wiebe function is considered a simple method which exists to calculate the heat release in an engine over the cycle. Detailed knowledge of the rate of pressure changes is required since the rate of heat release is calculated. However, the Wiebe function relies on the location of just three key regions in the combustion cycle; which are defined as the flame development process ($\Delta\theta_d$), the rapid burn angle ($\Delta\theta_b$) and the overall burn angle ($\Delta\theta_o$). These regions are all demonstrated in Figure 3.10 (Heywood 1988, Moxey 2014). Thus, an accurate estimate can be calculated from the spark location and burn duration. Eventually, the Wiebe function can be accurate enough to obtain the heat release, if accurate in-cylinder pressure data is available.

The first phase of the spark ignition combustion engines is characterised by the interval of the spark discharge and the time when a small but significant fraction (usually 10%) of the cylinder mass has burnt. This is called flame development or ignition delay (Ali and Saraswati 2014). There is usually a very small noticeable heat release from the charge at the CA10 region. The heat release rate is affected by mixture

state, composition around the plug and the charge motion (Heywood 1988, Ferguson and Kirkpatrick 2015).

The burning rate decreases where much of the useful energy in the fuel is expended as the flame front spreads to the cylinder walls in case of non-knocking conditions. However, the burning rate depends on the in-cylinder turbulence intensity of the charge. This is affected by turbulence in the charge, as this may speed up or slow down the burn rate. The bulk of the charge is consumed by the combustion here; traditionally up to 90% of the charge will have been burnt by the time this stage is complete – this 10-90% MFB period is referred to as the combustion duration (Ferguson and Kirkpatrick 2015).

The final stage is one in which the remaining charge is burnt off. This region can prove difficult to calculate correctly due to the complex nature of the interactions of the flame with the walls.

These flame development definitions seem fairly arbitrary, but vital, as they are required for the Wiebe function which is defined below:

$$x_b = 1 - \exp\left[-a\left(\frac{\theta - \theta_s}{\Delta\theta_t}\right)^{m+1}\right] \cdot (100) \quad \text{Equation 3.8}$$

where $(\Delta\theta_t)$ is the total duration of combustion; x_b is the mass fraction burnt; θ_s is the start of combustion; and a and m are adjustable parameters used to smooth the curve to match reality.

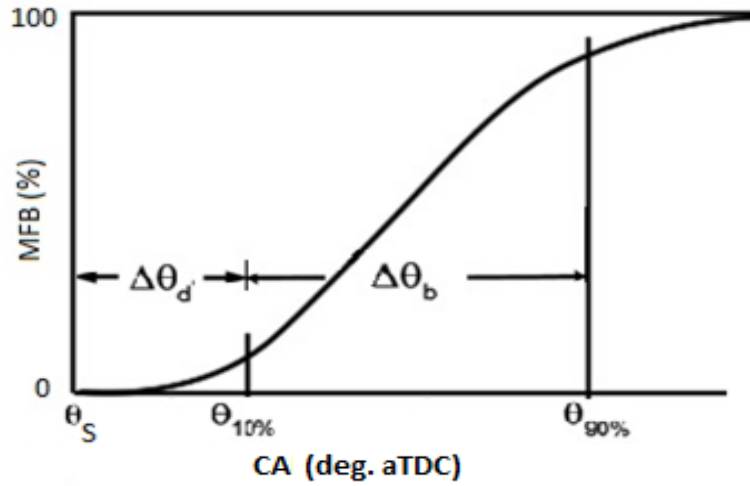


Figure 3-10 Key regions required by ROHR as flame development angle ($\Delta\theta_d$), rapid burning rate ($\Delta\theta_b$), shown as mass fraction burnt curve (Heywood 1988)

3.7.1.2 User Defined Heat Release Method (ROHR)

The first method, described by (Heywood 1988), assumes that combustion occurs over a finite time frame.

Theoretical pressure trace and heat release curve from an RCM cycle with the burn duration identified. The finite burn duration ($\Delta\theta_d$) extends from the start of combustion ($\Delta\theta_b$) to the end ($\Delta\theta_e$). The formula governing the energy in a system over small crank angle duration is expressed by:

$$\delta Q_{ch} = dU_s + \delta Q_{ht} + dW + \sum h_i dm_i \quad \text{Equation 3.9}$$

where:

δQ_{ch} – heat released from combustion

dU_s – internal energy of the fluid filling the engine cylinder,

δQ_{ht} – heat transferred to the engine walls,

$dW = pdV$ – work done by the fluid to the environment,

$\sum h_i dm_i$ – crevices losses in energy.

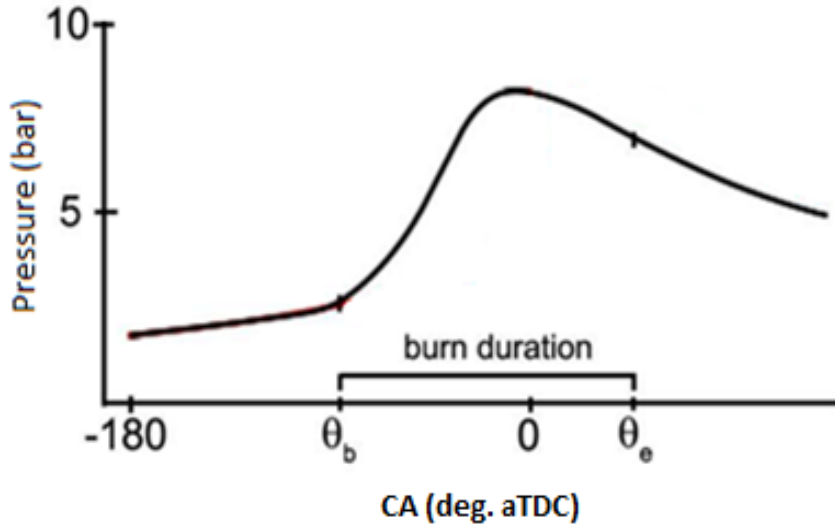


Figure 3-11 An example of general pressure trace and ROHR and combustion duration from RCM results at knock combustion

The internal energy increment considered as total differential from a product of mass m and the specific heat c_v and temperature T of the working fluid can be expressed by the equation:

$$dU_s = d(mc_v dT) = mc_v dT + mT dc_v + c_v T dm = mc_v dT + c_v T dm \quad \text{Equation 3.10}$$

Assuming that the c_v is constant and there is no mass transfer out the closed cylinder space $dm_i = 0$, dU_s can be determined as follows;

$$dU_s = mc_v dT \quad \text{Equation 3.11}$$

Hence, after rearranging the equation 3.9, its form is obtained for the net heat released δQ_{net} , which is not influenced by the heat losses δQ_{ht} to the walls.

$$\delta Q_{\text{net}} = \delta Q_{\text{ch}} - \delta Q_{\text{ht}} \quad \text{Equation 3.12}$$

next, taking the differential form of the equation of state as follows

$$Vdp + pdV = mRdT \quad \text{Equation 3.13}$$

Then, rearranging it to the form

$$mc_vdT = \frac{c_v}{R} (Vdp + pdV) \quad \text{Equation 3.14}$$

then, substituting it to the equation 3.11 and then to the equation 3.12. We finally obtain the equation 3.15

$$\delta Q_{\text{net}} = \left(\frac{c_v}{R} \right) Vdp + \left(\frac{c_v}{R} + 1 \right) pdV \quad \text{Equation 3.15}$$

Considering the relations (Eq. 3.16), (Eq. 3.17) and (Eq. 3.18) C_v and the universal gas constant (R) and both the specific heats

$$R = c_p - c_v \quad \text{Equation 3.16}$$

$$\gamma = \frac{c_p}{c_v} \quad \text{Equation 3.17}$$

$$\frac{c_v}{R} = \frac{1}{\gamma - 1} \quad \text{Equation 3.18}$$

The final equation for the net heat δQ_{net} over the crank angle increment $d\theta$ can be driven as follows:

$$ROHR = \frac{dQ_{\text{net}}}{d\theta} = \frac{1}{\gamma - 1} p \frac{dV}{d\theta} + \frac{\gamma}{\gamma - 1} V \frac{dP}{d\theta} \quad \text{Equation 3.19}$$

Where:

γ – ratio of the specific heats at constant pressure and constant volume, respectively,

P – in-cylinder combustion pressure,

V – in-cylinder volume,

θ – crank angle (CA)deg.,

Q_{net} – net heat released during combustion.

The equation 3.19 is applied for rate of heat release (ROHR) determination in the ICEs.

In accordance with this equation, combustion progress can be expressed by the cumulative heat Q_{net} , which can be determined through integrating it over the θ . If someone assumes that the Lower Heating Value (LHV) of the fuel does not change at elevated pressure and temperature, then the heat released from combustion process can be expressed as a product of the fuel LHV and the fuel mass burnt $M_F(\theta)$. Thus, progress in combustion can be quantitatively described by the normalized function as the MFB (Mass of fuel Fraction Burnt) defined as follows:

$$MFB(\theta) = \frac{M_\theta(\theta)}{M_T} = \frac{Q_{net}(\theta)}{Q_{net}} \quad \text{Equation 3.20}$$

Where:

M_F - mass of the fuel burnt since start of combustion up to the current crank angle θ ,

M_T - total mass of the fuel burnt in the single combustion event.

Although the MFB function is often used in the engine combustion analysis, difficulties might be encountered for anyone who wants to compute progress in combustion in the internal combustion ICEs on the basis of this equation 3.19 (Heywood 1988, Szwaja 2011, Ferguson and Kirkpatrick 2015).

In essence, this is the ratio of the cumulative heat release to the total heat release in the event. While it may not take into account the differences in temperature between the burnt and unburnt, (Yeliana, Cooney et al. 2008) showed that Rassweiler and Withrow method produced comparable mass fraction burnt curves as both the single-zone and two-zone models while being easier to solve (Heywood 1988, Stone 2012).

3.7.2 Thermodynamic Analysis

Thermodynamic combustion models can be considered in two different ways. First, the models are created to understand and predict the behaviour of the engines. This can be simulated by the researchers to figure out what may occur in the system without running the experiments. Second, the empirical data can be used to validate, and expand upon, the original data. Thermodynamic models can be referred to as either “one-dimensional” or “multidimensional. One-dimensional thermodynamic analysis operates on a single normal to the flow and uses a simplified description of both physical and chemical processes occurring in the combustion chamber - usually the Wiebe function. Multidimensional thermodynamic analysis uses some flow characteristics which are known as having been obtained via CFD or similar flow

modelling; which provide a greater understanding of the air/fuel mixing and subsequent combustion in three dimensions about the chamber (Galindo, Climent et al. 2011).

Prediction of the in-cylinder pressure and temperature are affected by the combustion process; thus, simulation of the combustion in ICEs becomes necessary to predict the engines' performance. There are several approaches to simulate combustion; such as, the computational technique which needs large computational time and effort. On the other hand, the Wiebe function (Wiebe 1956) is appropriate to be used in a 1D engine code; however, it lacks physical representation. This method is traditionally the most widely employed, the main drawback is the determination of the four Wiebe parameters needed to build up the in-cylinder rate of heat release (ROHR).

The first law of thermodynamics in the cylinder closed cycle with the aid of experimental data (mainly instantaneous in-cylinder pressure) should be obtained to determine the ROHR (Lapuerta, Armas et al. 1999). More models have been defined to simulate the open cycle to capture the in-cylinder trapped mass (Payri, Molina et al. 2006). Moreover, the ROHR determination can be copied with the empirical assistance and convenient use of theoretical models. The parameters which are used in the Wiebe function for different simulations still remain unclear; there are even several studies in the literature which did not help with the correlation for those parameters. Those empirical models have been developed for 0-90% mass fraction burnt angle (Lindström, Ångström et al. 2005, Bonatesta, Waters et al. 2010).

Here, in this study, a one-dimensional method of analysis is used, so that empirical methods can predict and then validate the experimental data due to absence of a fully

validated model of the charge motion for the RCM. Furthermore, due to the expense and physical difficulty involved with attempting to measure the burnt and unburnt gas temperatures needed for laminar burning velocity calculations, it was decided that using the commercial simulation software, AVL BOOST to model the engine and extract the required data would allow for characterising engine operation, without the need for high-end processing and time-intensive computations. At its core is an engineering code that is designed to analyse the dynamics of the pressure waves, mass flows and duct/flow interactions (Moxey 2014).

3.7.3 AVL BOOST Combustion Model Calibration and Validation

The RCM model needs to be calibrated with the parameters such as, air/fuel ratio, initial pressure and temperature, valve timing, compression ratio, piston motion and heat transfer. The calibration algorithm is shown in Figure 3.12.

These parameters are of high importance; thus, the RCM emulates only compression and partial expansion processes. Valve timing is not applicable in this machine due to the absence of both connecting-rod and crankshaft and consequently free movement of the piston.

The in-cylinder pressure trace and ROHR are two sources for models to be validated. As the curve has been specified in the SI Wiebe dialog box, it is expected to conform to the supplied data. Upon checking, this was found to be the case, with some

errors. However, when the in-cylinder pressure trace was superimposed onto the

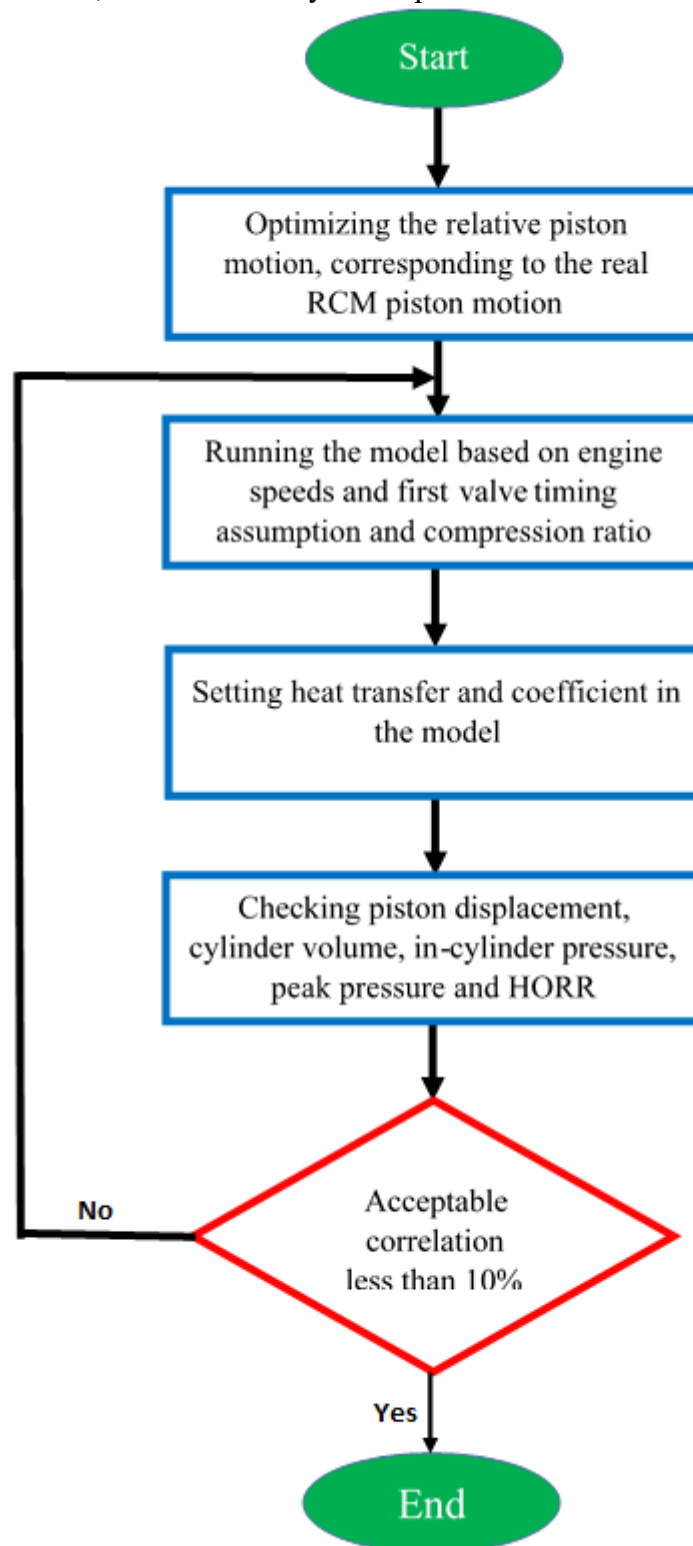


Figure 3-12 AVL BOOST calibration algorithm

empirical data it was clear that the AVL BOOST model was not accurate enough. The calculated ROHR is used to improve the accuracy of the model. Although influences

of the heat transfer and heat losses in ROHR calculation are not taken into consideration due to too many complexities, the ROHR is able to increase the reliability of the model. The ROHR is calculated on the experimental pressure trace and instantaneous volume obtained based on the piston motion. Therefore, as it is expected, we get better resolution and lower errors between the experiments and modelling. The results will be indicated in each section based on the fuels tested.

3.8 Experimental Test Procedure

Safety is the main issue which must be taken into account before the tests start. In the second stage, the mixture needs to be prepared. The mixture system needs to be warmed up to 50 °C before the start of the mixing. Meanwhile, the tank is flushed with N₂ for 3-4 times to ensure there are no gases from previous tests in the tank. Gas proportions must be specified in the mixture interface software and the software is then ready to start mixing. There is a chromatograph next to the mixing tank, examining the mixing accuracy.

There are some preparation procedures which are of high importance before starting the tests. As the oil can penetrate to the pneumatic area in the RCM, it can cause inaccuracy in the force applied by the piston. Before starting the tests, “removing oil from driving pressure” must be run. Furthermore, “calibration” of the piston position must be run before the test and after each 10 shots. This calibration helps to locate the piston at the exact position necessary.

The baseline operating conditions should be examined to identify the new recorded data are the same as the previously recorded accurate baseline. If there is a significant variation between the two, then the issue must be identified and resolved before repeating the baseline test. The procedure should be repeated until the engine results on the particular day conform to the previously determined baseline conditions.

Before starting the tests, the RCM cylinder needs to be warmed to 82 °C, to stabilize the combustion chamber's temperature; as an automatic thermocouple is used to measure and heat up the chamber because the temperature drops. The procedure of achieving the set-point will be explained in the following chapters.

Once the RCM is ready for real tests and producing reliable data, based on the mixtures, the fuel, and air and driving air pressures are loaded, respectively. Finally, the RCM is ready to operate. The driving air pressure is increased after each shot to achieve the threshold knocking operating condition. Once the post-processing data is released, and the pressure trace is no longer normal, then the driving air pressure must be reduced; this is called “knock threshold operating condition of the specified mixture”. The knock threshold operating conditions are repeated for 7 shots to investigate the consistency of the tests.

Chapter 4 - FEASIBILITY OF METHANE-PROPANE MIXTURES' COMBUSTION CHARACTERISTICS

4.1 Introduction

Nowadays, there are major initiatives to reduce dependence on fossil energy resources. These initiatives are focused on the large reciprocating engines, and often seek to replace conventional liquefied fuels with gaseous fuels.

Natural gas, as the high methane number container, is used in most gaseous; engines, while the price of this fuel increases, no longer it is beneficial to feed natural gas to the sectors. The manufacturers are limited by emissions' legislation. Therefore, alternative gaseous fuel behaviours should be investigated, to fulfil the new regulations and compete in the market.

Before using the new RCM for combustion-related studies, the air/fuel ratio and spark timing of the machine must be characterized. In the previous chapter, the experimental conditions, simulation assumptions and RCM operation have been expressed, and finally the test procedures were represented.

A large portion of this chapter is dedicated to assess the accuracy, repeatability and reproducibility (ARR) of a wide range of test conditions by investigation of the combustion characteristics of various mixtures of methane-propane, in order to provide high reliability of experimental data.

To investigate the ignition delay, combustion strategies have been conventionally used. Methane-propane mixtures have been investigated to figure out a systematic methane-propane reference curve. It helps to investigate the reaction of the unknown

gases by running them in the RCM, which reduces the practical experiments' expenses and the time consumed.

In this chapter, the experimental results of the combustion characteristics of the methane-propane and their blends have been presented. The rapid compression machine described in Chapter 3 was employed to measure the instantaneous in-cylinder pressure within the combustion chamber, during and after compression. From the measured in-cylinder, temperature, pressure of the ignition delay, peak pressure, EOC pressure and SOC pressure have been obtained.

In this chapter, the results are given in terms of pressures measured in the RCM during and after compression, as well as with ignition delays, which are derived based on the pressure traces.

The fuel and "air" were fed into the RCM in two different ways: first, fuel and air were fed into the chamber separately; second, the fuel and air were partially premixed in the separately heated mixing vessel for approximately half an hour to ensure proper homogeneous mixing. However, the mixing time increases as the number of mixing components rise. The partial pressure and required volume for each fuel injected into the mixing reactor were obtained from their mole fraction and total pressure for the certain energy content. These calculated values were always checked and they were within ± 100 Pa.

The required volume of each fuel injected into the mixing chamber was obtained from their mole fraction and total pressure; and the partial pressure obtained from the

addition of each individual fuel, was checked against the calculated partial pressure and the values were always within ± 100 Pa. To ensure each individual blend was fully vaporised, the settings were adjusted based on the lowest vapour pressure of the fuel component mixed.

4.2 Tests Fuels

Methane and propane with different blend proportions are used in this chapter to examine the ARR (accuracy, repeatability and reproductively) of the RCM; ultimately creating a methane-propane reference curve to investigate the highly unknown methane number (MN) gases. Thus, in pursuance of fulfilling this goal, methane and propane are selected due to the fact that based on the real engine results, this mixture has the most stable behaviour among the other higher MN blends.

Table 4.1 Properties of the gaseous fuels tested in this work with the RCM

Specifications	Base Methane (100%) Propane proportion mixture (%Vol.)			
Methane proportion (%Vol.) A	100	90	80	70
Propane proportion (%Vol.) B	0	10	20	30
AFR stoichiometric (Vol.)	9.52	10.95	12.33	13.7
Final fuel pressure (bar)	0.18	0.16	0.14	0.12
Final air-fuel pressure (bar)	2.28	2.24	2.2	2.18
X (number of moles of air per mole of fuel in mixtures)	9.52	10.95	12.37	13.8
LHV mixtures (MJ/nm ³)	35.88	41.61	47.34	53.07
Fuel temperature at mixing reactor	323 K			
Fuel temperature at chamber	354 K			

Ignition delays and peak pressures were measured in this study for methane and propane. The properties of methane-propane mixtures are summarized in Table 4.1.

4.3 Modifications Made to the RCM during the Research

The RCM used in this research is one of the first RCMs to operate based on the gaseous mixtures, so various techniques have been taken into consideration to figure out the best performance of the RCM and gain the most ARR results. It was required to examine the behaviour of the RCM under different conditions and various methods. The techniques maintain the possibility to improve the test bench with the desired operating conditions of the real engines. The modifications made to the RCM are explained in more details in the following subsections.

4.3.1 Combustion Cylinder and Chamber Heating Modification

The importance of temperature uniformity and stability in the test chamber is paramount when gathering peak pressure and compression ratio to support the RCM's reliability. Reference temperatures used to characterize the measurements must be accurately known, otherwise, there will be large errors in the results. Variation in the initial temperature is amplified, since the compressed temperature conditions are calculated, leading to inaccuracy of combustion peak pressure and compression ratio.

The in-cylinder temperature of the RCM was investigated to figure out the stable temperature condition in the chamber during the tests. As explained previously, heating elements are mounted through the piston liner and piston bowl. The exterior surface of the cylinder is also supported by a trace cable which can be heated up to 80 °C, as shown in Figure 4.1.



Figure 4-1 Trace heating cable system spinning through the outer surface of the RCM cylinder

The wall heating elements and piston bowl elements heated up to 110°C and 75°C, respectively. While the elements reached the set points after one hour, the temperature of the chamber was not stabilized even after three hours. According to the temperature gradient rise, it can be clearly seen that the heating set points were too high for being stabilized. Therefore, the set points were re-defined and reduced to 93°C and 80 °C; however, the RCM cylinder was pre-heated by a trace cable during the previous night to achieve 60 °C, as expressed in Figure 4.2. The interior heating elements were switched on and the system could stabilise itself at 80°C in less than two hours (Figure 4.4).

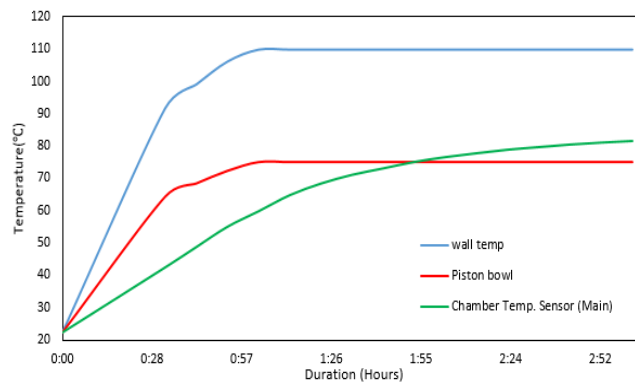


Figure 4-2 First test of temperature behavior of the pre-heating system in RCM, setting points of 110 °C and 75°C, without a trace heating cable

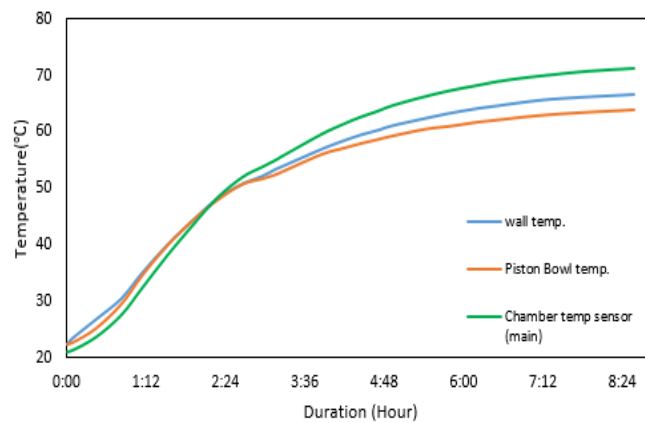


Figure 4-3 Temperature test behaviour of pre-heating system in the RCM, only with a trace heating

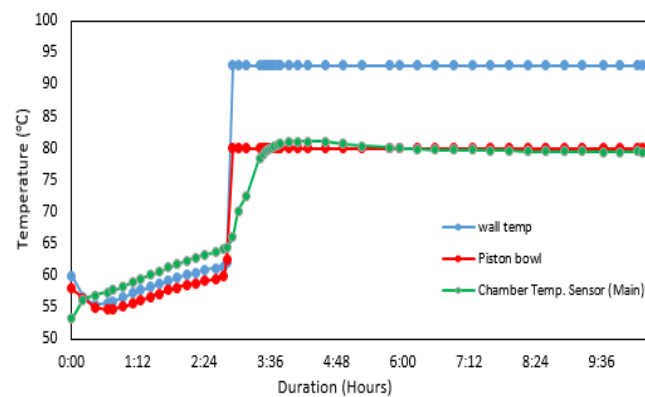


Figure 4-4 Temperature stabilizing tests of pre-heating system in RCM with setting points of 93°C and 80°C, with initial trace heating

4.3.2 Driving Pressure Accuracy Improvement

Two 10-litre air reservoirs are attached to the pneumatic chamber to support the initial pressure throughout the stroke in order to reduce the speed of the piston between 500 rpm and 2000 rpm (according to the Wartsila's engines). The pneumatic chamber is filled to a certain pressure by the compressed air at the beginning of the test. Fuel and air then are fed into the combustion chamber since this process lasts around 2-3 minutes. The filling period is enough for the compressed air in the pneumatic chamber to leak by 1 bar. Thus, the software is upgraded to re-fill the pneumatic reservoir to the certain pressure, after air/fuel are added into the combustion chamber.

4.3.3 Valve and Check Valve Modification

As the combustion chamber is vacuumed, the pressure difference before and after the air and fuel valves leaks if the valves' functionality fails. There was a random variation in the results and it found that there are two possibilities:

- Fuel leaks to the air pipeline
- Miss-functionality of the sealing component of the valves

There used to be a long distance between the check valve and the air valve. If the check valve fails to keep the fuel pressure in the combustion chamber, a small amount of fuel penetrates to the air pipeline; since the air valve starts filling the chamber, then the air-fuel ratio decreases. So, the air valve has been replaced exactly behind the check valve. Furthermore, the software has been updated to keep the valve closed, except during the air feeding period.

The valves used in the RCM can tolerate up to 300 bar. They function better as the pressure increases, while the fuel is fed into the cylinder to very low pressure, the leaking probability rises. It was found that there is a sealing component inside the valve which functions perfectly to around 500 shots and needs to be replaced afterwards.

4.3.4 Piston Damping Modification

As described in the previous chapter, the RCM is a single piston horizontal machine which is pneumatically driven by compressed air and damped hydraulically. The compressed air charge strongly depends on the mixtures tendency to knock. The fuel mixtures with high methane number (MN) have higher resistance against knocking and consequently higher driving pressure should be applied.

The damping issue has appeared since the heavier hydrocarbons chain has been used. The piston tube hits the RCM body after combustion and it leads to damaging the parts, since the methane has been mixed with small proportions of n-pentane. Therefore, a new method has been investigated. A check valve is placed in the driving volume section; it prevents the driving pressure releasing as fast as before. As the investigations represent in the following chapters, it has improved the damping issue.

4.4 Challenges and Limitation Related to the RCM's Performance

For many decades, different methods have been proposed and developed to ensure the ARR of the RCMs. There are some limitations that arose in practice, in achieving

the goals. Therefore, the main parameters which govern the operation of the RCM have been described in the following sections.

4.4.1 Ideal and Non-ideal RCM Operation

The accuracy and repeatability of the RCM results depend on how similar the operating conditions are arranged in the machine. The first aim after compression is to achieve a uniform temperature of the charge. It is possible to achieve this uniform temperature distribution by an adiabatic core assumption. It means that the core gas which is away from the thermal boundary layer is isentropically compressed to a uniform temperature. The thin boundary layer along the walls and the core charge is unaffected by the heat loss to the walls during and after compression. The unaffected area is called the core region, in which the temperature is assumed to be uniform.

To achieve this condition, the piston should be ideally compressed very quickly, in order to minimize the heat transfer between the core gas and the boundary layer. Thus, it is considered as homogeneous. The compression time for the RCMs typically are around 20-50 ms; however, the final half of compression is important because RCMs only simulate the combustion phenomenon of real engines. This time commonly is in the range of 1-5 ms. After compression, the reaction chamber volume starts increasing, with the piston pushing back towards bottom dead centre (BDC) instantaneously, with few rebounds.

4.4.2 Core Gas

Ignition delay times are usually measured by recording end of compression (EOC) pressure and temperature conditions. A high response dynamic pressure transducer is usually used to measure the pressure; it is installed with the reaction chamber wall. On the other hand, it is not possible to measure the temperature of the chamber instantaneously after the compression process; thus installing a thermocouple also might affect the aerodynamics of the flow in the chamber. Besides, non-intensive optical methods are difficult to set up and require extensive calibration. Subsequently, the adiabatic core hypothesis is an indirect method to determine the temperature.

This method has been previously validated experimentally (Das, Sung et al. 2012) and computationally (Mittal, Raju et al. 2008). The isentropic temperature of the gas in the core region at the end of compression can be obtained according to the following relation:

$$\int_{T_i}^{T_{ad}} \frac{1}{\gamma-1} \cdot \frac{dT}{T} = \ln (CR) \quad \text{Equation 4.1}$$

Where, T_i is the initial temperature; γ is temperature dependent specific heat ratio; and CR is the compression ratio.

As the piston in this RCM must travel twice as far as in normal engines, so the compression is not entirely isentropic, and it causes a little noticeable heat loss, resulting in lower values of pressure and temperature than the predicted by the isentropic process. Previous studies by (Desgroux, Gasnot et al. 1995) and (Griffiths, Halford-Maw et al. 1993) have shown that the adiabatic core assumption can be

reasonably met, by using an effective compression ratio modified by heat transfer to the wall. This effective compression ratio can be obtained by using the actual measured pressures within the core region by the following relation:

$$\frac{P_0}{P_i} = (CR)^\gamma \quad \text{Equation 4.2}$$

Based on this assumption, the end of compression temperature, T_o , is calculated from:

$$\int_{T_i}^{T_o} \frac{1}{T} \cdot \frac{dT}{\gamma-1} = \ln \left(\frac{P_o}{P_i} \right) \quad \text{Equation 4.3}$$

where P_i is initial pressure; P_o is end of compression pressure; and the other variables are the same as in Equation 4.1 (Materego 2015).

4.4.3 Effects of Heat Loss on RCM Operation

As the compression is not instantaneous, heat loss occurs because it is affected by compression time scales. Consequently, the pressure and temperature become lower than what is expected from the adiabatic calculations. According to the previous studies conducted on the RCM heat losses, pressure drops approximately 20%; it may increase since the ignition delay times have as longer delay (Goldsborough, Banyon et al. 2012). No ignition can occur since the ignition delay time excesses lead the heat loss to quench the chemical reactions. Although the measured ignition delay times are usually associated with the end of compression conditions of temperature and pressure, these conditions may not remain uniform during the delay time. Consequently, the measured delay times are not associated with end of compression conditions.

The compression process does not instantaneously occur and consequently, it leads to chemical reaction during the process (Griffiths, Halford-Maw et al. 1993, Cox, Griffiths et al. 1996, Mohamed 1998). Slow compression causes increasing temperature leading to chemical reactions. Thus, the compression time, particularly t_{50} , acts as a limiting factor for accurate delay time measurements of very reactive fuels (Materego 2015).

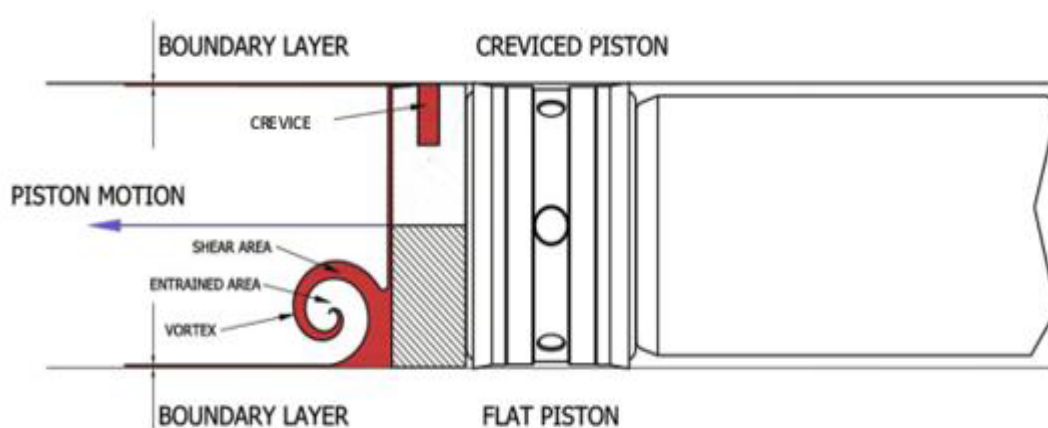


Figure 4-5 Piston motion creates roll up vortex during compression in lower section and containment of boundary layer through a crevice (upper section) through proper design (Sung and Curran 2014)

In an ideal condition, the mixture is assumed to remain homogeneous within the chamber before, during and after compression. However, the mixture's homogeneity is affected by the complex flow inside the chamber, which is affected by the temperature distribution, due to the high speed of the piston's movement when suddenly brought to rest at the end of the compression process.

According to several studies (Lee and Hochgreb 1998, Würmel and Simmie 2005, Mittal and Sung 2006), results show the generation of a roll-up vortex, caused by the

piston scraping off the cold boundary layer during compression. It results in inhomogeneous mixing between colder gas from the cylinder wall and hotter gases in the core zone; however, this can't be exactly characterised. To cope with the issue, RCMs have been specially designed with crevices on the sides of the piston, leading to suppression of the vortex formation during the compression. It finally causes the limiting of the displacement of the colder gas to the core zone. Sung and his colleagues used this method to suppress the issue as shown in Figure 4.5 (Sung and Curran 2014). Besides, Würmel predicted the temperature field by using CFD, and showed improvement when a creviced piston head was used. There was a more uniformly distributed temperature in the combustion chamber, as shown in Figure 4.6 (Würmel and Simmie 2005).

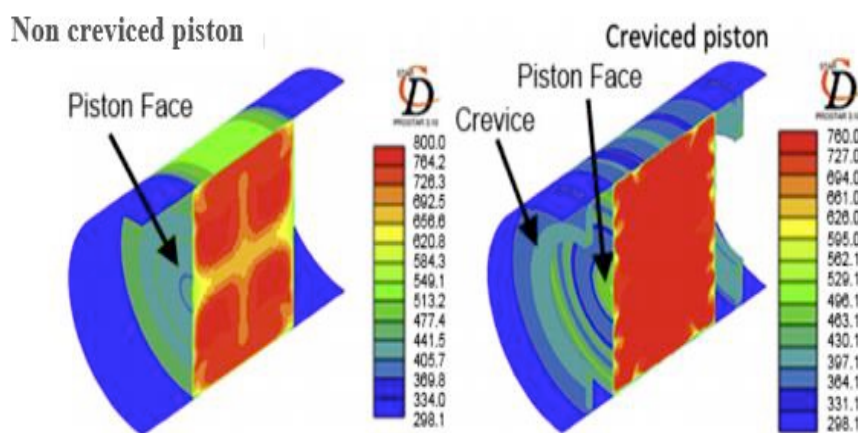


Figure 4-6 Comparison of predicted temperature fields at 10.4ms from the end of compression for N₂ gas using creviced and non-creviced piston heads (Materego 2015)

4.5 Test Condition and Test Methods

Peak pressure and compression ratio were measured in the RCM for different propane proportions blended with methane (baseline); since the threshold operating conditions of the fuels were adjusted by changing the driving pressure. The mixtures' reactivity changes were prepared with dry air containing 21% O₂ and 79% N₂. The compressed temperatures and pressures are attained through a combination of changes in compression ratio and by changing the initial temperature and pressure of the charge. Initial temperatures were changed by temperature investigation discussed in section 4.4.1; and 81 °C (±2) was selected to ensure complete fuel vaporization, which has been confirmed using GC/MS analysis.

In this study, a spark plug was mounted in the RCM pre-chamber to ignite the mixture; while in most of the research carried out on RCMs, it has not been used. Besides, as mentioned previously, an RCM has a variable compression ratio due to the free movement of the piston (absence of con-rod). Thus, the spark timing is of high importance. Two methods were chosen: first adjust the spark timing with respect to 155 mm aBDC (after bottom dead centre) and second; 10 mm bTDC (before top dead centre). The test was done with lambda 1.5 for this investigation.

On the other hand, from the spark timing investigation it found that lambda 1.5 could not produce ARR, thus, it was necessary to investigate the lambda which could produce ARR. Therefore, ultra-rich-to-lean mixtures were prepared. Ignition delay, combustion occurrence and their errors were investigated. The proper lambda and spark

timing were adjusted and finally, reactivity mixture tests were selected with lambda 1.2 and spark timing of 10 mm bTDC, as concluded according to the results.

Experimental results then were calibrated and validated with the models simulated in AVL BOOST platform to investigate the heat release rate for selected mixtures.

4.6 Lambda Investigation based on the Methane-Propane Mixture

It was found that lambda needs to be finely-tuned, in order to reduce the misfiring combustions and reduce errors of both peak pressure and compression ratio. It was assumed it would be most preferable to start the tests with very lean mixtures and continue to the very rich mixtures. It helps to figure out the combustion interval occurrence. The ignition delay and peak pressure were investigated. Lambda was chosen based on the longest to the shortest possible error in the ignition delay time.

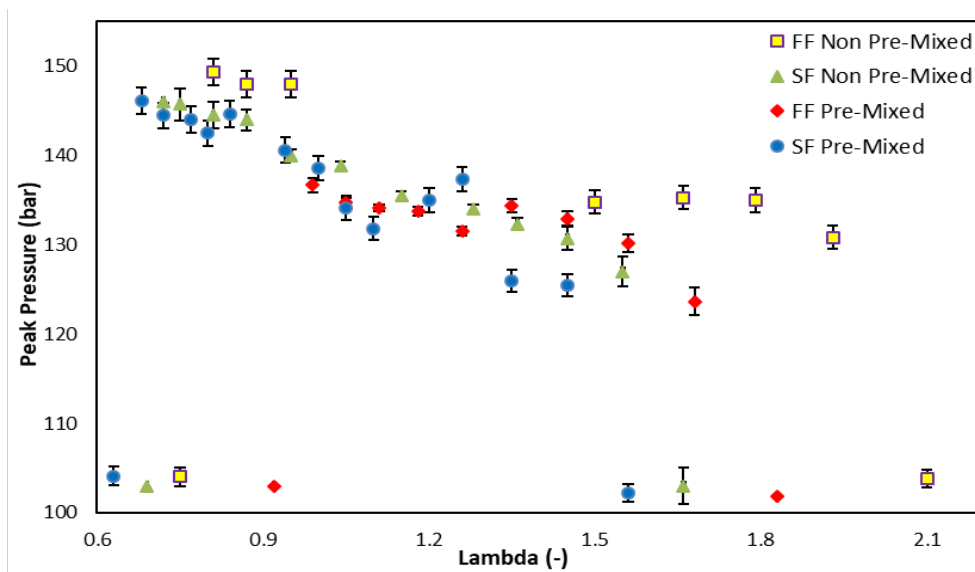


Figure 4-7 Effects of slow and fast flow rate and lean-to-rich mixtures on the peak pressure and ARR

Ignition delay times show how fast chemical reaction occurs and mixtures burn during the combustion process. Figure 4.7 shows as the lambda goes away from stoichiometric condition. As the mixture approaches towards either leaner or richer conditions, the repeatability and accuracy of the results drop. Several tests were carried out to investigate the proper flow rate of filling fuel into the cylinder; in pursuance of fulfilling this goal, a throttle was mounted to check the flow rate of the mixtures. The mixture was fed into the combustion chamber in the range of lambda 0.7 to 1.9, since the flow rate was changed to a fast, normal and slow rate.

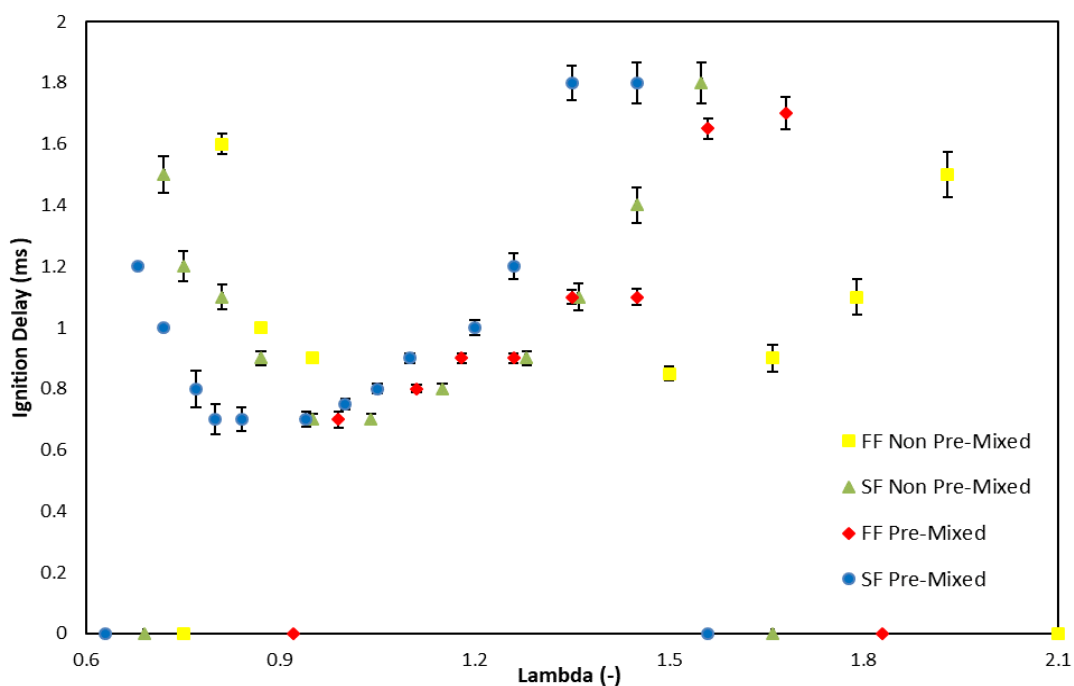


Figure 4-8 Effects of slow and fast flow rate and lean-to-rich mixtures on the ignition delay time and ARR

Here, ignition delay is important to investigate the homogeneity of the mixtures at the end of the compression, which represents the reactivity of the mixtures before combustion occurs. Moreover, as the ignition delay time rises, it may increase the probability of either not completing combustion or misfiring. Stoichiometric mixtures,

as well as rich mixtures close to stoichiometric, have the most reactivity to combust and propagate the mixture; while, either ultra-leaner or -richer mixtures have longer ignition delay times, as shown in Figure 4.8 (SF: Slow Filling; FF: Fast Filling). In the highlighted region, fuel takes only 0.7 ms to combust, since in the other regions delay takes 1.8 ms to ignite. Besides, the proper time for ignition delay in normal SI engines is 0.5-0.8 ms.

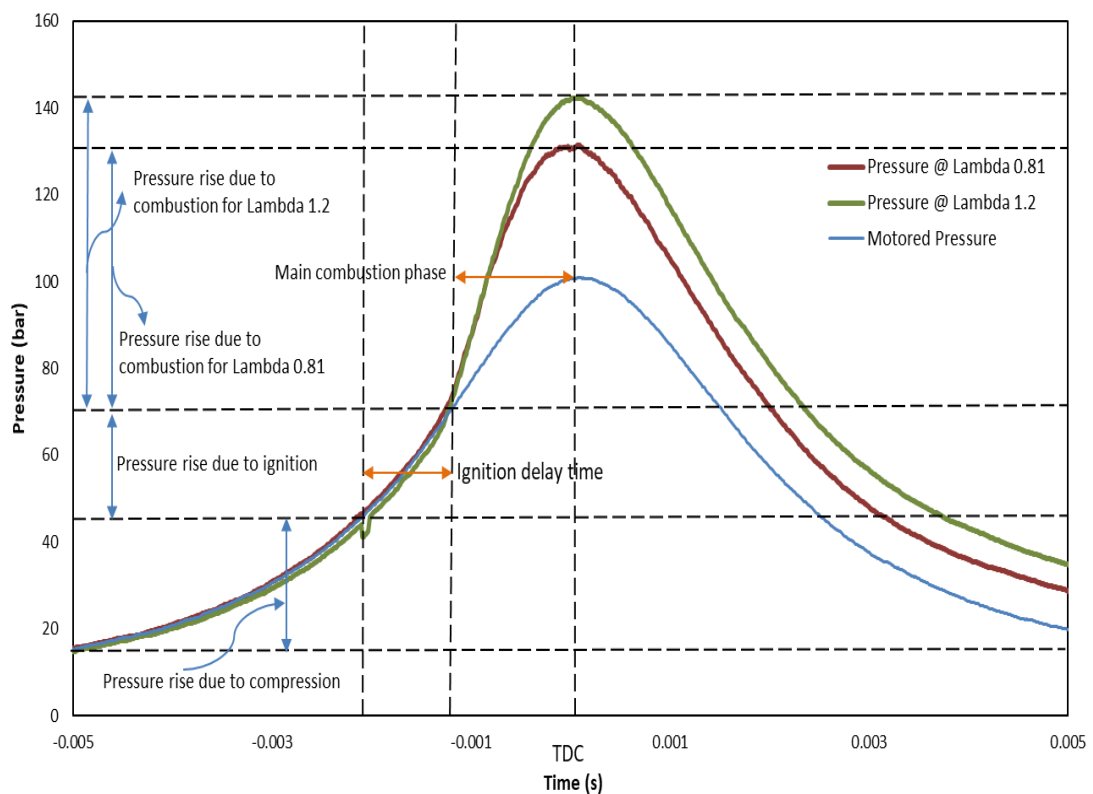


Figure 4-9 An example of a typical pressure trace of the mixture filling the chamber with a fast flow rate and lambda of 0.81, 1.2 and motored pressure

Here there is an example of how the compression, ignition timing and combustion phases were assumed and calculated. In the RCM, the piston starts moving toward TDC, so that the first 20 mm moves very slowly and then it is shot very fast based on the charged driving air pressure. The compression process is assumed as the period of

fast piston movement and lasts until the spark plug ignites the fuel and the piston reaches TDC. There is a very short gap between spark ignition and start of combustion (SOC), named the ignition delay. The steepest pressure rise point is considered as the main combustion phase and the combustion starting point, as shown in Figure 4.9.

4.7 Variable Spark Timing

Spark timing is one of the important parameters necessary to increase the power and fuel economy. It is adjusted before top dead centre (bTDC), discharging the energy prior to the clearance volume (TDC), since one of the purposes of the advance spark timing is for the fuel to be burnt completely, while it produces the highest possible power to expand the combustion chamber.

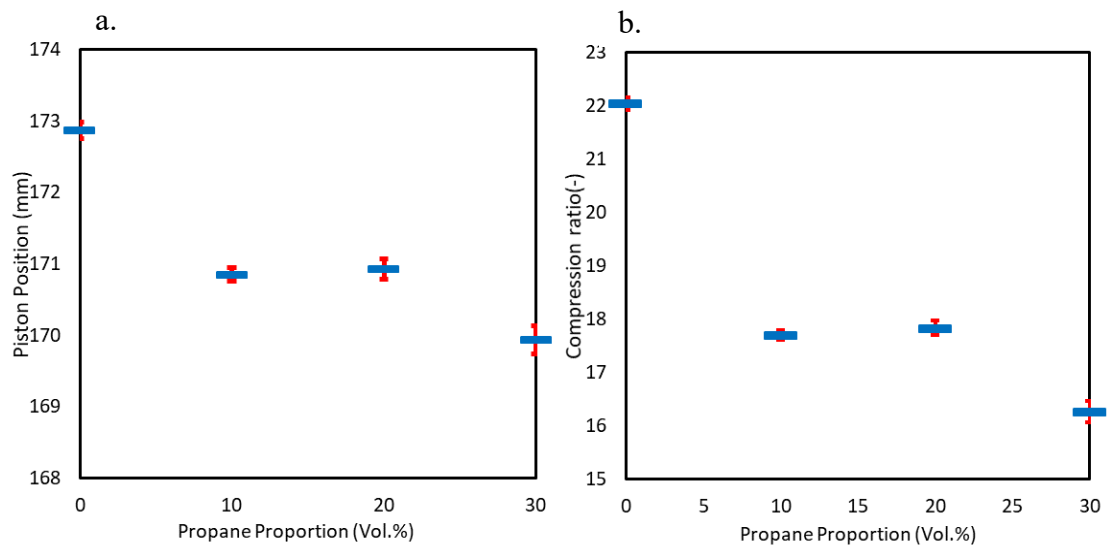


Figure 4-10 (a) Piston position (b) calculated compression ratio: of the RCM tests with a spark timing constant of 155 mm aBDC, with blending different propane proportions in the methane.

In the literature, the RCMs used in most studies are based on compression without a spark plug. In this study, a new set-up was used and a spark plug equipped on the centre of the cylinder head. Different strategies were used to find out the effects of the spark timing and then adjust the optimum spark time advance. First, the spark timing was set at 155 mm aBDC. This assumption was taken due to the uncertainty of the piston stroke as mentioned previously, it was affected by the mixtures' reactivity.

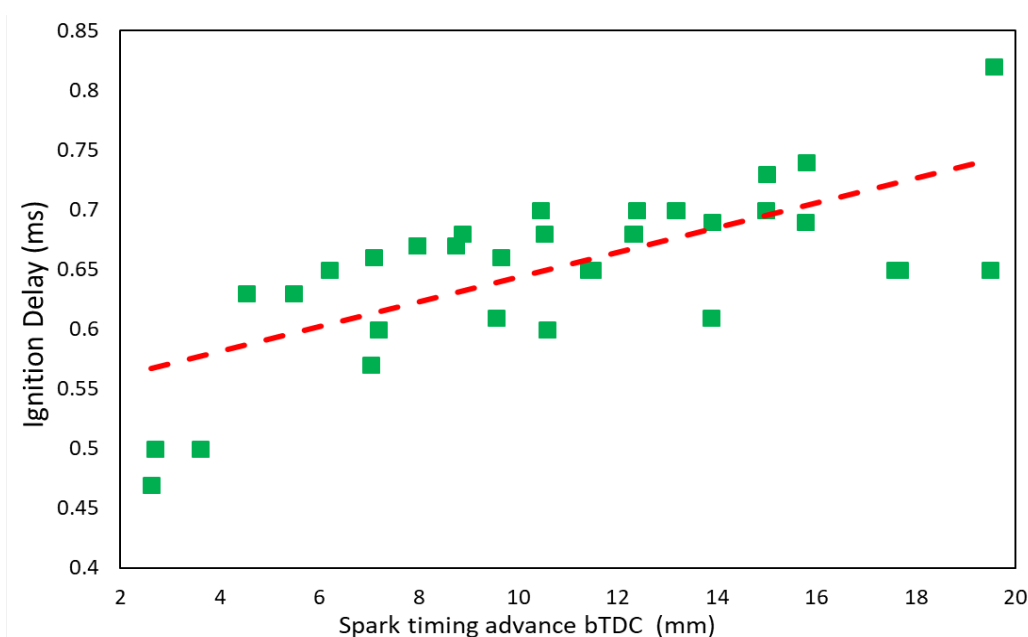


Figure 4-11 Influences of the variable spark timing on ignition delay of the mixture of methane 50% and ethane 50%

It is obvious that methane has the highest knock resistance. Knocking probability increases as heavier hydrocarbon (here, propane) is blended into the methane; consequently, both peak pressure and compression ratio reduce. Piston position and compression ratio are shown in Figures 4.10(a) and 4.10(b), respectively. Piston position and compression ratios demonstrate as propane content increases, mixtures are more prone to knock, however, there are some inaccuracies, so that in an 80% methane

and 20% propane mixture, piston moves further than in a 90% methane and 10% propane as it can be clearly seen in Figure 4.10(a). As the compression ratio is obtained with respect to the piston motion, CR has also the same behaviour, as shown in Figure 4.10(b).

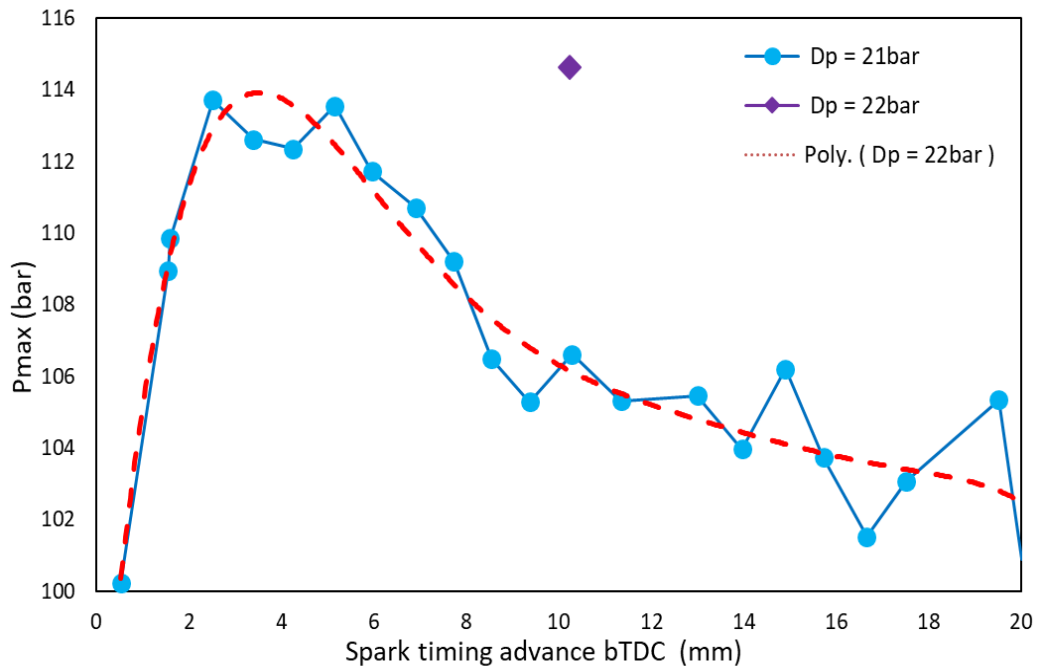


Figure 4-12 An example of the influences of the variable spark timing on the peak pressure since the spark varies from 1 mm bTDC to 20 mm bTDC with the mixture of methane 85% and propane 15%

According to the observations and investigation conducted on the spark timing of the RCM, (155 mm aBDC), it found that the piston stroke and CR fluctuates with different mixtures of methane and propane. In addition, the ignition delay and the timing of the spark vary for each mixture. Thus, another method has been investigated. In this method, spark timing has been set according to the TDC; this means that the piston and spark always have a constant distance. The optimum spark timing advance also has been taken into account. The mixtures have been tested with various spark timing advances. The spark timing sets were from 1 mm bTDC to 20 mm bTDC. For

instance, this distance for all tests is 10 mm bTDC, which is obtained from the following investigations.

There is a limitation on the RCM which affects the spark timing. As the piston is not connected to the connecting-rod, consequently, it hits the piston tube even with the damping system, then the aim is to keep the peak pressure occurring close to TDC. Ignition delay for different mixtures at various spark timings has been investigated to figure out the proper ignition delay as in real spark ignition engines, shown in Figure 4.11. Figures 4.12 and 4.13 present the peak pressure of the two different mixtures, to obtain precise studies of the spark timing influences.

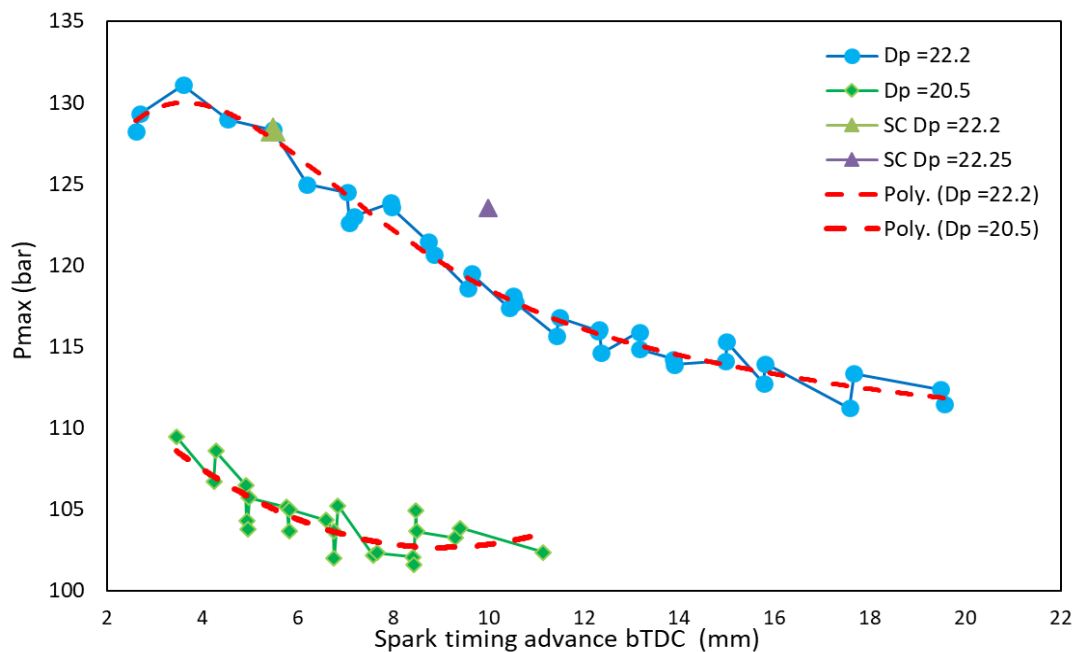


Figure 4-13 An example of influences of the variable spark timing on the peak pressure trace with different driving pressure of 20.5 bar and 22.2 bar in the mixture of 50% methane and 50% ethane; (SC: self-Combustion)

Driving air pressure acts to either speed up or slow down the piston speed in the RCMs. The driving air pressure for the spark timing investigations is 21 bar, which covers all the range of the advancing timings. According to the tests, ignition delay increases from 0.45 ms to around 0.85 ms, as the spark timing is advanced from 2.5 mm to 20 mm bTDC. Spark timing should be either retarded or advanced until the mixture cannot ignite and is not burnt.

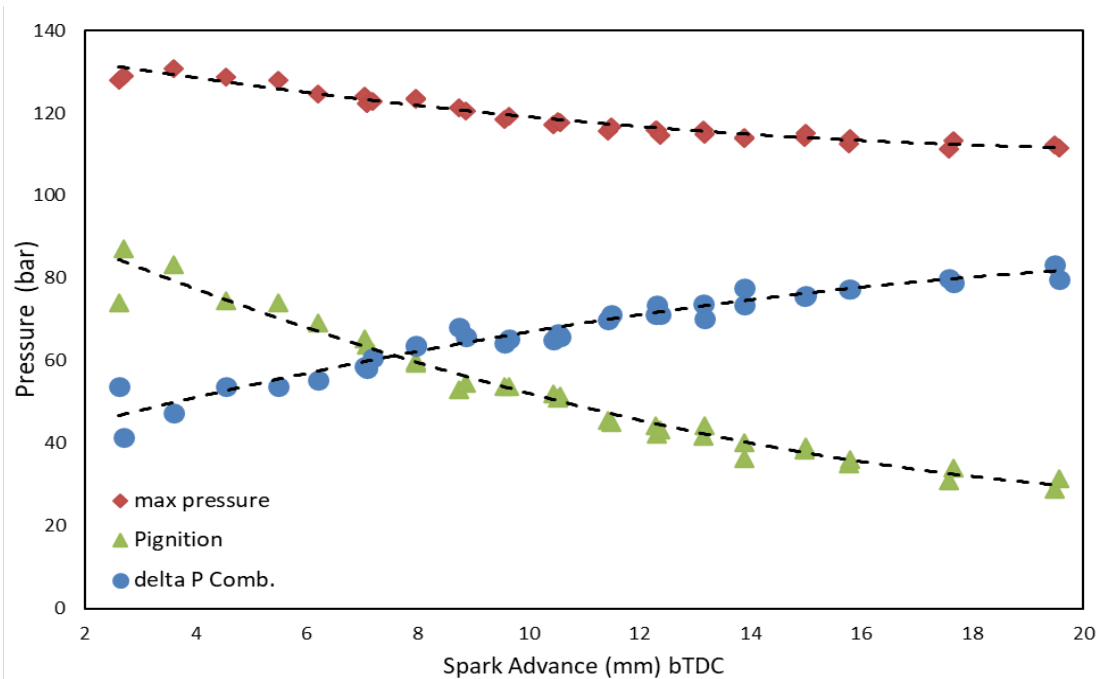


Figure 4-14 Detailed initial conditions of the mixture containing 50% methane and 50% ethane for variable spark timings.

The spark timing tests were investigated with different driving pressures and different mixtures, to examine if either of these changes affect the spark timing adjustment. Figure 4.14 indicates the pressure curve with different spark timings. Peak pressure is affected by the driving air pressure; for instance, peak pressure with driving pressure of 22.2 bar behaves almost the same as peak pressure with driving pressure of 20.5

bar. However, it is not possible to combust the mixture when the spark timing is retarded more than 11 mm bTDC. (SC means self-combustion)

Meanwhile, the knock threshold point of the mixture with 6 mm and 10 mm bTDC spark timings has been investigated. It was found that the mixture is more prone to meet the knocking condition since the spark occurs far away from the TDC. Figure 4.13 demonstrates that the mixture meets the self-combustion point with a spark timing of 5.3 mm bTDC and lower driving pressure of 22.2 bar; when the spark timing was increased to 10 mm, the driving pressure was increased to 22.25 bar.

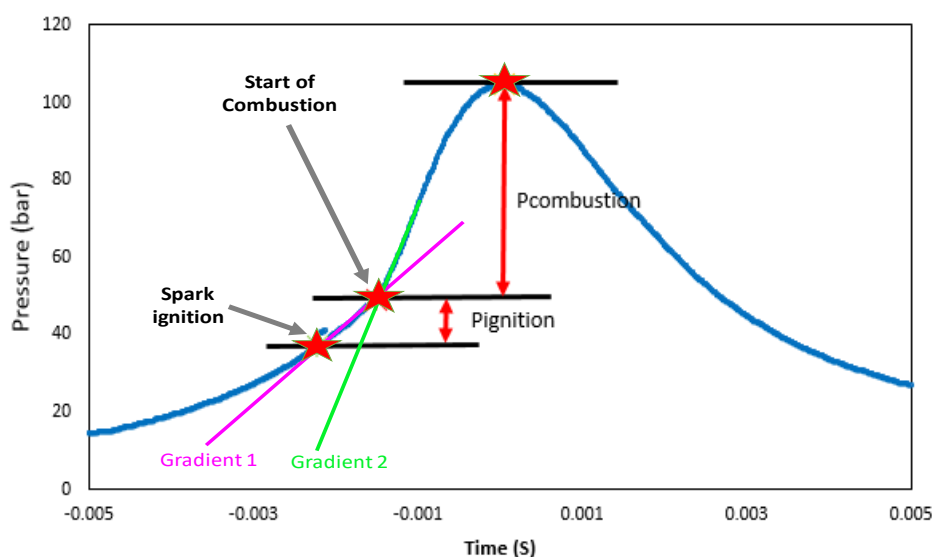


Figure 4-15 An example of detailed pressure trace (pressure rise due to compression, spark ignition and main combustion) of mixture including 50% methane and 50% ethane

Pressure rise is categorised into three different groups due to: compression, ignition and chemical reactions caused by the mixture. These pressure rises have been identified for various spark timings in Figure 4.14. It indicates that since the spark timing is close to the TDC, the mixture has enough time to be compressed and pressure

due to compression rises; however, the energy release due to combustion reduces proportionally to the recorded peak pressure.

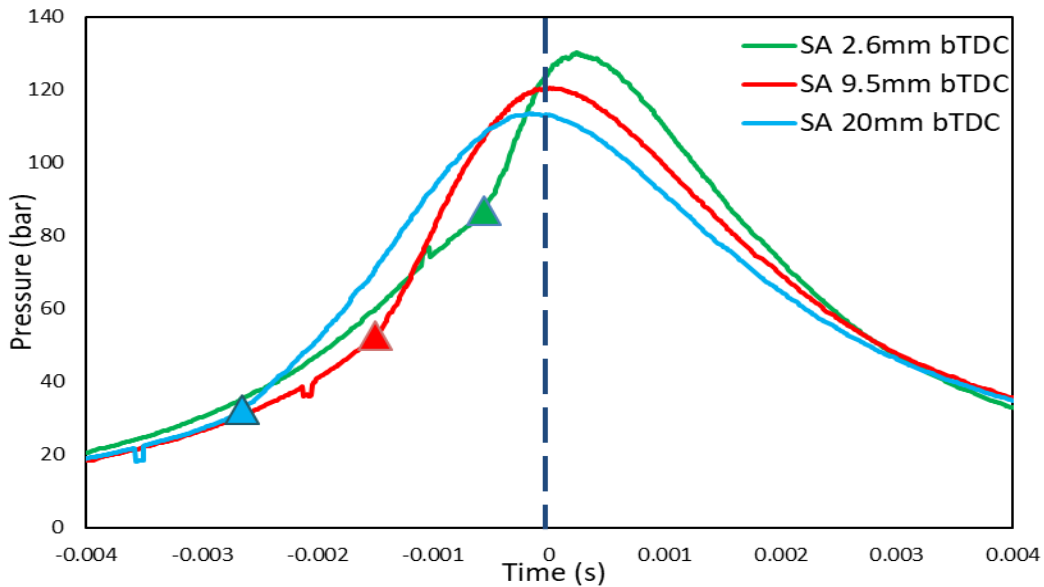


Figure 4-16 Examples of pressure trace when the spark timing is varied from 2.6 mm bTDC to 20 mm bTDC for the mixture of 50% methane and 50% ethane.

An ignition delay measurement technique has been identified to integrate the measurements. As shown in Figures 4.15 and 4.16, it is assumed that the intersection (coincidence) of the two gradients (purple and green lines) represent the starting point of the combustion. To be more precise, the highest pressure rise of the pressure trace shows the start of combustion. The time interval between the spark ignition and the starting point of combustion is called the ignition delay time. Furthermore, Figure 4.16 with three different spark timings, confirms that peak pressure occurs at TDC, since the spark timing has been set to 10 mm bTDC; while, peak pressure for either 20 mm bTDC or 2 mm bTDC occurs before and after TDC, respectively. It is perilous that the spark ignites close to the TDC due to absence of a con-rod in the RCM. Also, it is not appropriate to ignite the mixture, since the pressure and temperature are not at the proper condition, due to the earlier ignition and lower compression ratios.

4.8 Simulation Assumptions

4.8.1 Basic Model

The AVL BOOST modelling platform allows users to create a network of ducts, junctions and orifices leading to and from the combustion cylinder. Once the model is

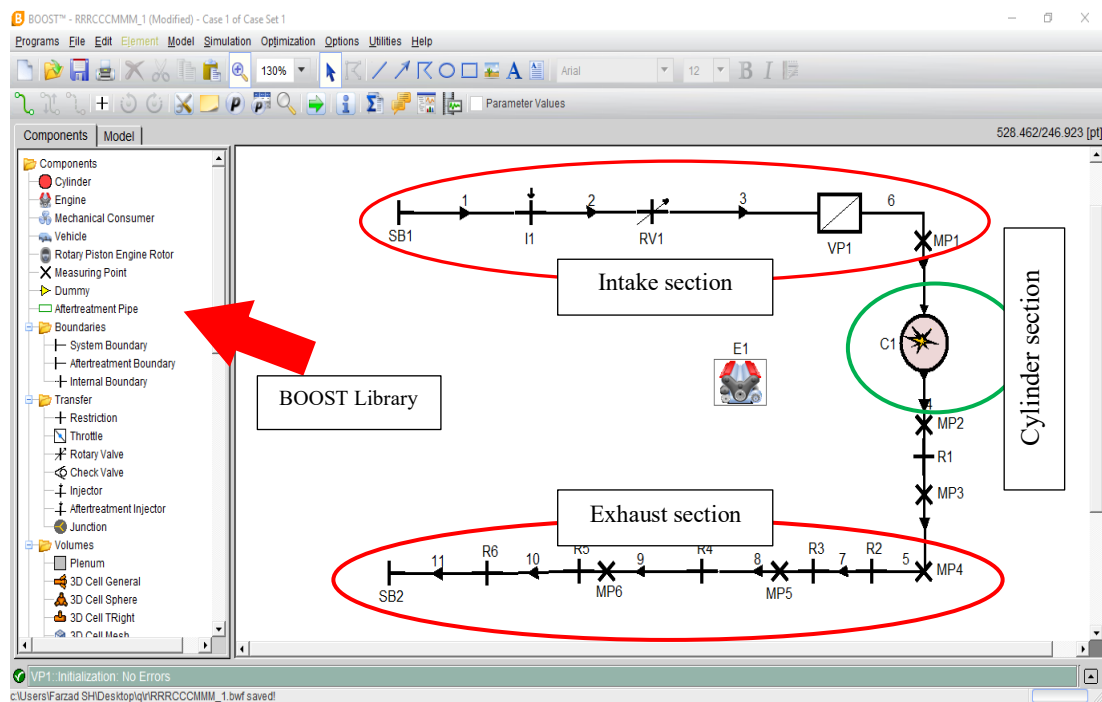


Figure 4-17 A view of the RCM model created in AVL BOOST, identifying the sections of the model (intake and exhaust ducts and cylinder)

built, the geometric data can be aligned to the various modelled parts and the operating parameters can be set in place. The AVL BOOST provides the facilities in the library, so that the user can specify the fuel to be used, control the iteration process of the solver, or add/create library parts for use in the model. Parts are added via a drag-drop system and linked by automatically created ducting. This ducting initially is created with zero dimensions requiring the user to go back and manually add them in (Version 2010, Alqahtani, Shokrollahi Hassanbarough et al. 2015).

4.8.2 Inlet and Exhaust

A close view of the created model has been shown in Figure 4.17. The inlet, exhaust and cylinder systems of the RCM have been highlighted. All dimensions have been entered into the platform for an accurate model to be formulated.

Figure 4.17 is a close view of the model to be solved in AVL BOOST with the inlet and exhaust systems inside the areas named 1 and 3, respectively. All dimensions from the two systems must be logged and entered precisely into the platform for an accurate model to be formulated. In the inlet system the first library item is the 'ambient' condition (here referred to as 'mixing tank') which is where the starting ambient pressure and temperature are recorded (Moxey 2014). The third area in Figure 4.18 indicates the exhaust duct. The exhaust duct is attached to the exhaust valve and

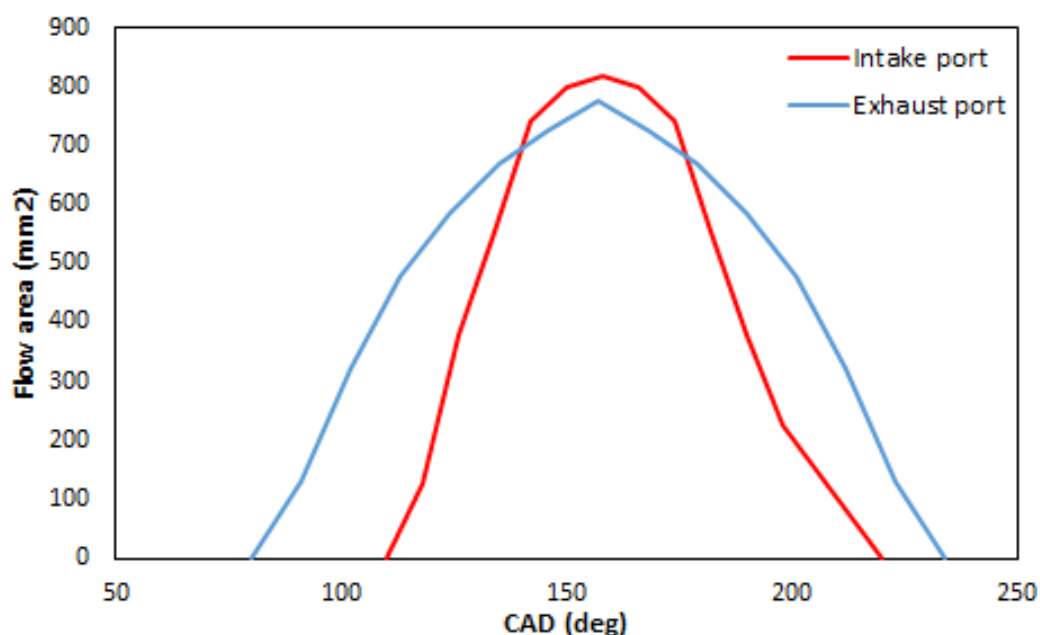


Figure 4-18 Valve timing profile which is used in the AVL BOOST platform to model the RCM induction and exhaust processes.

then the final duct is over 1000 mm long and represents the exhaust duct reaching up, expelling the gas out of the lab.

There is a difference in both intake and exhaust valves and the cylinder of the RCM compared with real two-stroke engines, in which the valves in both the intake and exhaust system are not mounted exactly to the cylinder head. There is short distance which leads to a higher dead volume during the combustion. As the valve timing has no meaning in the RCM, intake and exhaust valve timing profiles are defined as shown in Figure 4.18.

4.8.3 In-cylinder Modelling

It is quite vital to have a successful validated model with an accurate inlet and exhaust system in the AVL BOOST platform; however, the information surrounding the cylinder is also equally important for obvious reasons. The fundamental variables and parameters such as the bore, stroke, compression ratio, the con-rod length and the clearance height must be defined. The most efficient method of modelling the engine is to sweep from inlet to exhaust, as the inducted charge would, altering and calibrating data along the way. The interaction between the inlet manifold and the cylinder is an important part of the model simulation. Valve lift profiles have a highly important role. If the valves are situated too low in the cylinder and don't match those of the real RCM, then the two sets of the results will never align. In this work, because the RCM is custom-built, a spread-sheet of valve lift position to crank angle does not exist; thus, a valve lift of the two-stroke engine with the same dimensions is used. Here also, a user

can specify the amount of lash or bounce in the valves and move the profile in the cycle.

This stage was repeated for the exhaust profile.

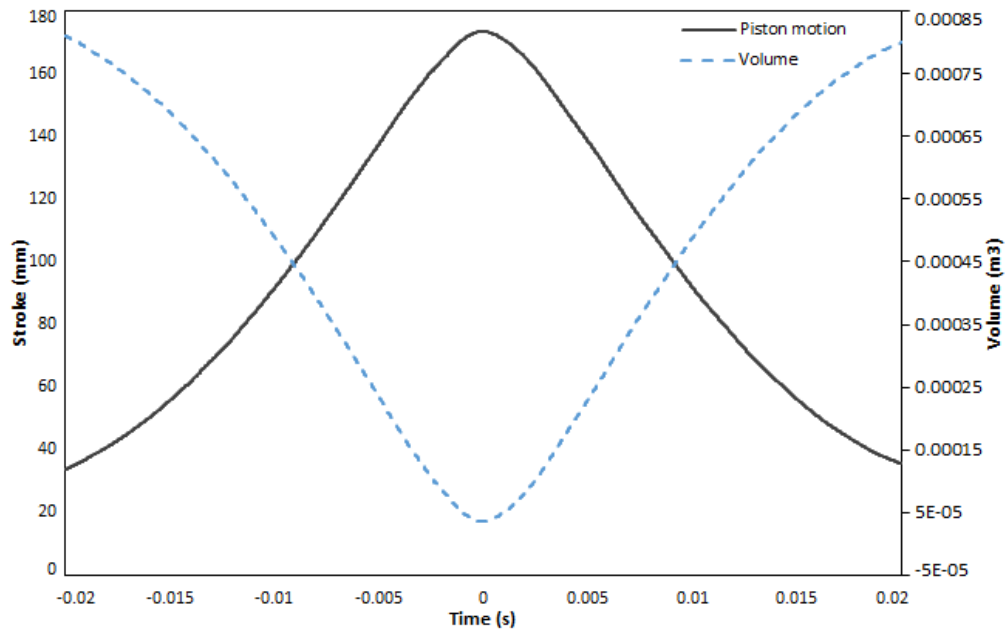


Figure 4-19 Piston movement and volume of the cylinder in the RCM, after the piston starts moving rapidly for the mixture containing pure methane

In the cylinder modelling section, the motion of the piston is vital. It indicates at each crank angle the location of the piston. In the RCM, the piston motion was described before, there is no connecting-rod and piston is driven freely by the charged compressed air. Therefore, it is crucial to identify the position of the piston at a certain time and convert to the crank angle (usable form in the AVL BOOST platform). It is the only way to import the data into the cylinder section of the AVL BOOST platform. The piston's motion profile is more beneficial due to the special feature of the RCM with a longer stroke of 180 mm. The piston motion in each test is varied and

consequently the compression ratio is changed. The piston motion and compression ratio can be affected by changing the driving pressure (Shown in Fig. 4.19).

The final element is the combustion mode. Here, from the several combustion profiles, the Weibe function and heat release data are selected. First, the model is simulated in the Weibe function and then the model is developed for the calculated ROHR of the experiments.

4.9 Results

4.9.1 Simulation and Experimental Results

Methane and propane have been blended with different proportions. Tests have been carried out in the RCM to study the combustion characteristics of various mixtures of the methane and propane. The tested mixtures include pure methane; 90% methane plus 10% propane; 80% methane and 20% propane; and 70% methane and 30% propane. In the first attempt, the knocking threshold operating conditions of the aforementioned mixtures have been investigated as shown in Figure 4.20. Driving pressure increases to move the piston faster as well as compress the mixture more. It continues since the either self-combustion or knocking occur. Then the last normal pressure trace would be considered as the threshold operating point. The detailed influences of the propane content mixed into the methane are explained later.

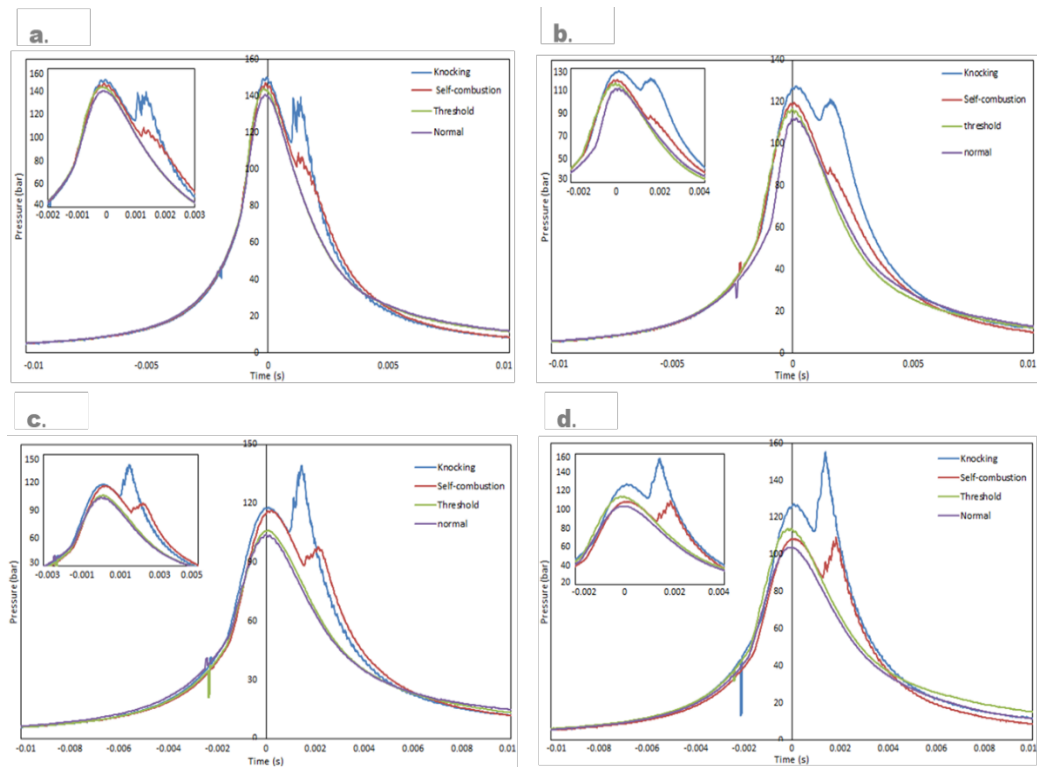


Figure 4-20 Approaching the knock threshold operating condition of the mixtures containing: a. pure methane; b. methane 90% and propane 10%; c. methane 80% and 20% propane; and d. methane 70% and 30%

Ignition delay and the temperature of the mixtures at the EOC process have been obtained for both threshold and knocking operating conditions. The EOC temperature decreases at a constant rate as the propane content in the mixture increases for both threshold and knocking conditions. For knock threshold operating conditions, the EOC temperature decreased from 800 K to 720 K, as the propane content in the mixture rose from 0% to 30%. Ignition delay time of the mixtures varies from 1.4 ms to 0.8 ms, when the mixtures contain higher proportions of propane. The IDT in knocking conditions behaves almost the same as IDT in knock threshold conditions; however, it varies unexpectedly when the propane content rises to 25% (Shown in Fig. 4.21).

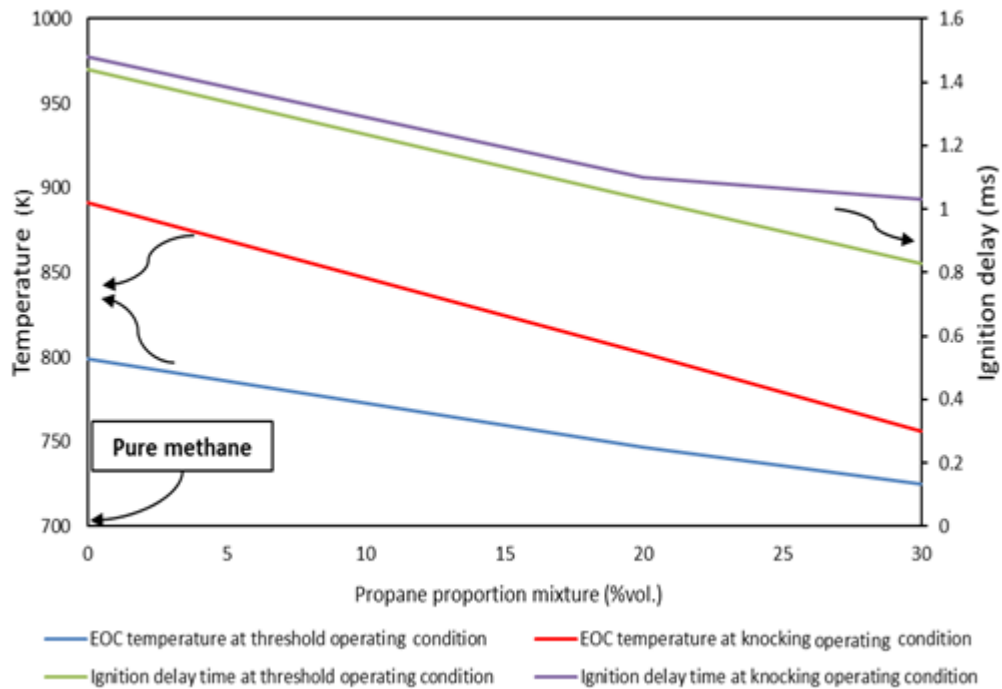


Figure 4-21 Ignition delay time for the methane-propane mixtures and temperature of the mixtures at the EOC process

Figure 4.22 indicates the results simulated in AVL BOOST and they have been validated by the results measured in the experiments. In this approach, the start of combustion and combustion duration should be identified to simulate the combustion. This approach provides a pre-defined ROHR for combustion of the mixture. In addition, the piston motion of the RCM should be obtained and converted precisely with respect to the crank angle. Thus, Figure 4.22 (b) has been drawn to validate the pressure changes with respect to the volume changing based on the piston motion.

The heat release rate for different mixtures of the methane and propane has been investigated, as shown in Figure 4.23. In this approach the utility interface panel of the AVL BOOST was used; thus, the obtained pressure and piston motion of the RCM

from the experiments were entered into the panel, and the heat release rate of the mixtures was calculated.

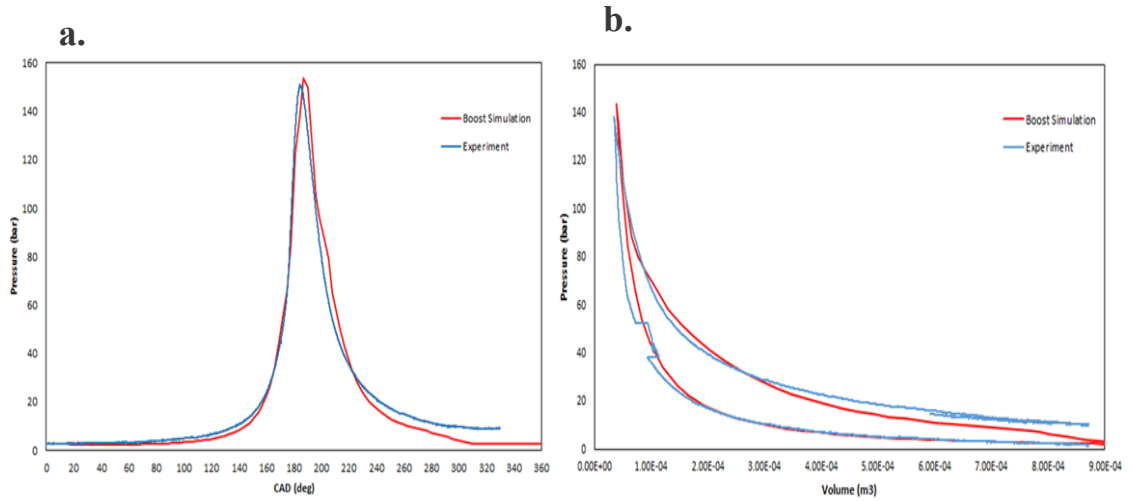


Figure 4-22 Comparison of the experimental and simulation investigation of the pressure trace and volume of the chamber in the RCM, since the Wiebe mode is used in the combustion model

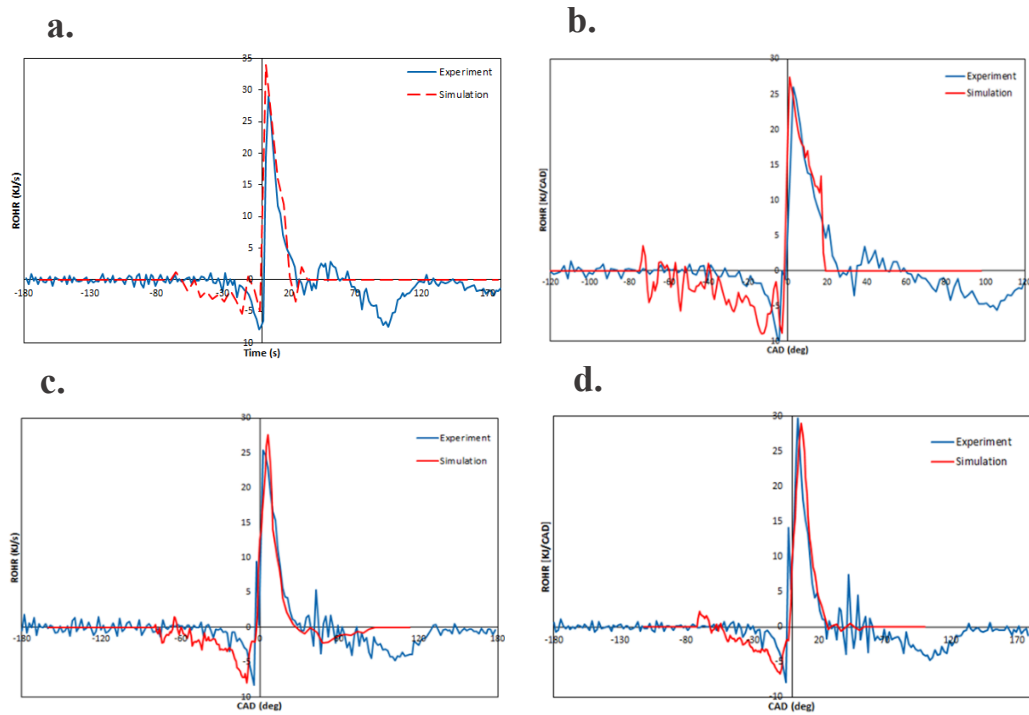


Figure 4-23 Comparison of the ROHR Experimental and simulation investigation for different mixtures of the methane and propane

4.9.2 Knock Intensity Results

Knock intensity calculation procedure for different mixtures of the methane and propane has been investigated, as shown in Figure 4.24. The knock intensity for all proportions of methane and propane with different intensities were presented. First step of this analysis was to separate the high frequency pressure oscillations (HFPO) with a high-pass digital filter with the cut-off frequency of 7 kHz which the frequency



Figure 4-24 Procedure used to identify the knocking intensity of the methane-propane mixtures with different driving pressure

is the same in these cases as it depends on the combustion chamber diameter. The method of pressure frequency and knock intensity determinations are expressed as a MATLAB manuscript in Appendix A. The in-cylinder pressure vs time, the band pass filter and power spectrum were depicted in fig. 25 a, b and c for pure methane. In fig. 25 d, e and f the knock metric analysis of 10% propane mixed in 90% methane was shown. Respectively, the fig. 26 a, b and c show the amplitude of knock intensity since the proportion of the propane increases from 10% to 20% and consequently the methane content reduces to 80%. Finally, the fig. 26 d, e and f present the knock intensity of the 30% propane blended in 70% methane.

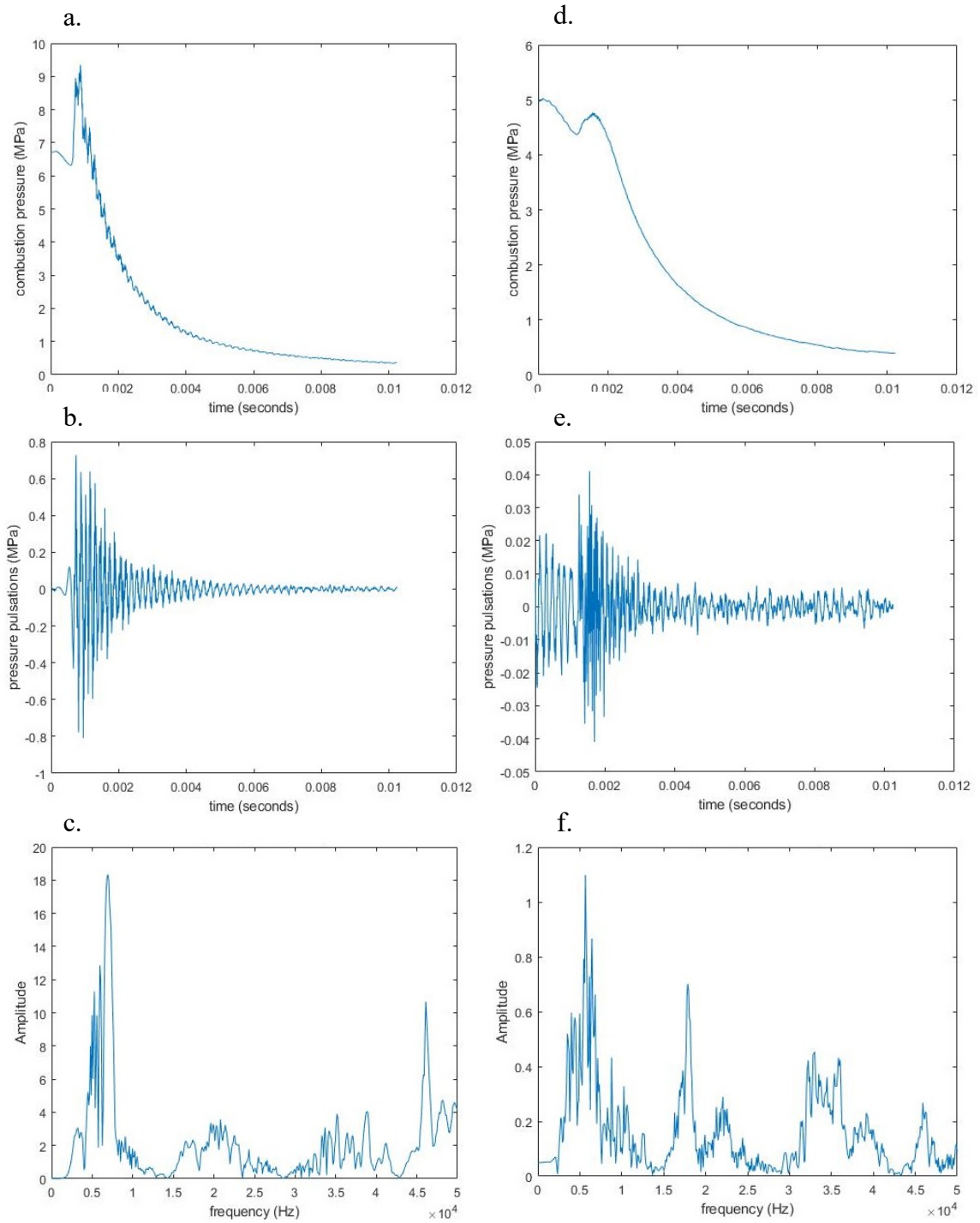


Figure 4-25 a. In-cylinder pressure, b. spectrum of pulsation and c. knock intensity for pure methane; d. In-cylinder pressure, e. spectrum of pulsation and f. knock intensity for 90% methane mixed in 10% propane

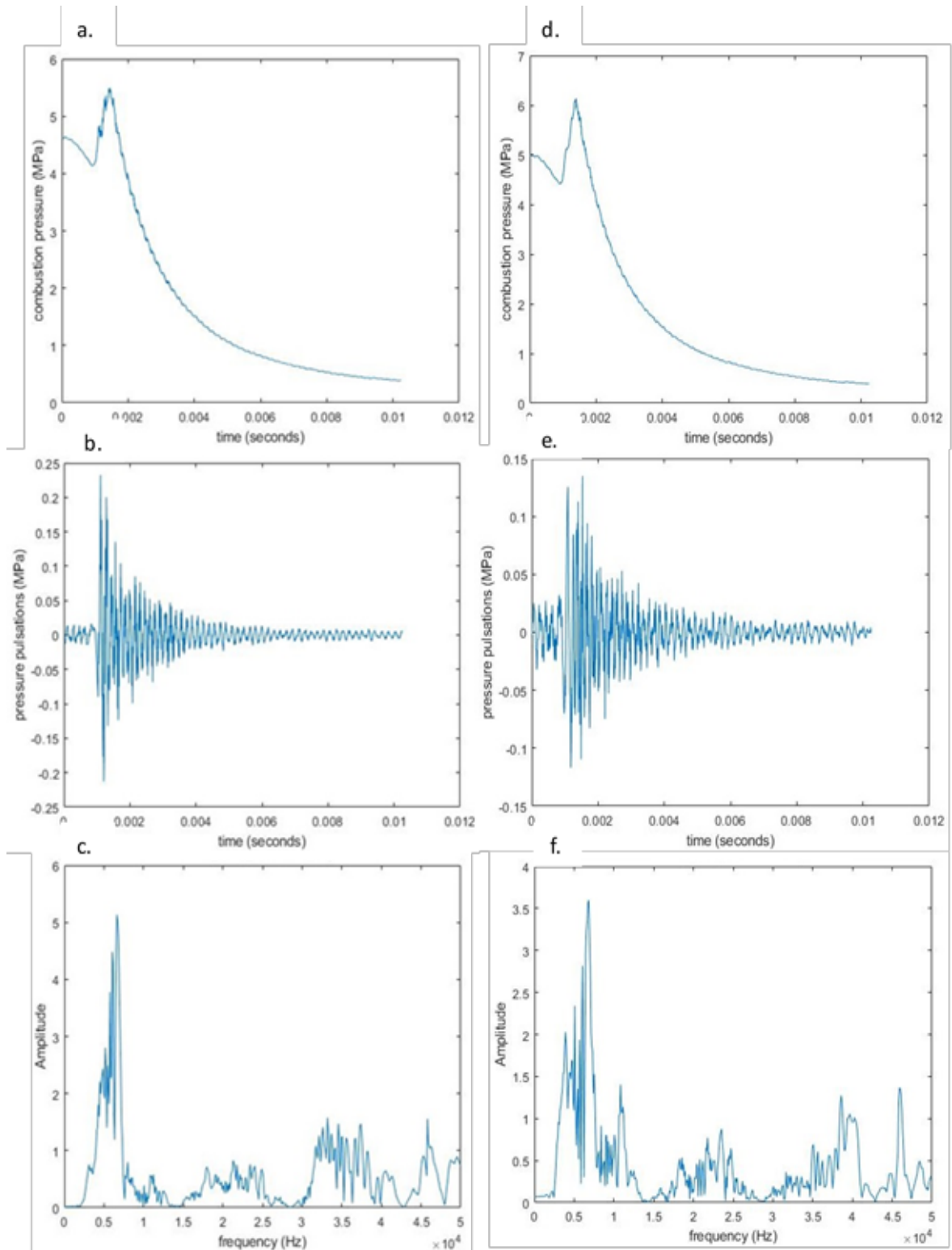


Figure 4-26 a. In-cylinder pressure, b. spectrum of pulsation and c. knock intensity for 80% methane plus 20% propane; d. In-cylinder pressure, e. spectrum of pulsation and f. knock intensity for 70% methane plus 30% propane

4.9.3 Optimized Methane-Propane Reference Curve

4.9.3.1 Pressure Methane-Propane Reference Curve

The RCM was developed in this study and new techniques were used to integrate the RCM's behaviour, since the mixtures had been changed. The test results of the peak pressure for different methane/propane mixtures are summarised in Figure 4.27. There are seven different approaches to investigate the methane/propane reference curve; each set represents an improvement as well as better correlation with methane/propane behaviour. Tests were run with pure methane and then propane was blended into the methane. Energy content, spark timing, lambda, temperature stabilization, sensor calibrations, software updating, air-fuel premixing, driving air pressure development, induction system and practical improvements were some of the upgrading works done during this study.

For test set 1, the mixtures were run at lean mixture condition. Air and fuel were mixed in the cylinder separately and the spark timing was set at 155 mm aBDC. The results show that there were some huge uncertainties in peak pressures, since propane was blended into the methane. There were obvious uncertainties in compression ratios, which represents the variant spark timings. The piston fluctuated unexpectedly for different mixtures.

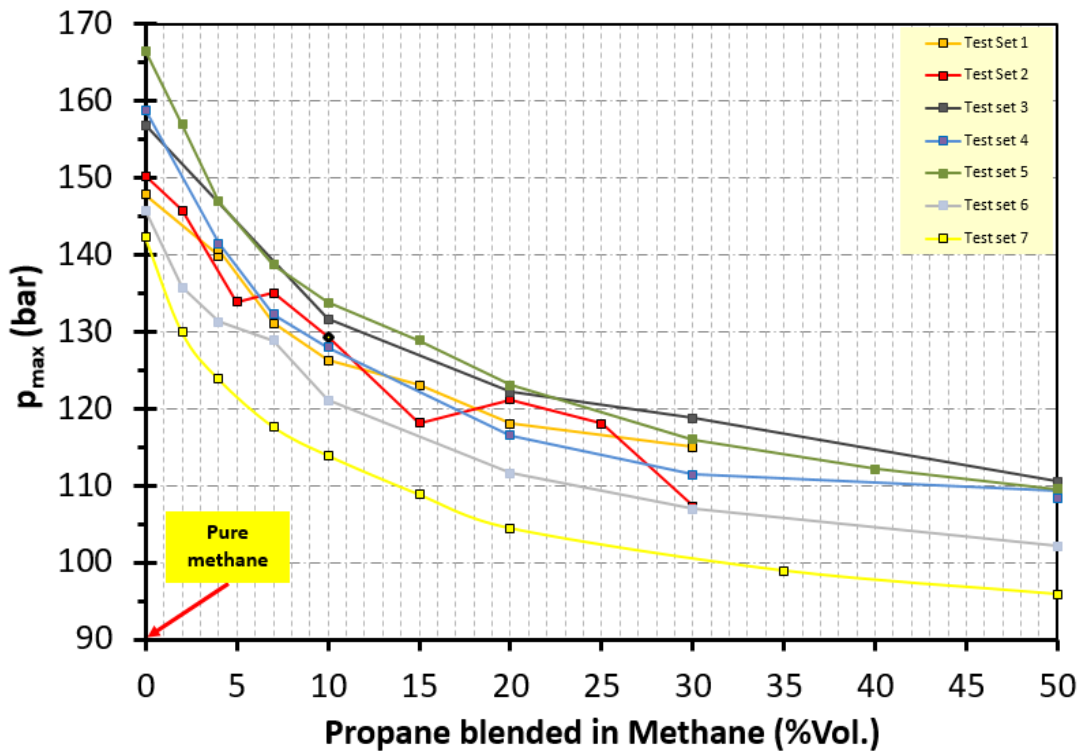


Figure 4-27 Summarised peak pressure measurement of the methane-propane mixtures for different methods used to achieve the final smooth reference curve

For test set 2, peak pressure and compression ratio of the pure methane had the highest range of 150 bar and 24, respectively. However, the peak pressure and compression ratio plunged to around 100 bar and 18, correspondingly, when 30% propane was blended into 70% methane. Although there was a descending trend, there were some strange behaviours for mixtures containing 95% methane and 5% propane, and 85% methane and 15% propane mixtures. The results showed swings in both pressure and compression ratio, caused by non-uniform distribution of the heat across the cylinder. The temperature varied at all points, and especially at those aforementioned points. The temperature recorded higher (+10 °C) than the set point (110 °C) at 95% methane and 5% propane, and at 85% methane and 15% propane mixtures.

In test set 3, the temperature issue was solved and it was concluded to reduce the temperature to 80 °C in the cylinder. To fulfil the goal, heating elements, trace heating cable and isolation covers were installed and examined. According to the pressure curve, there was a clear improvement in the accuracy of the peak pressure results since the tests run at 0%, 10%, 20%, 30% and 50% propane blended in the methane. The compression ratio still did not have an acceptable correlation; there was a practical problem with the piston displacement sensor and driving air pressure. The piston displacement sensor needed to be repaired. There was also a higher driving charge air pressure to produce the same compression ratio as in the previous tests. After some investigations, it was found that the driving volume first was filled by compressed air and the air and fuel were inducted into the cylinder. There was enough time to leak around 1 bar in the driving volume section; thus, the software was upgraded to fill the driving volume just before the piston shot towards TDC.

In test set 4, a new ultimate level of the peak pressure and compression ratio after improvement was recorded. Peak pressures of 10%, 20% and 30% propane contents dropped around 3, 5 and 9 bar. Compression ratios at 10%, 20% and 30% propane contents also slumped severely in comparison with test set 3. These low peak pressures and compression ratios demonstrated richer mixtures than the set points with lambda 1.5. According to the further investigations done on the ignition delay and the repeatability of the tests from lean-to-rich conditions, the most reliable lambda with the Wartsila's RCM, was found as 1.2, detailed investigations were described in section 4.7.

The new test set 5 focused on the premixed strategy with energy content of 5.5 kJ and the in-cylinder temperature was set at 82°C. The peak pressure trend followed a smooth pattern and with apparent improvement; so that the highest peak pressure belonged to the pure methane. As the propane content increased, resistance of the mixtures against knocking diminished. In test set 5, it appeared that peak pressure for pure methane reached 166 bar. Peak pressure decreased to 135, 123, 117 and finally 110 bar as 10%, 20%, 30% and 50% propane blended into the 90%, 80%, 70% and 50% methane, respectively. Consequently, peak pressure reduction expressed less resistance of the mixtures against knocking.

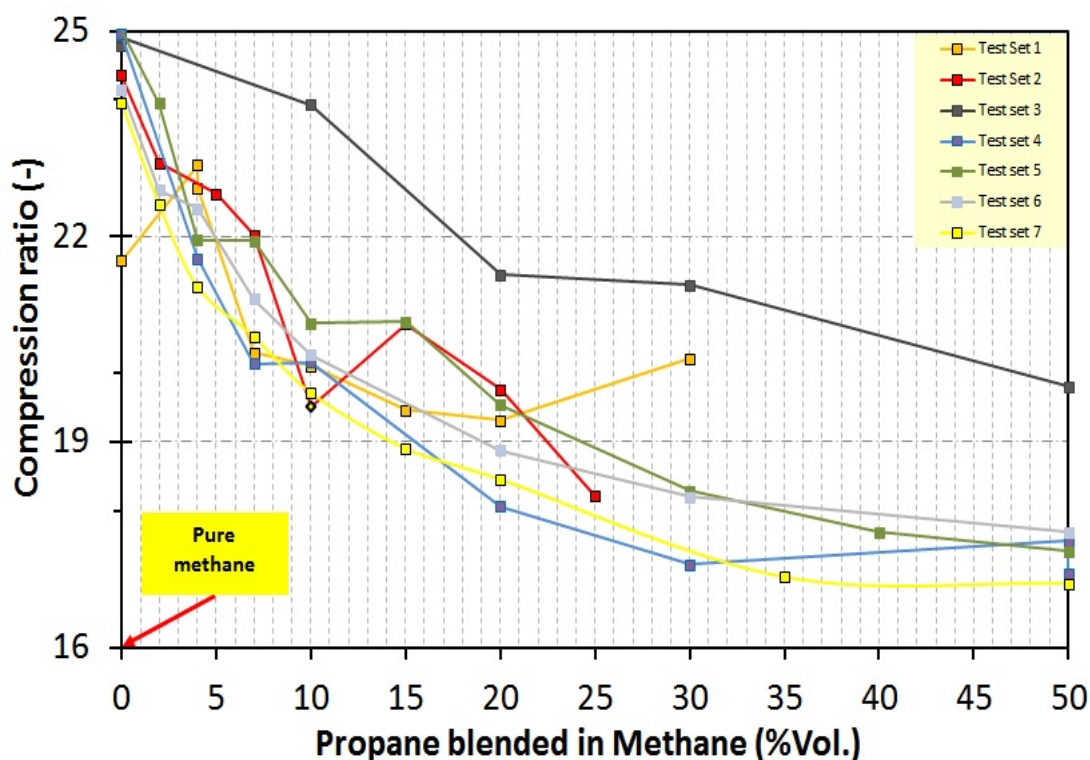


Figure 4-28 Summarised compression ratio measured from the methane-propane mixtures for different methods used to achieve the final smooth reference curve

In test set 5, compression ratios for various propane proportions were not identified, as there were some errors between 5% and 7% propane, 10% and 15%

propane, as shown in Figure 4.28 (green line). There was a practical issue and by adjusting a regulator before the fuel valve, the pressure was set to feed the fuel always with 0.5 bar, so that in the next test set, the most accurate results were achieved.

In test set 6, the temperature of the fuel and air from the mixing tank to the RCM cylinder was stabilized at 81°C, by using a trace cable, thermocouple and heat exchanger. Moreover, a new check valve was installed on the RCM to increase the damping effect. The results of test set 6 were much smoother (grey line). However, there were some inaccuracies between the mixtures with 5% and 10% propane in both peak pressure and compression ratio graphs; which it was due to miss-functionality of the check valve mounted after the combustion chamber to prevent high pressures damaging the air valve. Also, it was found that there was a bug in the RCM's software leading to leak the fuel in the air pipeline. Therefore, it was replaced just before the check valve, leading to reducing the dead volume as much as possible.

For the lateral test set, the RCM was ready to produce the most reliable smooth methane/propane reference curve. There were several modifications made to the RCM, as a result of the knock threshold operating condition for the methane/propane blends which were shown in Figure 4.28, test set 7 (yellow line). Peak pressure and compression ratio for various propane, methane blends were investigated as; for the pure methane they were recorded as 142 bar and 24, respectively, by which demonstrates the highest possible methane number of the test sets. As the propane proportion increases, resistance of the mixtures against knocking reduces and it is more prone to experience knocking. To be more precise, peak pressure and compression ratio

dropped to 114 bar and 19.7, respectively. By blending 10% propane into 90% methane it reduced approximately 20% the resistance of the mixture against knocking with respect to both pressure and compression ratio. The mixture's resistance against knocking, dropped to 105 bar in peak pressure and 18.2 in compression ratio (around 8% reduction) as the propane content increased to 20%. The reduction trend continued to 98 bar and 17 for peak pressure and compression ratio, respectively, as the propane content increased to 35% in the mixture. There was a slight reduction in peak pressure and compression ratio for the 50% propane and 50% methane mixture; peak pressure was 96 bar and the compression ratio was 16.7, which it is equal to 3% reduction with respect to 35%propane content in the mixture.

4.9.3.2 Methane Number Reference Curves

Methane number indicates the knock tendency of the mixtures. It is important to understand the knock resistance of the mixtures when they are used in engines, as the mixtures have different constituent gases like methane, ethane, propane and butane.

The methane numbers of the tested mixtures are shown in Figures 4.29 and 4.30. There were used different methods used which are available in the market to calculate the methane number; Wartsila's methane number calculator and EN1627 methane number calculator. The figures represent the combination of the theoretical and experimental approaches to the knock tendency of the mixtures. All figures represent that the methane number is reduced as the propane content in the methane is increased. It continues to a point where the engines are not capable of combusting the mixtures;

however, the EN methane number calculator is able to calculate the methane number of the mixtures with a higher propane content of 50%. Both peak pressure and compression ratio parameters are analysed to find more precise method to investigate the other unknown mixtures with this methane/propane reference curve.

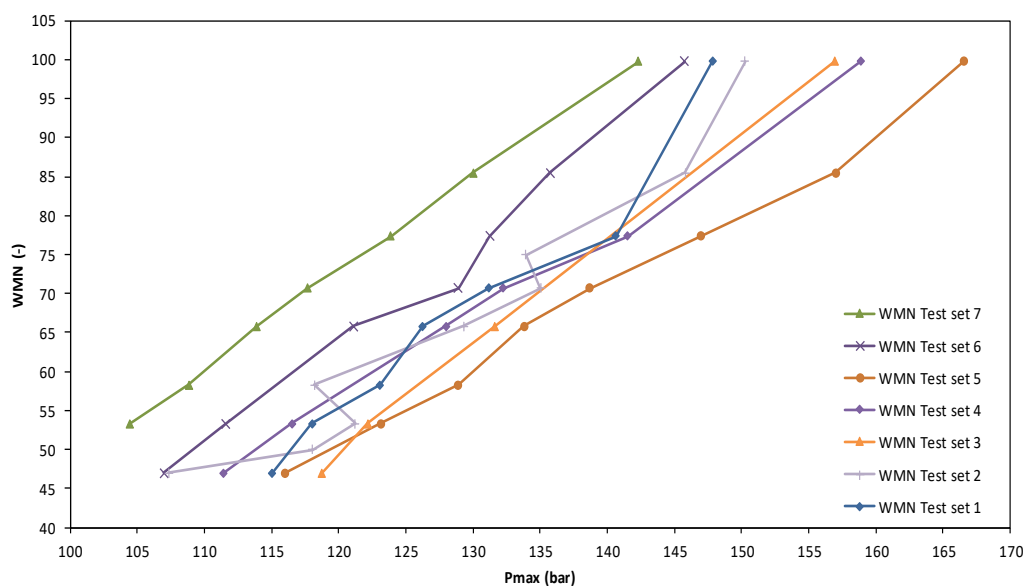


Figure 4-29 Summarized measured peak pressure and calculated MN for the methane-propane mixture tested in the RCM

As explained in the previous chapter, there were several attempts made to achieve the best smooth methane/propane reference curve correlated with Wartsila's real engine. It was interesting to determine the methane number of the methane/propane mixtures and plot them then with respect to the peak pressure and compression ratio. Figure 4.27, WMN vs Pmax, shows that pure methane has the highest methane number of 100 with 142 bar. The methane number drops steeply to 85 with peak pressure of 130 bar, when only 2% propane is blended into the methane. The methane number reaches 76, when 4% propane proportion is added into methane. This pattern continues with higher propane proportions; however, the rate of reduction is decreased. Wartsila's

methane number calculator is capable of determining close to 53, where the peak pressure is 105 bar.

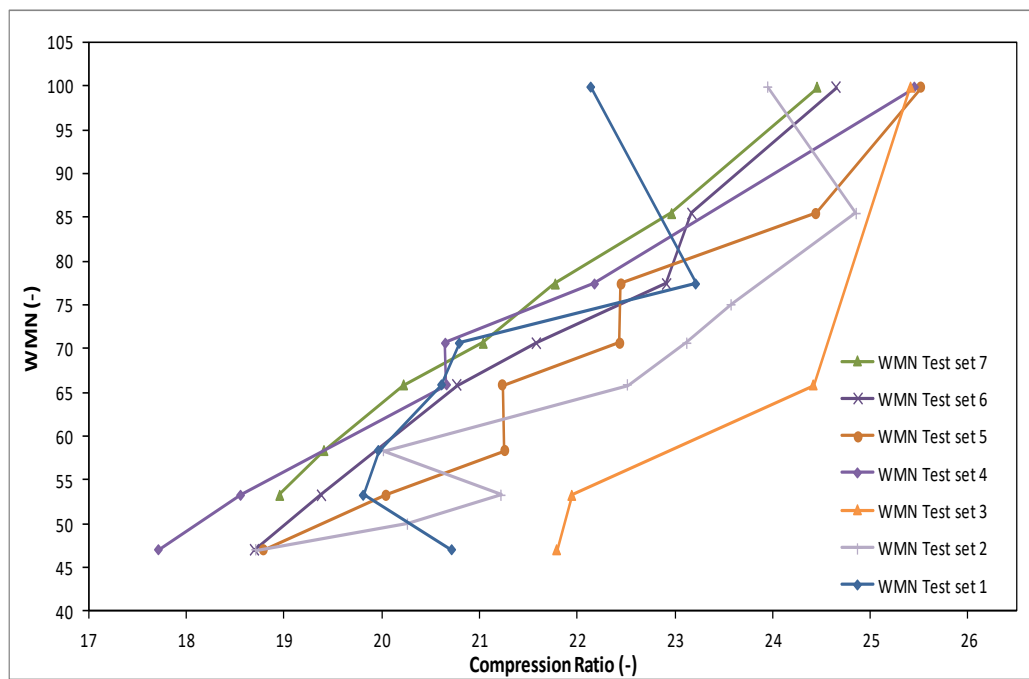


Figure 4-30 Summarized measured compression ratio and calculated MN for the methane-propane mixture tested in the RCM

Generally, the methane number shows a downward trend as the propane proportion increases, by considering all 7 test sets, except for some inaccuracies. All tests represent the same pattern as the peak pressure and compression ratio. It should be pointed out that some mixtures don't follow the same integrated pattern as the other mixtures; for example, there are some fluctuations at 135 bar, 165 bar and 130 bar in test set 2, test set 5 and test set 6, correspondingly. Thus, those points express a higher knock tendency, while the calculated methane number doesn't prove.

Compression ratios of the RCM for each individual test were determined in order to have better understanding of the mixtures' behaviours. It helps to study the combustion characteristics of the mixtures deeply. According to Figure 4.28, showing WMN vs CR, the compression ratio depicts more fluctuations than the pressure graph. These fluctuations might be due to either the piston free movement of the piston toward TDC, or inaccuracy in the displacement measurement sensor.

Generally, the trend follows the same pattern as the pressure graph. In most cases, the compression ratio is achieved in the range of 24 to 25 and also ends up to the same range of 18.5 to 19.5 for the same mixture proportions, except test sets 1 and 2. As explained previously, in test set 1 and 2, the piston moves aimlessly, due to both variable spark timing and inaccuracy in lambda.

4.10 Conclusion

The intension was to investigate the methane/propane mixtures combustion characteristics in the RCM. This study was conducted to figure out the possibility of making a methane/propane reference curve. This approach attempts to generate a comprehensive reference curve to examine all unknown gaseous fuels.

The combustion characteristics of the methane/propane mixture were investigated. According to the study, the spark timing was set 10 mm before TDC, so that combustion peak pressure occurs as the piston reaches TDC. In addition, lambda was investigated to find out at which air-fuel ratio, RCM is able to produce the best ARR. According to

the results, λ was set at 1.2 and was examined by checking the repeatability of the mixture at ignition condition, peak pressure and compression ratio. These three parameters showed that λ 1.2 can produce the best reliable results with the equipment at the Wartsila lab.

from another point of view, to have better understanding of the RCM, a model was created in AVL BOOST, a 1D simulation platform. The model was created by two different combustion methods. These models can predict the behaviour of the RCM in reality, however, the model is not completely independent of the experimental data. The simulation results show good correlations with the RCM results.

Methane has the highest methane number and knock resistance with respect to the peak pressure and compression ratio parameters. Although the mixtures tendency to knock increase by blending propane into the methane, a higher amount of propane proportion in the methane affects it less than a lower proportion of propane. To be more precise, peak pressure and compression ratio of less than 10% propane drops more than peak pressure and compression ratio of the 10-20% propane content in the methane. The peak pressure and compression ratio drops are almost constant between 30% and 50% propane proportion.

**Chapter 5 – STUDY OF
COMBUSTION
CHARACTERISTICS OF
METHANE BLENDING
WITH ETHANE AND
BUTANE IN AN RCM**

5.1 Introduction

Engines with gas fuel flexibility are presently of interest to the power generation and combustion research communities, due to the variation in fuel composition, which is expected to increase with the decrease in fossil fuel supply and the increasing use of gaseous fuels. Such variations can be due to dissimilarities in the fuel source itself or to the advent of gaseous fuels currently being developed at a fast pace. The primary fuel for industrial gas turbines is natural gas (Healy, Curran et al. 2008); which is the source of about one quarter of the world's primary energy today and is expected to be so until 2030 (Spadaccini and Colket Iii 1994). Natural gas has a low greenhouse gas signature, is energy efficient and is easy to use, in that the infrastructure needed is already in place. Although natural gas is mostly methane (CH_4), higher-order hydrocarbons such as ethane (C_2H_6) and butane (C_4H_{10}) can be presented depending on its origin, extraction, and transport processes (Healy, Curran et al. 2008).

Natural gas has been used during recent years, but it is not always economical to use due to the price of the energy. Thus, it is necessary to investigate the possibility of other unknown gaseous fuels. There are so many reasons for gaseous fuels to replace liquid fossil fuels. They significantly produce much less pollutant emissions such as particulate matter (PM), unburned hydrocarbon (HC) and carbene monoxide (CO) (Saharin 2013).

In this chapter, the secondary reference mixture is tested to investigate new reference methane-ethane and methane-butane reference curves. These fuels were

selected to compare with those from the results of the real Wartsila engine. For this, experimental ignition delay time, peak pressure and compression ratio for different lean fuel mixtures with $\lambda = 1.2$ were obtained from the RCM at the Wartsila Fuel Laboratory.

5.2 Tested Fuels and Fuel Properties

In this chapter, different proportions of ethane and butane were blended into the methane, separately. To be more precise, methane and ethane were mixed with different volumetric proportions as summarised in Table 5.1 and then methane and butane were mixed with different volumes as summarised in Table 5.2.

Table 5.1 Properties of the gaseous fuels tested in this work with the RCM

Specifications	Base Methane (100%) Ethane proportion mixture (%Vol.)			
Methane proportion (%Vol.) A	98	85	50	0
Ethane proportion (%Vol.) B	2	15	50	100
AFR _{stoichiometric} (Vol.)	9.66	10.59	13.09	16.66
Final fuel pressure (bar)	0.18	0.16	0.13	0.10
Final air-fuel pressure (bar)	2.27	2.24	2.19	2.14
X (number of moles of air per mole of fuel in mixtures)	11.59	12.7	15.7	19.99
LHV mixtures (MJ/nm ³)	36.50	40.12	50.12	64.36
Fuel temperature at mixing reactor	323 K			
Fuel temperature at chamber	354 K			

Table 5.2 Properties of the gaseous fuels tested in this work with the RCM

Specifications	Base Methane (100%) Butane proportion mixture (%Vol.)			
Methane proportion (%Vol.) A	99	97	95	90
Butane proportion (%Vol.) B	1	3	5	10
AFR _{stoichiometric} (Vol.)	9.73	10.2	10.6	11.6
Final fuel pressure (bar)	0.18	0.17	0.16	0.15
Final air-fuel pressure (bar)	2.27	2.27	2.26	2.25
X (number of moles of air per mole of fuel in mixtures)	11.7	12.2	12.7	14
LHV mixtures (MJ/nm ³)	36.6	38.2	39.8	43.7
Fuel temperature at mixing reactor	323 K			
Fuel temperature at chamber	354 K			

5.3 Test Conditions and Test Methods

In this study, peak pressure, compression ratio, ignition delay and EOC temperature were measured in the RCM for various ethane and butane proportions blended into the methane (as a baseline fuel), separately. The knock threshold operating conditions of the mixtures were adjusted by changing the driving pressure. The mixtures' reactivity changes were prepared with dry air containing 21% O_2 and 79% N_2 . The compressed temperatures and pressures were attained through a combination of changes in compression ratio. Initial temperatures were adjusted by the temperature investigations discussed in section 4.4.1; and 81 °C (± 2) was selected to ensure complete fuel vaporization, which has been confirmed using GC/MS analysis.

In this study, a spark plug was mounted in the RCM pre-chamber to ignite the mixtures; while in most of the research carried out with the other RCMs, it has not been

used. Besides, as mentioned previously, the RCM has a variable compression ratio due to the free movement of the piston (absence of crankshaft). According to the investigations done in the previous chapter regarding the best possible RCM performance, spark timing was chosen as 10 mm bTDC, lambda was approximately chosen as 1.2 and the energy of the mixture was held constant at almost 5 kJ.

Based on the feedback resulting from the RCM performance, in the previous chapter (Chapter 4), the driving pressures have been selected so that the heavy knocking combustion no longer occurs. It is due to the probable damages which happen to the cylinder head, piston and piston tube in the driven section.

5.4 Experiment Conditions

Ignition delay, peak pressure and compression measurements have been made in the RCM for methane-ethane and methane-butane mixtures at the $650\text{ K} \leq T_{EOC} \leq 800\text{ K}$ and lambda approximately 1.2. The compressed pressure also was changed based on the charged driving pressure. All reactive charges have been prepared with dry air, 21% O₂ and 79% N₂. The compressed temperatures and pressures are attained through a combination of changes in compression ratio and by changing the pressure of the charge. Initial temperatures were selected as 81 °C (±2) to ensure complete fuel vaporization, which has been confirmed using GC/MS analysis. All information was described in detail in Chapter 3. Based on the Figures 5.5 and 5.11, it is seen that the tests are focused on the low temperature and low-to-moderate pressure regions.

5.5 Results and Discussion

5.5.1 Methane-ethane Mixtures

This chapter focuses on investigation of blending methane in two different hydrocarbons of ethane (lighter than propane) and butane (heavier than propane). Here, the same methane-propane procedure was used, to investigate the methane-ethane and methane-butane mixtures, however, the proportions of the mixtures were different. First the methane-ethane results have been presented and then the results of the methane-butane are shown correspondingly. The results display the procedure of the knocking combustion approach as well as the repeatability of the RCM results based on different mixtures. In the next attempt, the analysis of the combustion characteristics for each mixture is discovered.

Methane and ethane were blended in different proportions as shown in Table 5.1. Ethane was added into the methane in four different volumetric proportions: 2%, 15%, 50% and 100%. For each mixture, the partial pressure of the fuel and air based on λ 1.2 and an energy content of 5 kJ were calculated.

It was aimed to operate the RCM with different methane-ethane mixtures at knocking threshold conditions. The air-fuel ratio and energy content of the mixture were kept constant to have the same energy amount for the tests. The driving pressure acts like a connecting-rod in real internal reciprocating engines.

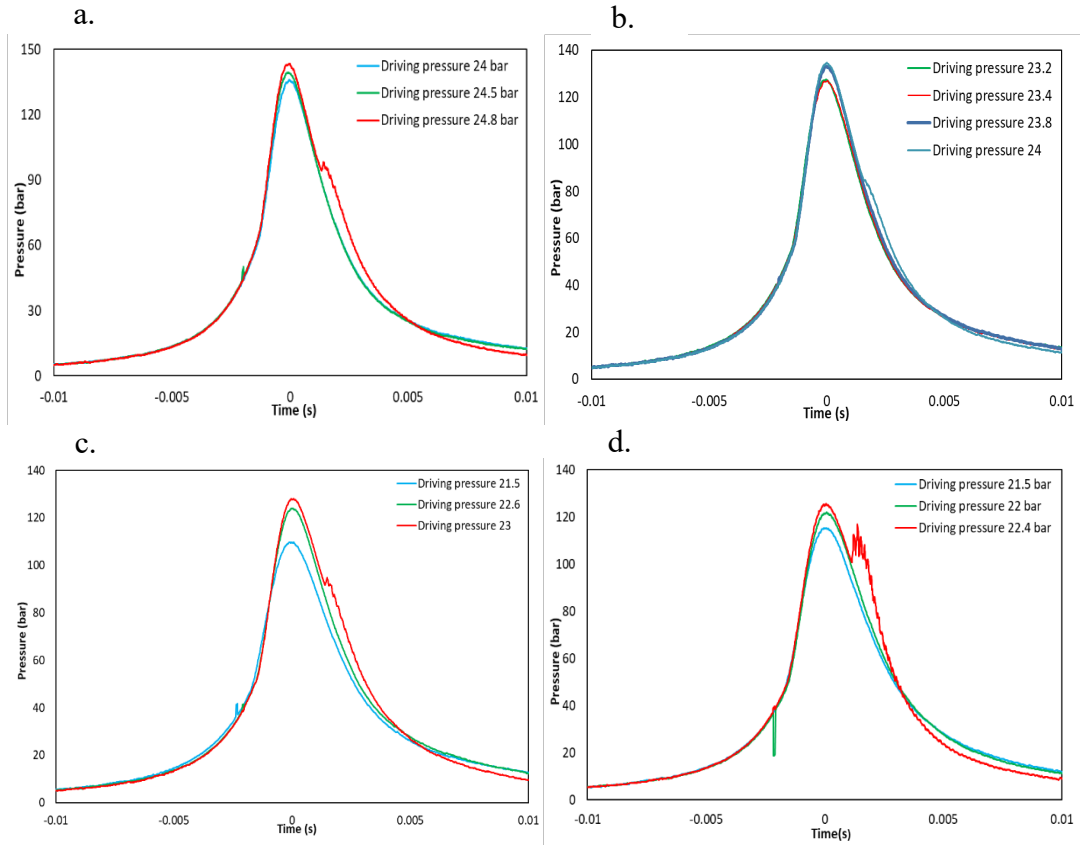


Figure 5-1 Approaching to the threshold operating condition of the mixtures containing: a. 98% methane plus 2% ethane; b. 85% methane plus 15% ethane; c. 50% methane plus 50% ethane; and d. pure ethane

In the RCM, compression ratio varies by changing the charged driving pressure. As the compression ratio increases, the mixture is more prone to knock. The pure methane number as presented in Chapter 4, has the highest tolerance against knocking and has the highest methane number. Thus, it is obvious for it to have the highest driving pressure producing the highest compression ratio. As the ethane proportion increases in the mixture, the knocking resistance of the mixtures reduces. As Figure 5.1 shows, driving pressure drops from 24.5 bar to 22 bar as the ethane proportions in the mixtures increase from 2% to 100% for normal combustion at knock threshold operating points.

The repeatability of the RCM with different mixtures, was investigated in Figure 5.2. The tests for each mixture were run seven times, to obtain the repeatability of the mixtures. Figure 5.2 shows the pressure trace of the methane-ethane mixtures. The peak pressure and compression ratio for each test were measured and the errors were calculated.

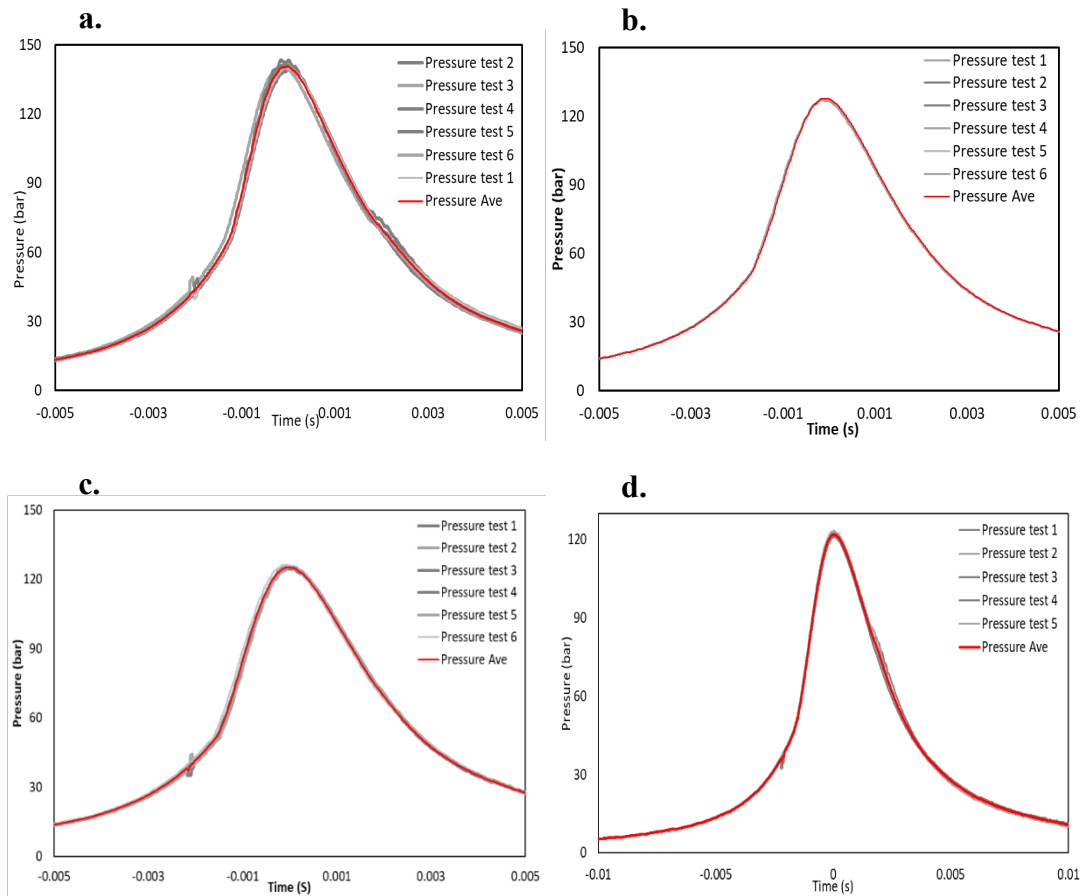


Figure 5-2 Repeatability tests of pressure trace for the mixtures containing of: a. 98% methane and 2% ethane; b. 85% methane and 15% ethane; c. 50% methane and 50% ethane; d. pure ethane

In Figure 5.3, the initial pressure of the ignition, pressure at SOC and the peak pressure are shown. The ignition pressure reduces from 40 bar to almost 32 bar as the ethane proportion increases from 2% to 100%. There is a delay between ignition point and start of combustion called the ignition delay time. The ignition delay time causes a pressure rise, shown in the second level (ignition delay pressure rise) with medium dark colours (Figure 5.3).

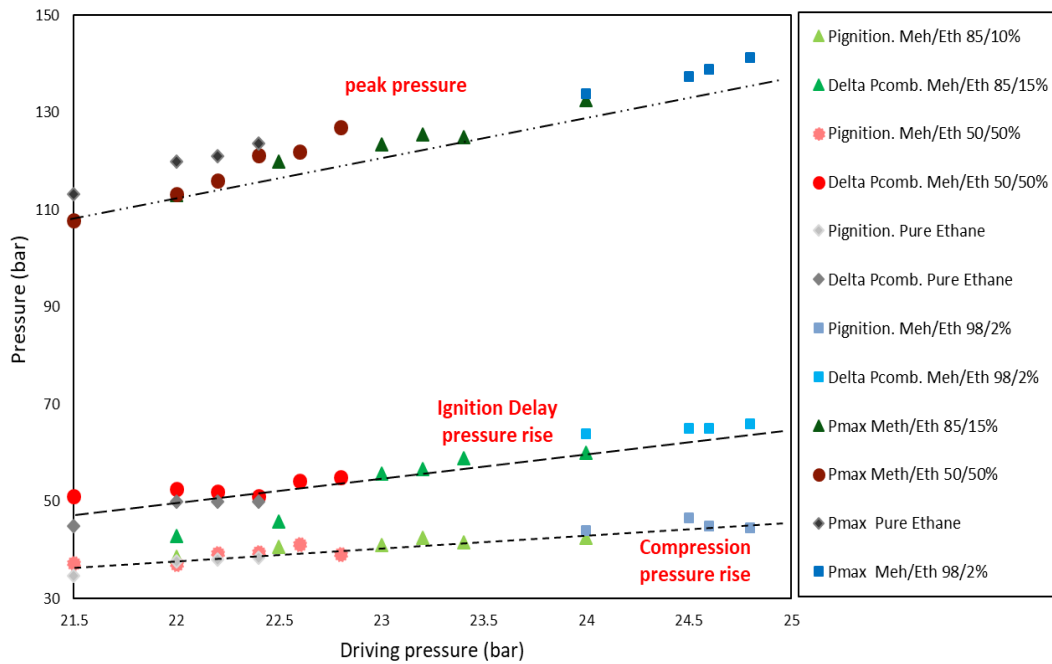


Figure 5-3 Detailed pressure (caused by compression, ignition and chemical reaction) of mixtures containing: 98% methane, 2% ethane; 85% methane 15% ethane; 50% methane 50%, ethane and pure ethane

Table 5.3 Peak pressure and compression ratio relative errors occurring during the repeatability test

Description	Methane98% Ethane 2%	Methane85% Ethane 15%	Methane50% Ethane 50%	Ethane 100%
Peak pressure error (%)	0.9	1.58	0.42	0.8
Compression ratio error (%)	1.4	0.87	0.51	0.89

Peak pressure and compression ratio, as the most important parameters during the combustion, have been investigated. Figure 5.4 shows the peak pressures of various methane-ethane mixtures versus the compression ratio. At knock threshold operating condition, the following results were obtained. The mixture of 98% methane and 2% ethane has the highest peak pressure of 139 bar and compression ratio of 25. The averaged peak pressure reduces to 128.5 bar and a compression ratio of 23, as the ethane proportion in the mixture increases to 15% by volume (methane 85%). The mediocre

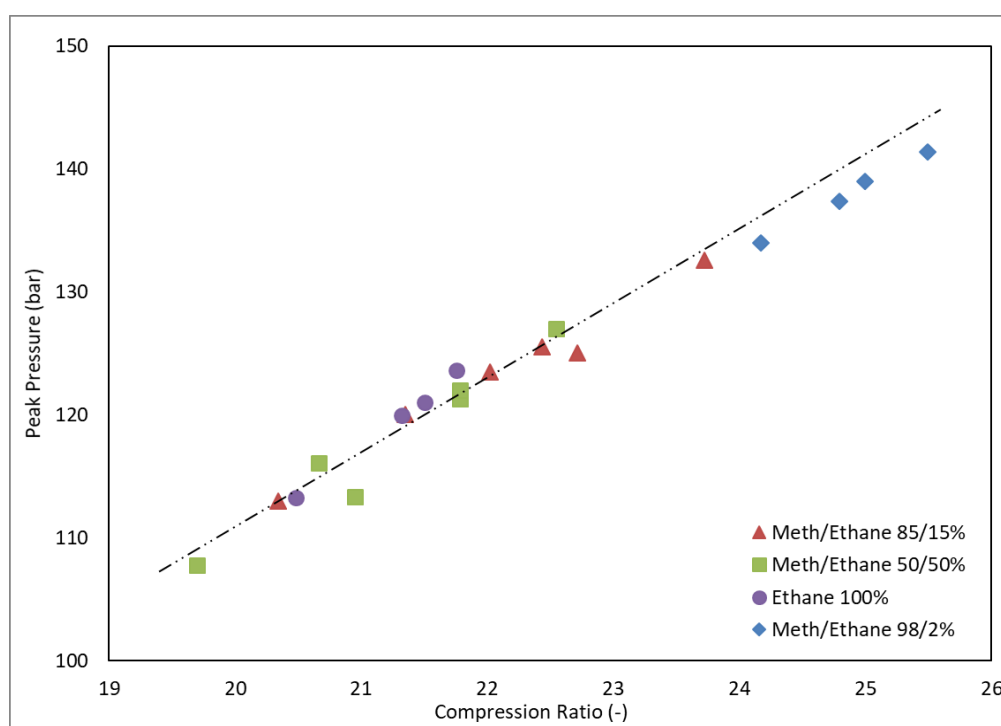


Figure 5-4 Peak pressure of the methane with different ethane proportions, since compression ratio increases at knock threshold operating condition

peak pressure drops to 123.5 bar and 22.2 for compression ratio, when the methane and ethane have been mixed in equal proportions of 50%. The peak pressure of pure ethane combustion in the RCM falls to 120 bar in pressure and 21.4 in compression ratio.

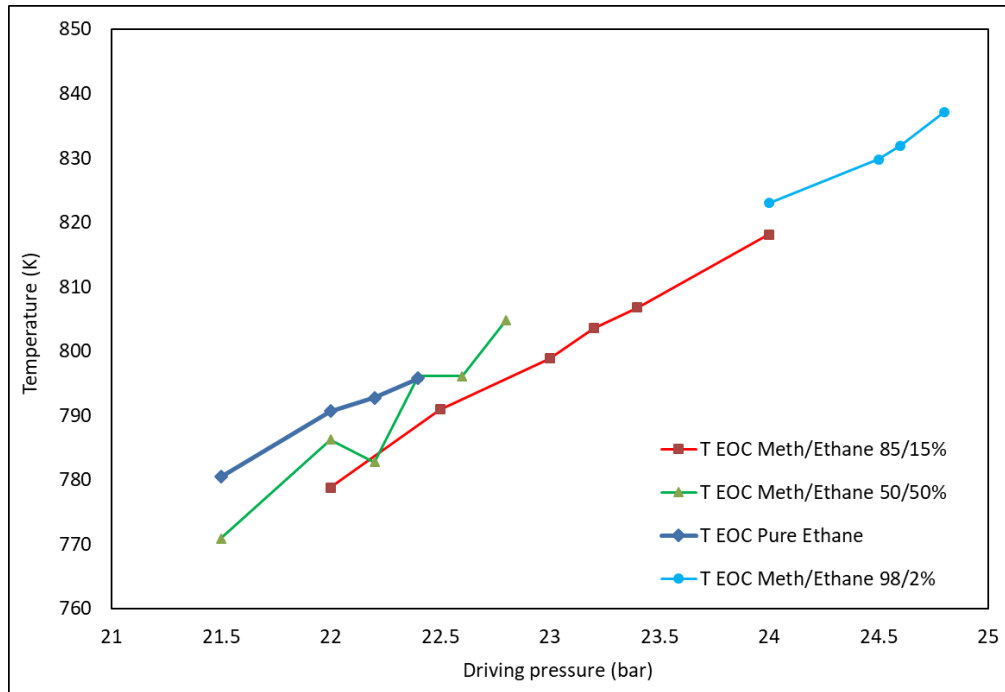


Figure 5-5 EOC temperature of the mixtures containing: 98% methane plus 2% ethane; 85% methane plus 15% ethane; 50% methane plus 50% ethane; and pure ethane

The pressure and temperature of the tests should be recorded and checked, to adjust the same compression pressure like in a real engine. In Figures 5.5 and 5.6, the temperatures and pressures at the end of compression process are presented, respectively. As the ethane content increases from 2% to 100% in the mixture, pressure at the EOC reduces from 70 bar to 58 bar at the knock threshold operating conditions. The temperature of the mixtures at the end of the compression process reduces from 830 to 780 K, as the ethane ascends from 2% to 100% ethane (pure ethane) as shown in Figure 5.5.

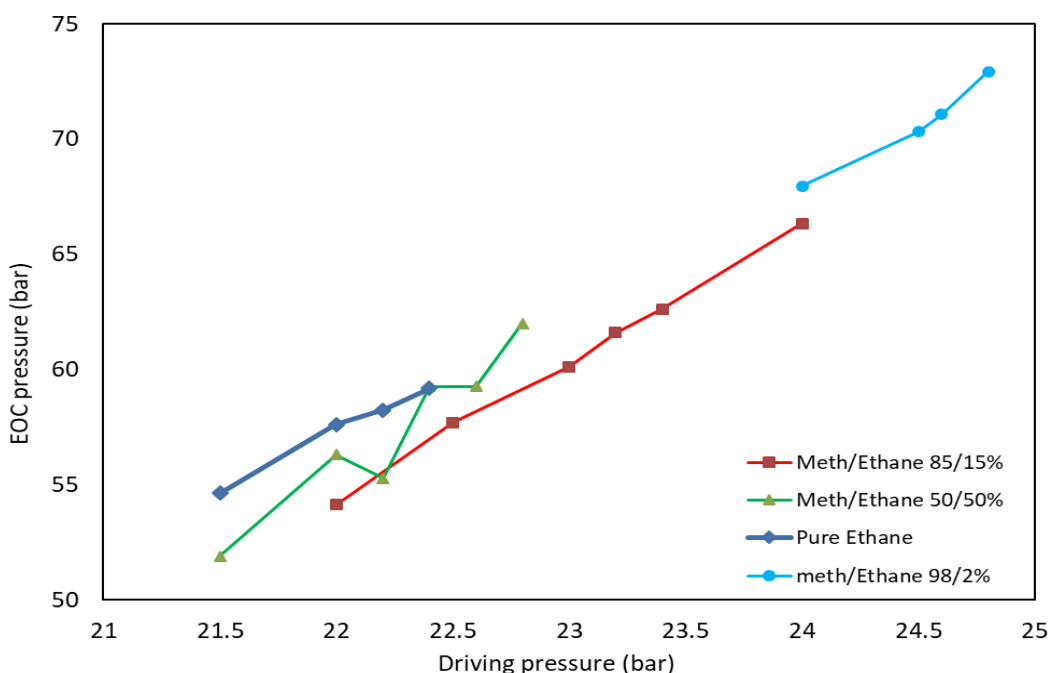


Figure 5-6 EOC Pressure for the mixtures containing: 98% methane plus 2% ethane; 85% methane plus 15% ethane; 50% methane plus 50% ethane; and pure ethane

In spark ignition engines, the duration of the ignition lag affects the knocking tendency of the RCM. If the ignition lag is longer than the time required for the flame front to burn through the charge, there will be no knocking. However, if it is shorter than the time required for the flame to propagate through the charge (and the temperature of the charge is greater than the auto-ignition temperature of the fuel), detonation can occur. So, to avoid detonation, a longer ignition lag is preferred accompanied by a high auto-ignition temperature as far as the fuel properties are concerned. Figure 5.7 shows the ignition delay of the various proportions of the methane-ethane mixtures. The figure shows the ignition delay time of 98% methane blended into 2% ethane, reducing from 73 ms to 66 ms, since the driving pressure which has a direct correlation to the compression ratio increases from 24 bar to 24.8 bar. The ignition delay for 15%, 50% and 100% ethane content falls from 71 ms, 67 ms and 62 ms to 58 ms, 55 ms and 58 ms, respectively at threshold operating conditions.

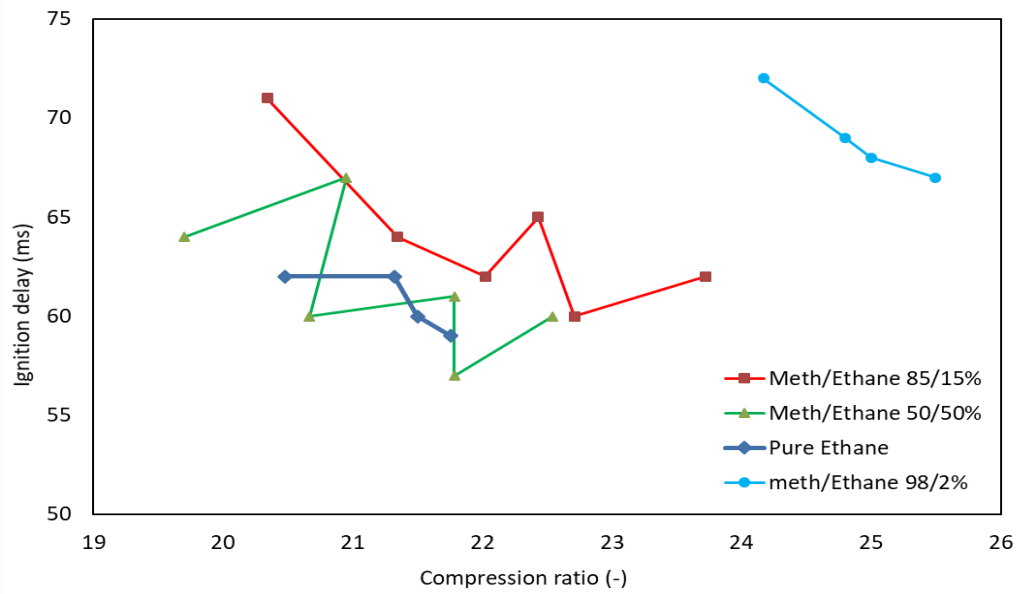


Figure 5-7 Ignition delay of the mixture containing of different proportions of methane and ethane with respect to compression ratio

The heat release rate was calculated in MATLAB using the pressure obtained from experimental data of the RCM and the volume using the piston motion of the RCM during the experimental tests. The pressure and volume were obtained from one

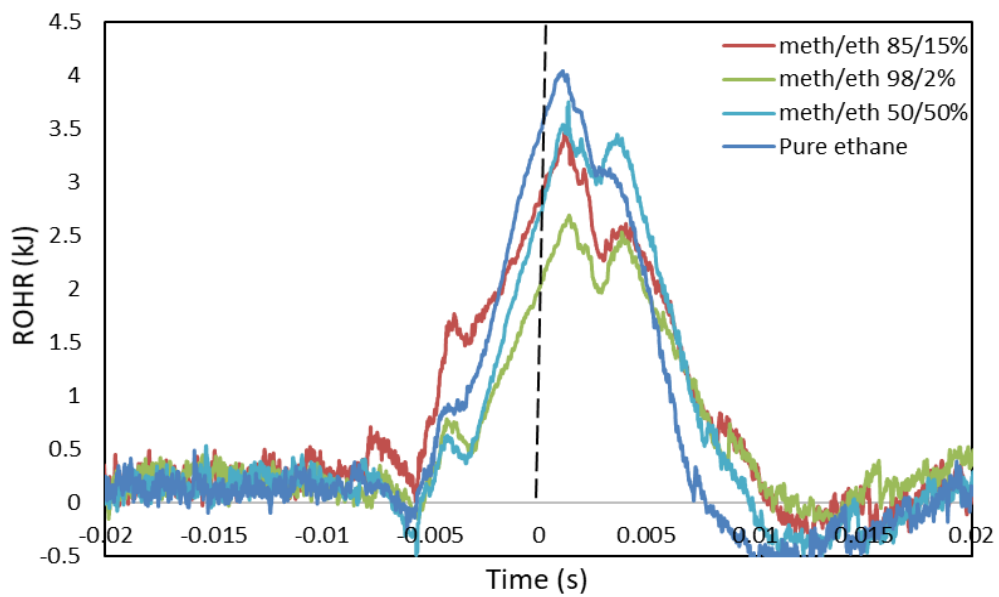


Figure 5-8 Rate of heat release for different proportions of methane-ethane mixtures

cycle with an increment of 0.1 ms. The rate of heat release of the methane-ethane mixtures is indicated in Figure 5.8.

5.5.2 Methane-butane Mixtures

Methane and butane have been blended into different proportions as shown in Table 5.2. Butane was mixed into the methane with four different volumetric proportions: 1%, 3%, 5% and 10%. For each blend, the partial pressure of the fuel and air based on λ 1.2 and an energy content of 5 kJ have been calculated.

The knock threshold operating conditions of various proportions of methane-butane mixtures have been investigated by recoding the pressure trace of the mixtures as well as the piston displacement. The points are shown in Figure 5.9 (a to d). Figure 5.9 a. shows the mixture containing 1% butane added into 99% methane (by volume). The driving pressure increases until either self-combustion or knocking occurs in the chamber, then the highest driving pressure leading to normal combustion is selected as the knock threshold point. For instance, the driving pressure has been set at 23.5 bar, 23.8 bar and 24.4 bar, respectively to reach the first knocking level, then the last test with a normal pressure curve is selected as the threshold operating point for the mixture. Driving pressure of 23.8 bar with normal combustion is selected as the threshold point for the 1% butane plus 99% methane mixture.

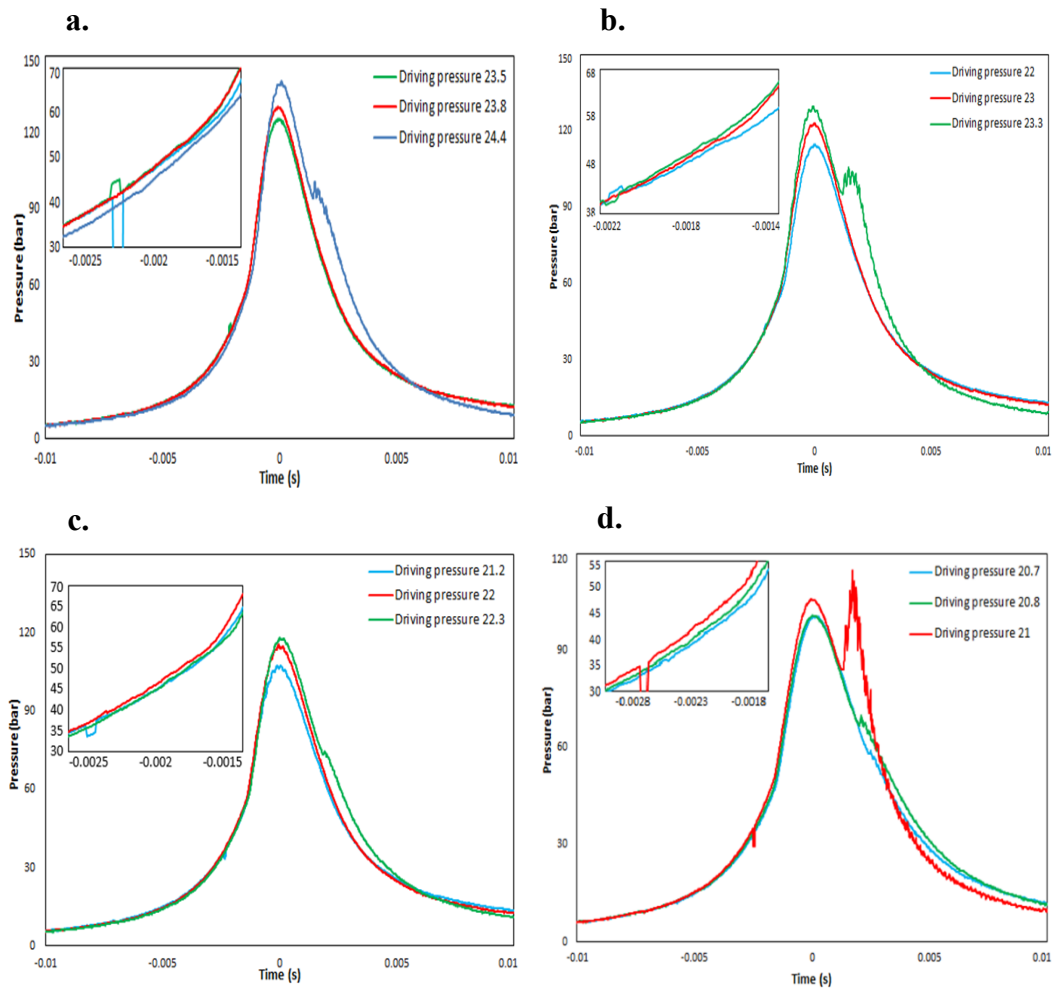


Figure 5-9 Approaching to the threshold operating condition of the mixtures containing: a. methane 99% and butane 1%, b. Methane 97% and butane 3% c. methane 95% and butane 5% d. methane 90% and butane 10%

The tendency of the mixture to knock increases since the butane content in the mixture rises to 3%. Driving pressure reduces to 23 bar for the threshold operating point. The abnormal combustion occurs when the driving pressure rises to 23.3 bar.

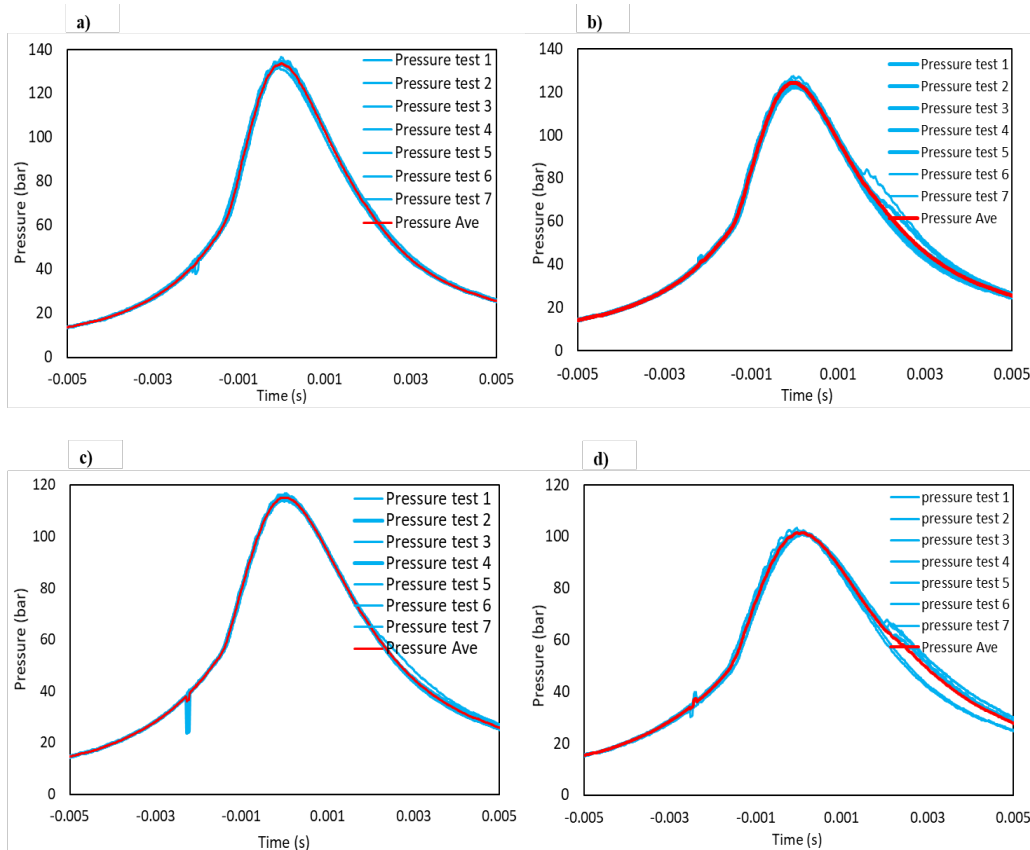


Figure 5-10 Repeatability tests of pressure trace for the mixture containing: a. methane 99% and butane 1%; b. methane 97% and butane 3% c. methane 95% and butane 5% d. Methane 90% and butane 10%

Since the butane content in the mixture increases to 5%, the mixture needs less charged driving pressure for compressing the mixture. For instance, driving pressure reduces to 22 bar to meet the normal combustion in the RCM, while the pressure sensor recorded very light self-combustion by increasing the driving pressure to 22.3 bar. As Figure 5.9 shows, the initial pressure level of different driving pressures causes variation in the mixtures' temperature. The compressed mixtures have a higher temperature because driving pressures increase.

Table 5.4 Calculated relative errors for the mixture at TDC for pressure trace and compression ratio

	Methane99% Butane 1%	Methane97% Butane 3%	Methane95% Butane 5%	Methane90% Butane 10%
Peak pressure error (%)	1.19	1.22	0.73	0.80
Compression ratio error (%)	0.55	0.65	0.74	1.0

The tendency of the mixture to knock increased since the content of the butane in the mixture increased to 10%. The driving pressure needs to be adjusted to find out the threshold operating point for the mixture containing 90% methane and 10% butane. Thus, the driving pressure is reduced to 20.7 bar to prevent either self-combustion or knocking. The smaller window in Figures 5.9 indicates the influences of the driving pressure on the pressure where spark and main combustion occur. It shows that pressure increases 3.5 bar at the start of combustion, since the driving pressure rises by 1 bar. Increasing 3.5 bar at the SOC raises the peak pressure by 5 bar, which results in knocking after TDC, as the temperature of the front flame propagation increases before the flame propagates throughout the chamber.

The repeatability of the RCM with different mixtures of methane and butane has been investigated and shown in Figures 5.10 (a to d). Tests for each mixture were run seven times to obtain their repeatability. The peak pressure and compression ratio for each test was measured and the errors at TDC were calculated. The errors for each mixture are shown in Table 5.4.

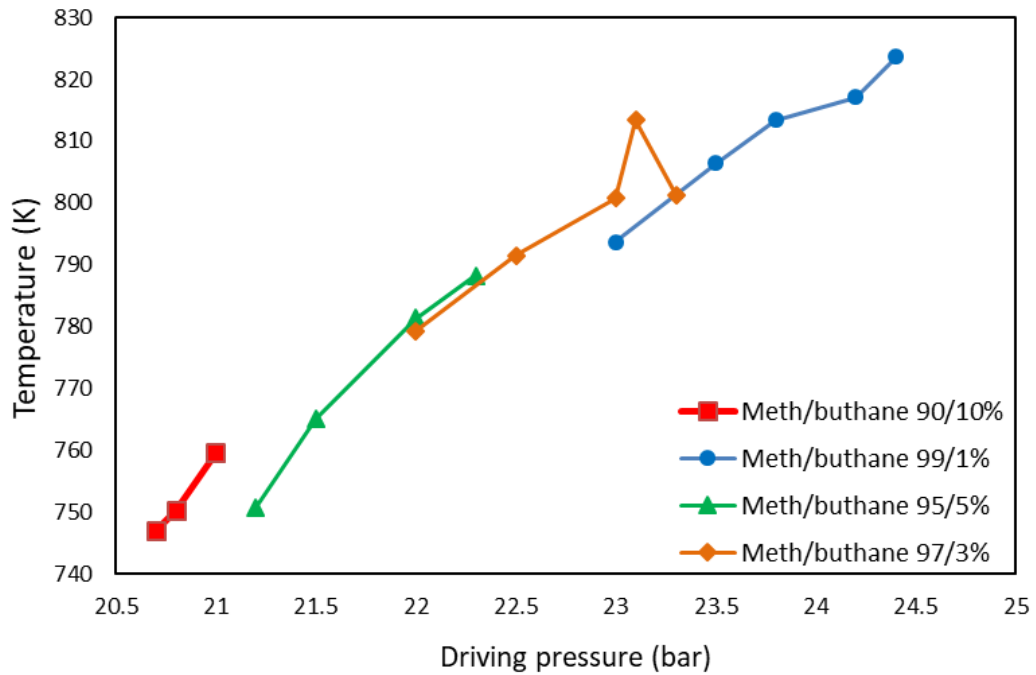


Figure 5-11 Influences of driving pressure on EOC temperature for mixtures containing 99% methane plus 1% butane; 97% methane plus 3% butane; 95% plus methane 5% butane; and 90% methane plus 10% butane

Figure 5.11 exhibits the influence of the EOC temperature for various proportions of butane mixed into the methane. The reduction trend of the EOC temperature is the same as for the EOC pressure. As the butane content increases from 1% to 3%, the EOC temperature drops from 820 K to 800 K; the reduction trend continues, reaching 780 K as the proportion of the butane increases to 5%. The EOC temperature declines to 750 K when the butane content rises to 10% in the mixture. The tendency of the mixture to knock soars as the mixture is compressed due to the higher content of butane. For instance, driving pressure reduces from 24.5 bar to 21 bar when the butane content

increases from 1% to 10%, respectively. It means that the mixture should be run with lower compression ratios.

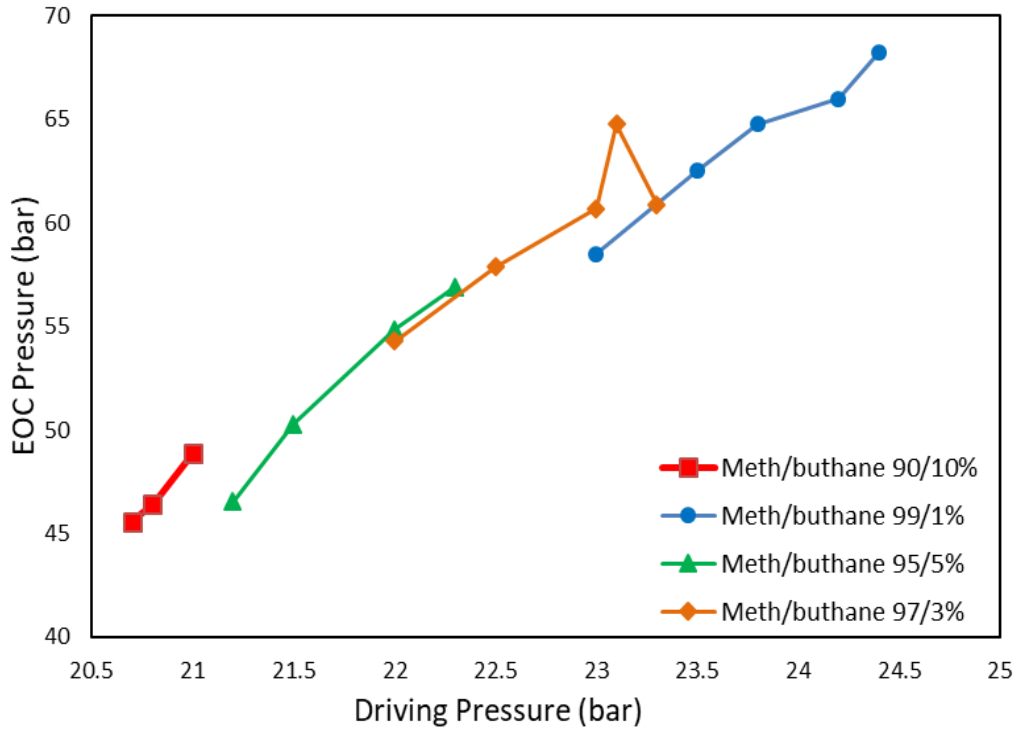


Figure 5-12 Influences of driving pressure on EOC pressure for mixtures containing 99% methane plus 1% butane; 97% methane plus 3% butane; 95% plus methane 5% butane; and 90% methane plus 10% butane

Figure 5.12 demonstrates the effects of driving pressure on EOC pressure for the mixtures containing methane and butane. The EOC pressure reduction for all mixtures of methane and butane is almost constant. For instance, EOC pressure reduces from 67 bar to 48 bars, as the butane content increases from 1% to 10%. As the butane content in the mixture increases, driving pressure should be reduced from 24.5 bar to around 20.5 bar, due to knock prevention.

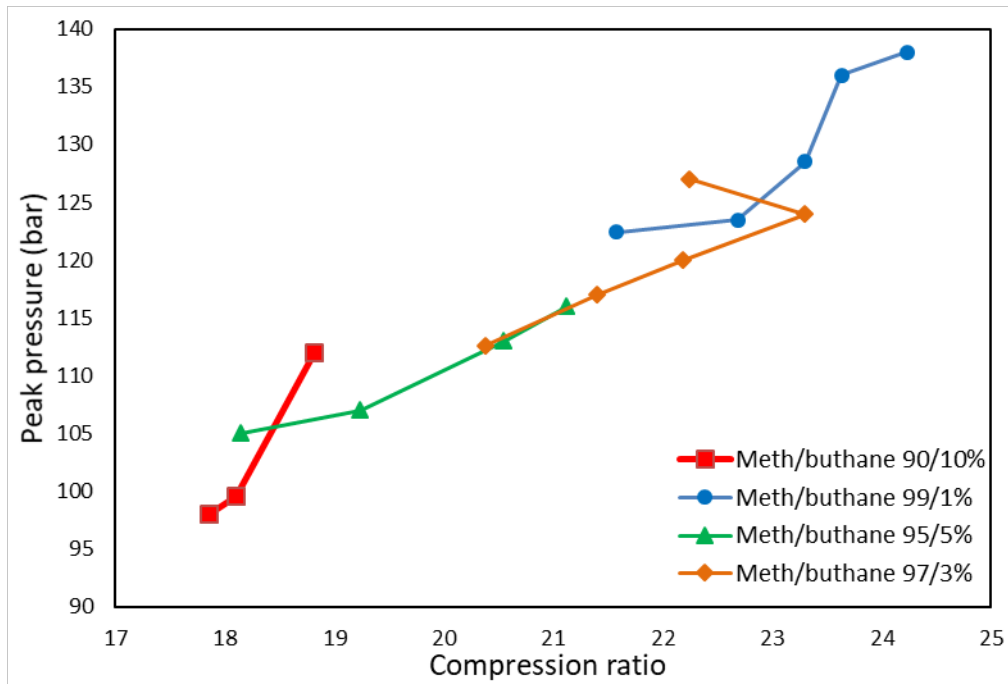


Figure 5-13 Influences of compression ratio on the peak pressure of the mixtures containing 99% methane plus 1% butane; 97% methane plus 3% butane; 95% methane plus 5% butane; and 90% methane plus 10% butane

Figure 5.13 shows the influences of the compression ratio on peak pressure for the mixtures containing methane and butane. At knock threshold conditions, peak pressure reduces with almost constant rate, but there are some fluctuations in 99% methane plus 1% butane. Peak pressure reduces from 135 bar to 125 bar, as the butane increases from 1% to 3%. Peak pressure continues to drop from 115 bar to 100 bar when the butane proportion rises from 5% to 10%.

The heat release rate was calculated in MATLAB using the pressure obtained from the experimental data of the RCM and the volume using the piston motion of the RCM during the experimental tests. The pressure and volume were obtained from one cycle

with increments of 0.1 ms. The rate of heat release of methane-ethane mixtures is indicated in Figure 5.14.

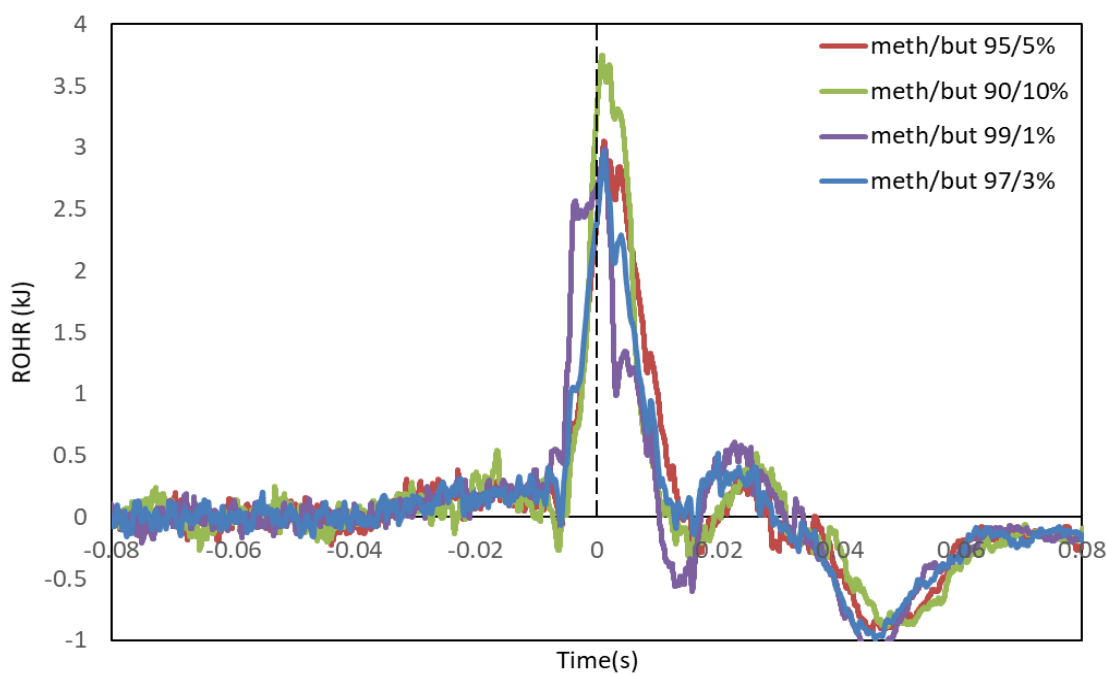


Figure 5-14 Rate of heat release for different proportions of methane-butane mixtures

5.5.3 Pressure Methane-ethane and Methane-butane Reference Curves

Figure 5.15 presents the summary of the tests done according to this chapter. The figure compares the resistance of a lighter and a heavier molar mass fuel blended into methane (the most difficult gaseous fuel to knock). In general, methane-butane mixtures are more prone to knock in comparison with methane-ethane mixtures. It is possible to mix higher proportions of ethane into methane, while only 10% (volume) of butane can be blended into it. For instance, the mixture containing 98% methane and 2% ethane causes more than 3 bar decrease in peak pressure, which means lower

resistance to knock; however, blending of 1% butane into the (99%) methane decreases the peak pressure of the mixture to 132 bar. Blending higher proportions of ethane into the methane has a lower impact on the mixture's tendency to knock. This has been proven by the results obtained by the RCM, so that the peak pressure is reduced more than 10 bar for 8% ethane additive, although the peak pressure reduces to 124 bar when the ethane content increases to 50%. The peak pressure drops to 120 bar when pure ethane is tested in the RCM. There is a reduction in the rate of decreases as the ethane proportion increase.

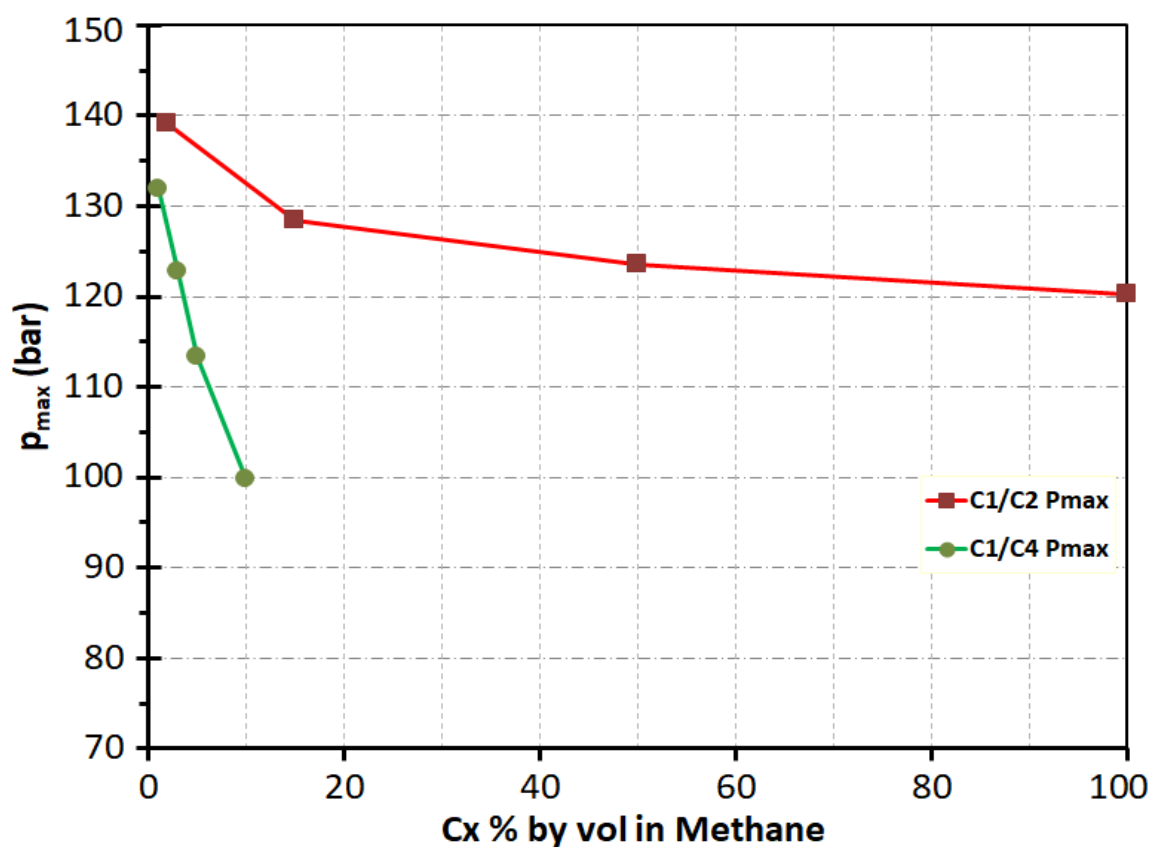


Figure 5-15 Summary of peak pressure for different proportions of methane-ethane and methane-butane mixtures

Butane is the next fuel which has been mixed into methane. The oxidation of various proportions of methane-butane mixtures have been examined and summarized

in Figure 5.15. Lower proportions of butane can be capable of being blended into the methane, due to its higher knock tendency. The peak pressure of the methane-butane mixtures experienced very sharp decreases as the small proportions of butane were blended in. To be more precise, peak pressure drops from 142 bar to 132 bar, when 1% butane is blended into the pure methane. The trend continues by blending 3% butane into the methane, and the peak pressure declines to 123 bar. By increasing the butane proportion to 5% in volume, there is a reduction of 9 bar and peak pressure stays at 114 bar. The highest possible amount of butane which would blend into the methane is 10%, and it is combustible in the RCM. the peak pressure drops to 100 bar, when the 10% butane content is tested.

5.5.4 Compression Ratio Methane-ethane and Methane-butane

Reference Curves

To ensure the reliability of the RCM, several parameters should be investigated. Compression ratio is one of the parameters which here can check the accuracy of the peak pressure. Compression ratio was calculated based on the piston movement and the geometries provided by the manufacturer. The RCM piston detectors were calibrated every 10 shots, in order to reduce the inaccuracies.

The compression ratio of 98% methane and 2% ethane stood at 25.1. This compression ratio reduces to 23.2, when the ethane content reaches 15% in volume. There is around an 8% reduction as the methane content reduces from 98% to 85%, and the ethane content increases from 2% to 15%. The reduction in compression continues

to 22.2, when the mixture contains 50% ethane and 50% methane. The rate of reduction is halved and it reduces to 4%, in comparison with the mixture of 2% ethane and 98% methane. The compression ratio stays slightly lower than 21.5 for pure ethane; the compression reduced by around 3.5% in comparison with the previous mixture.

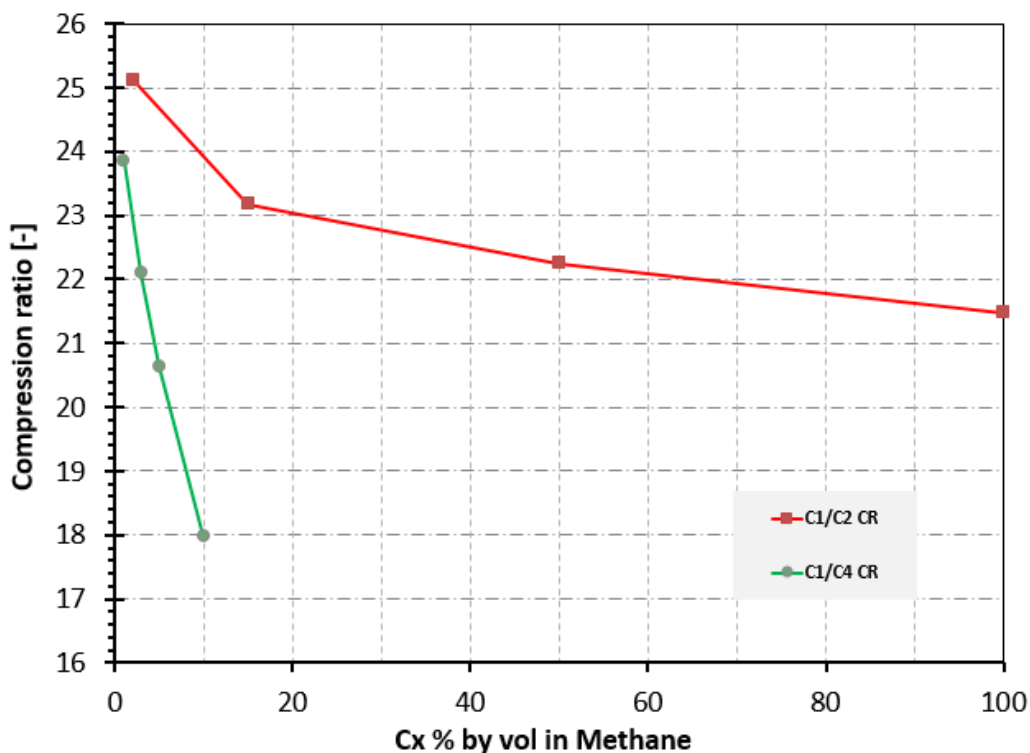


Figure 5-16 Summary of compression ratio for different proportions of methane-ethane and methane-butane mixtures

The trend when mixing butane into the methane is the same as for the methane-ethane mixtures; however, the rate of the variations is completely different. To be more precise, the mixture of 1% butane and 99% methane is compressed much less than what it was with 2% ethane and 98% methane and the compression ratio of the mixture stood at point 23.85. The compression ratio of the 3% butane and 97% methane reduces to 22; it shows a 7.7% decrease in compression ratio of the higher butane proportion. Since the proportion of the butane in the methane increases to 5%, the compression

ratio drops about 6.6%, reaching 20.6. It is interesting since the butane content is doubled, the compression ratio is achieved to 18, and this means that the compression ratio is reduced by more than 12%. The compression ratio data have been represented in Figure 5.16.

It can be clearly seen that ethane has higher resistance against knocking in comparison with butane, so that it can be compressed more and consequently higher compression ratios have been produced. Besides, the compression ratio drops only 3.6 units from 25.1 to 21.5, since the proportion of the ethane increases from 2% to 100% ethane; however, the compression ratio declines about 5.8 units from 23.8 to 18, when the butane is blended into the methane from 1% to 10%.

5.5.5 Methane Number Reference Curves

Figure 5.17 shows the calculated methane number of the various mixtures based on the peak pressure measured in the RCM. The methane numbers were calculated based on two different methods: The Wartsila and EN19625 standard.

The methane number of pure methane is set at 100 to show its highest possible resistance against knocking, since the fuels (heavier hydrocarbons) added into the pure methane cause a reduction in tolerance of the mixtures against knocking. According to both Wartsila and EN standard MN calculators, when 2% ethane is blended into methane, the methane number reduces to 94. The methane number of the new mixture containing 15% ethane and 85% methane is 77 with Wartsila MN calculations, while

the methane number of the same mixture is lower than Wartsila's MN calculation, and reaching 74. Since the content of the ethane in the mixture goes higher than 50%, the MN drops faster. To be more precise, when the mixture contains 50% ethane and 50% methane, the MN suddenly drops to 61 based on Wartsila, and 55 based on the EN standard calculations, due to the lower peak pressure from the tests done by RCM. The MN of the pure ethane drops with the rate of the 50% ethane and 50% methane mixtures and it reaches 51 and 44, based on the Wartsila and EN standard methods, respectively.

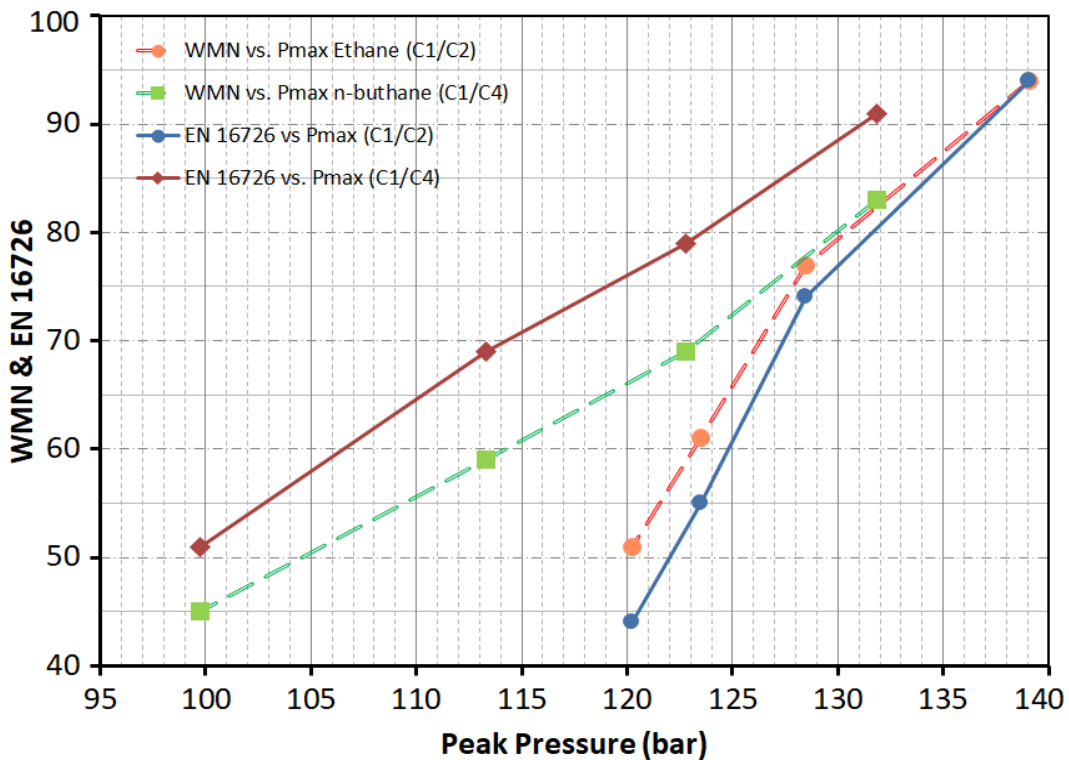


Figure 5-17 Methane Number calculated by two methods (WMN, EN 16726) for methane-ethane and methane-butane W.R.T peak pressure

The MN of the methane-butane mixtures based on the peak pressure has been analysed. It shows that since the butane was added into the methane, the MN reduction has almost a constant rate. Thus, the MN is 88 and 91 for the 1% butane and 99% methane mixture based on the Wartsila and EN standard methods, respectively. The

MN stays at 69 (Wartsila method) and 79 (EN standard), when the butane content increases to 3% in the mixture. According to the Wartsila MN calculation, MN drops to 59 and 45, with a mixture of 5% butane plus 95% methane and 10% butane plus 90% methane tested in the RCM, respectively. Based on the EN standard method, the MN decreases to 69 and 51, when the same mixtures of 5% butane and 10% butane are blended into 95% and 90% methane, respectively.

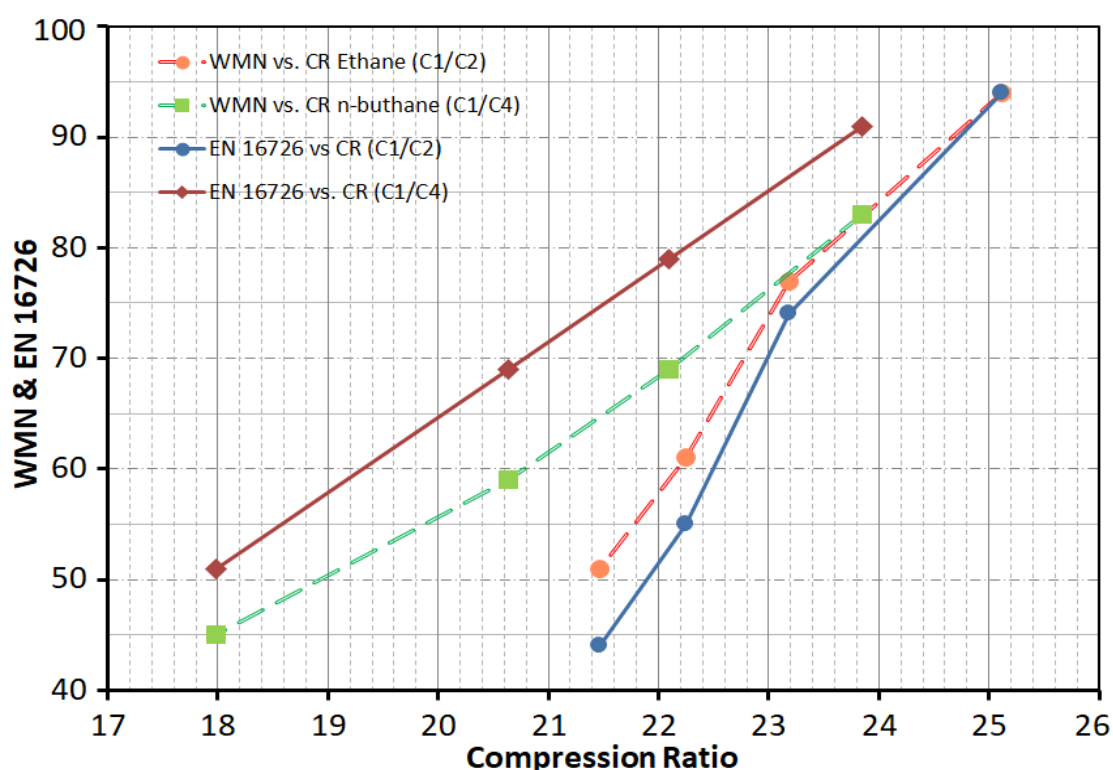


Figure 5-18 Summarized calculated compression ratio and calculated MN (WMN, EN 16726) for the methane-ethane and methane-butane mixtures tested in the RCM

Figure 5.18 displays the methane number of two different fuels blended into the methane as a baseline fuel, based on the compression ratios extracted from the RCM tests. The MNs are compared with different parameters to also examine the reliability of the machine. According to Figure 5.18, the graphs follow the same trend. The trend

of the mixtures is downward with the same rate, while the methane-ethane mixture with a higher proportion of 50% ethane has larger reduction.

5.6 Conclusion

The influences of adding ethane and butane into the methane on the combustion process have been characterized in this chapter. First, ethane as the lightest hydrocarbon after methane was mixed into the methane. Second, the butane as a heavier hydrocarbon was blended into the methane to study the combustion behaviour of the mixtures.

Tests were carried out to investigate the influences of blending ethane and butane separately into the methane as the threshold operating conditions were studied by using the RCM. The mixtures were compressed by increasing the driving pressure to meet the knocking combustion. Then the lower level of the driving pressure leading to normal combustion was selected as the threshold operating condition. In the next step, the repeatability of these points was examined. According to the results, the driving pressure drops as the ethane and butane content in the mixtures increases. The driving pressure reduces the peak pressure and compression ratio.

The resistance of the mixture reduces as the ethane and butane are blended into the methane. Although the ethane content can be increased to 100% in the mixture, the butane content as a heavier hydrocarbon, is limited to 10%. The ignition delay time of the mixtures having a higher butane proportion is shorter, due to the higher activity of the butane.

**CHAPTER 6 – STUDY OF
COMBUSTION
CHARACTERISTICS OF
BLENDING N-PENTANE IN
METHANE BY USING AN
RCM**

6.1 Introduction

The next generation of advanced propulsion systems will struggle to combine dramatically enhanced power output with high efficiency and control; pushing combustion to occur at the very limits of flammability and stability for a specific fuel. There is a potential challenge ahead in terms of achieving combustion stability for active combustion enhancement by the introduction of new and alternative fuel blends, which can exhibit a drastic variation in combustion characteristics depending on the operational conditions.

Lighter hydrocarbon fuels (ethane, propane and butane) blended into the pure methane investigated in Chapters 4 and 5 exhibit an increase in the tendency of the mixtures to knock, which leads to range and load limitations for power plant engines operating on the mixture (Allen 2012).

The purpose of this study is to investigate the effects of the presence of diverse proportions of pentane mixed in the pure methane on the combustion process in the RCM. Preparation of the mixture for an experimental platform is of high importance, due to the fact that n-pentane should be injected into a mixing tank separately, as well as carrying the vaporised mixture into the chamber.

6.2 Tested Fuels and Fuel Properties

In previous chapters, different proportions of ethane, butane and propane (separately) were blended into the methane (baseline), and then the combustion characteristics of each mixture were studied. Combustion characteristics such as peak pressure, compression ratio, ignition delay, pressure and temperature of the mixture at the end of the compression process were investigated. Here, in this chapter, it is aimed to mix a heavier fuel of n-pentane with the methane. Table 6.1 summarises the properties of the fuels investigated in this study. The fuels have been ordered and stored at Wartsila Fuel Laboratory in Vaasa, Finland.

Table 6.1 Properties of n-pentane which was mixed with methane in different proportions

Property	Methane (CH ₄) in gaseous form	N-pentane (C ₅ H ₁₂) in Liquid form
Molecular formula	CH ₄	C ₅ H ₁₂
Heat of combustion	55.5 MJ/kg	104.6 MJ/kg
Flash point	−188 °C	−49.0 °C
Boiling point	−161.49	35.9 to 36.3 °C
Molar mass	16.04 g·mol ^{−1}	72.15 g·mol ^{−1}
Density	0.657 g·dm ³	0.626 g *0.001 dm ³

Figure 6.1 shows the mixing reactor and a valve attached (highlighted in the figure in red) to inject the liquid n-pentane into the mixing tank. The operator will be asked to specify the fuels needed to be mixed. The reactor must be flushed and then vacuumed before n-pentane is added in the program panel. After flushing and vacuuming, n-pentane should be injected as the first fuel in the tank. The detailed procedure has been

explained previously in Chapter 3. Figure 6.2 shows the syringes and n-pentane bottle required to inject it into the mixing reactor.



Figure 6-1 Mixing tank with valve equipped to inject the liquid n-pentane into the mixing during the process



Figure 6-2 N-pentane bottle and syringes for injection to the mixing reactor

The n-pentane was blended into the methane with different proportions as shown in Table 6.2. the n-pentane was added by 0.5%, 1%, 2% ,3%,4% and 8% into the 99.5%,

99%, 98%, 97%, 96% and 92% methane, respectively. The energy content of all the mixtures was kept constant at of 5 kJ, as well as lambda also at a constant 1.2. The detailed properties of the mixtures and proportions created in the reactor for the tests are represented in Table 6.2.

Table 6.2 Properties of the methane and n-pentane with different proportions

Lambda 1.2	Energy Content (5kJ)	Base Methane (100%) N-pentane proportion mixture (%Vol.)					
Methane proportion (%Vol.) A		99.5	99	98	97	96	92
N-pentane proportion (%Vol.) B		0.5	1	2	3	4	8
AFR _{stoichiometric} (Vol.)		9.662	9.805	10.091	10.376	10.662	11.80
X (number of moles of air per mole of fuel in mixtures)		11.595	11.766	12.109	12.452	10.66	11.80
LHV mixtures (MJ/m ³)		36.4	36.97	38.07	39.17	40.27	38.01
Final fuel pressure (bar)		0.18	0.18	0.17	0.17	0.16	0.147
Final air-fuel pressure (bar)		2.27	2.27	2.27	2.26	2.25	2.23

6.3 Experimental Methods

As already mentioned in Chapter 3, different proportions of ethane and butane fuels (separately) blended into the methane were investigated, corresponding to the average initial temperature of 81°C. Initial temperature is essentially defined by the RCM heating elements mounted inside the piston and cylinder walls. Here, in this chapter, pentane as a heavier hydrocarbon active fuel is blended into the methane. The creation of a premixed fuel and air charge requires preheating of the mixture to 50°C, leading to vaporisation of all the mixtures. However, the heat must be carefully applied to the system because excessive temperature leads to concerns regarding thermal decomposition increased by the conventional use of a mixing vessel, which is heated for several hours during batch pre-mixture preparation and testing.

In this study, a different method for preparing an active charge directly in the RCM has been proposed and characterised. The method has been specifically designed for creating pre-mixtures with non-volatile fuels, and it provides an efficient means for measuring combustion characteristics at a broad set of test conditions.

Table 6.3 Comparison of the methods used to adjust the 85%methane and 15% n-pentane mixtures

Description	Peak Pressure (bar)	Compression ratio (-)	Driving pressure (bar)	Stroke (mm)	Lambda	LHVf (kJ)	Comments
Original	114	19	20.6	180	1.2	5	Hitting the BDC of RCM
Method 1	79	15	22.7	180	1.6	5	Leaner-high error-easy combustion changes to knocking
Method 2	64	16.7	18.2	180	1.6	3.8	Leaner-high error-lower LHV-easy combustion changes to knocking
Method 3	61	20.5	16	180	1.6	3	Leaner-high error-lower LHV-easy combustion changes to knocking
Method 4	51	16.7	10.5	180	1.2	2.5	Lower LHV-extremely higher errors
Method 5	80	14.1	17.3	120	1.2	5	Extremely high error-lower stroke
Method 6	68	>45	12.4	120	1.2	1.67	Extremely low LHV-high CR- high error-not meeting SC-KN conditions.

From the piston position data extracted from the tests of 15% n-pentane blended into 85% methane, it was found that the piston hits the BDC since it is bounced by the released energy of the mixture, as shown in Figure 6.4. Although it cannot affect the combustion phenomenon, it can damage the RCM. Therefore, different methods have been proposed and then tested to overcome the issue. These methods have been explained in Table 6.3. Meanwhile, a check valve and throttle valve have been installed in the driving tank section, due to the fact that there are two driving tanks to slow down the piston speed to the range of 500 rpm to 2500 rpm; but as the driving pressure reduces it cannot act as a damper and the piston hits the body.

To run the tests with pentane proportions blended into the methane, driving pressure should be reduced; consequently, it cannot react as a damper since the piston travels speedily towards the BDC and it heads towards hitting the bottom of the cylinder and can cause damage to the RCM. Different methods were proposed to overcome the issue as summarised in Table 6.3. The stroke was held constant at 180 mm in methods 1 to 4, while the energy content of the fuel and lambda are changed. In these methods, the issue was solved, however, another issue appeared. There was no gap between the normal and knocking combustion phases. This is due to inhomogeneity of the mixture in leaner conditions between the mixture and air in the chamber, so that only a 0.1 bar increase in driving pressure leads to heavy knocking.

In methods 5 and 6, the stroke was reduced to 120 mm (lowest possible stroke in the RCM) to find out the effects of the shorter stroke on the combustion of the mixtures. According to the results, tests failed to specify the threshold conditions of the tested

mixture since the piston hit the TDC before abnormal combustion occurred. Moreover, errors increase with higher proportions of the n-pentane in the mixture, even when the lambda reduces to 1.2.

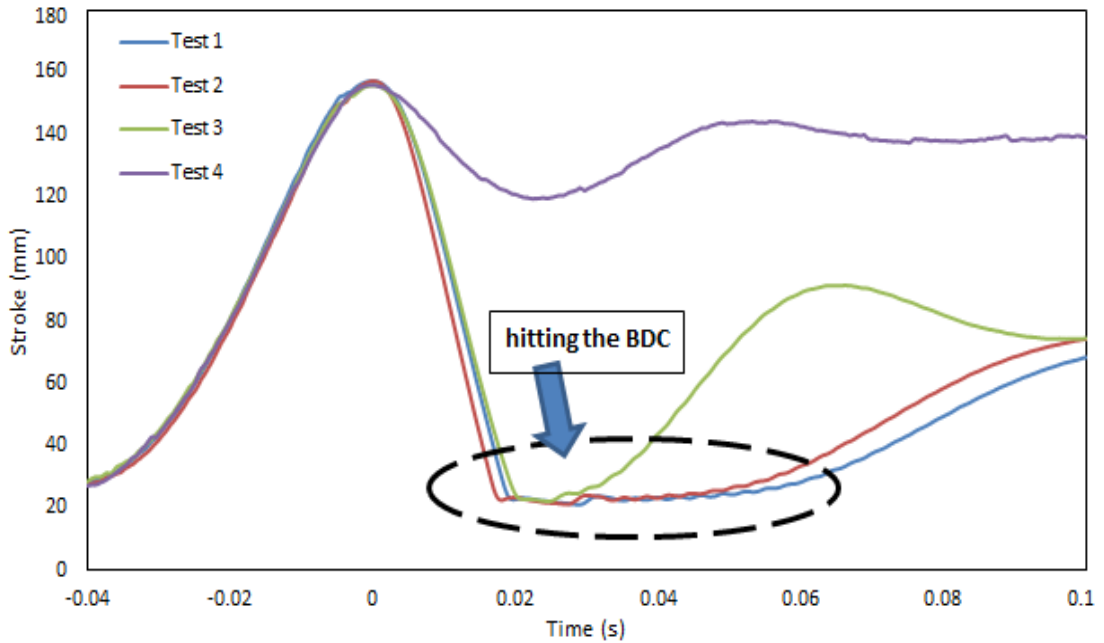


Figure 6-3 Influence of the higher content of the pentane mixture in the RCM, piston hits the BDC

To solve the issue, since the RCM operating conditions are not affected by the changes, four parameters of the stroke, lambda, final charge pressure and energy content of the fuel have been changed. These changes have been made to find the best method. Each method has some advantages and disadvantages. The most important issue with which the RCM team was concerned was keeping all operating parameters and conditions constant in all experiments. Therefore, the original method was performed; however, a check valve and throttle valve were installed and adjusted. The throttle valve was adjusted so that the driving air pressure was trapped in the main driving pressure tank, acting as a damper and then it prevented damage to the RCM.

6.4 Results and Discussion

For the new tests with the new preparation of the mixture and a new check valve and a new throttle valve installed in driving section of the RCM, it is desirable to investigate the behaviour of higher proportions of pentane blended into the methane. It is a good starting point to consider the effects of the lowest possible content of pentane blended into methane on the combustion characteristics of the mixture. These results have been validated in the AVL BOOST software and based on the assumption that they serve as an additional direct comparison for data measured in the RCM.

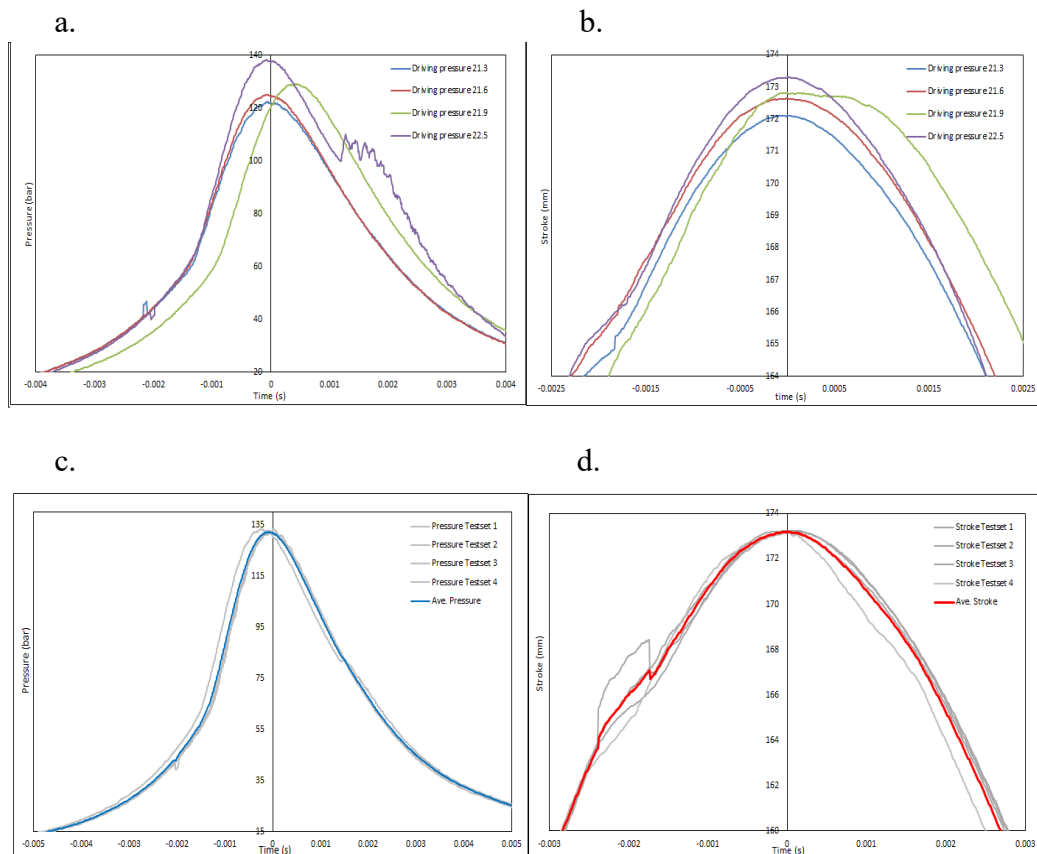


Figure 6-4 Study of the mixture containing 99% methane plus 1% n-pentane:
a. approaching to the knock threshold operating condition by adjusting the driving pressure; b. piston motion closed to TDC with adjusting the driving pressure; c. pressure repeatability investigation at knock threshold condition;
d. stroke repeatability investigation at knock threshold condition

In general, one way to obtain the knocking threshold operating point of various mixtures is to increase the compression ratio of the engine, since the other conditions are held constant. In the RCM, the compression ratio can be varied to increase the initial compressed temperature (and pressure) of the mixtures. Increasing the compression ratio is possible since the driving pressure increases. This is the strategy which has been used in this study, increasing the driving pressure to lead the mixture to be more prone to knock.

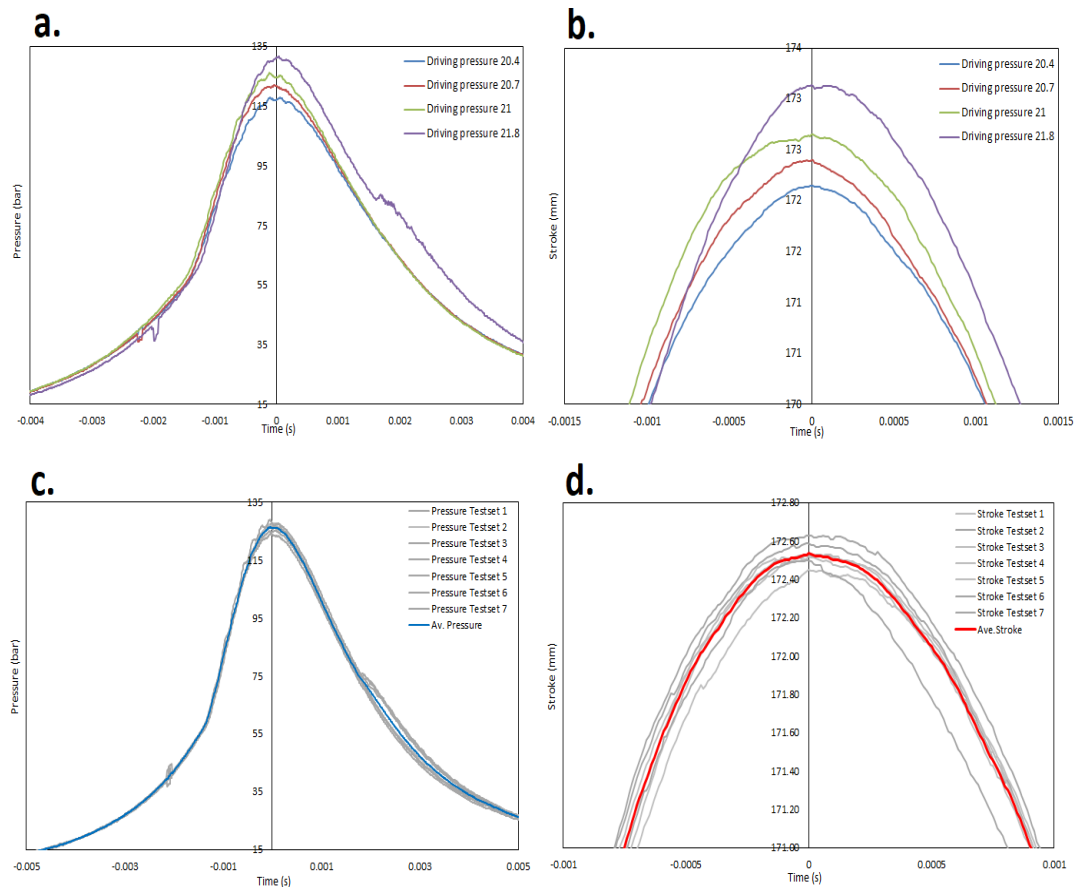


Figure 6-5 Study of the mixture containing 98% methane plus 2% n-pentane:
a. approaching to the knock threshold operating condition by adjusting the driving pressure; b. piston motion closed to TDC with adjusting the driving pressure; c. pressure repeatability investigation at knock threshold condition; d. stroke repeatability investigation at knock threshold condition

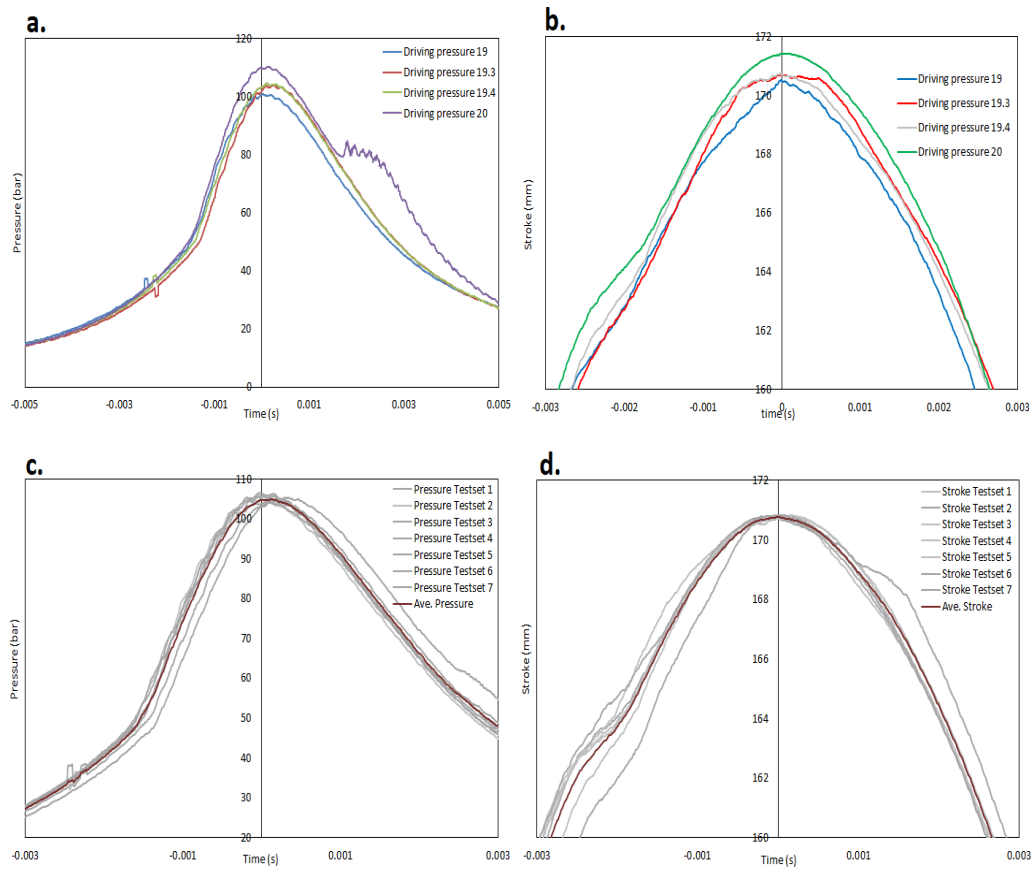


Figure 6-6 Study of the mixture containing 96% methane plus 4% n-pentane:
a. approaching to the knock threshold operating condition by adjusting the driving pressure; b. piston motion closed to TDC with adjusting the driving pressure; c. pressure repeatability investigation at knock threshold condition; d. stroke repeatability investigation at knock threshold condition

Figures 6.4 to 6.8 exhibit the pressure, piston position and repeatability test data measured in the RCM for lean conditions of lambda 1.2 at threshold operating condition, since the pentane content increases to 0.5%, 1%, 2%, 3%, 4% and 8%, respectively in 99.5%, 99%, 98%, 97%, 96% and 92% methane. It should be noted that all the mixtures are mixed with air during the mixture preparations to obtain better homogeneous air-fuel mixtures.

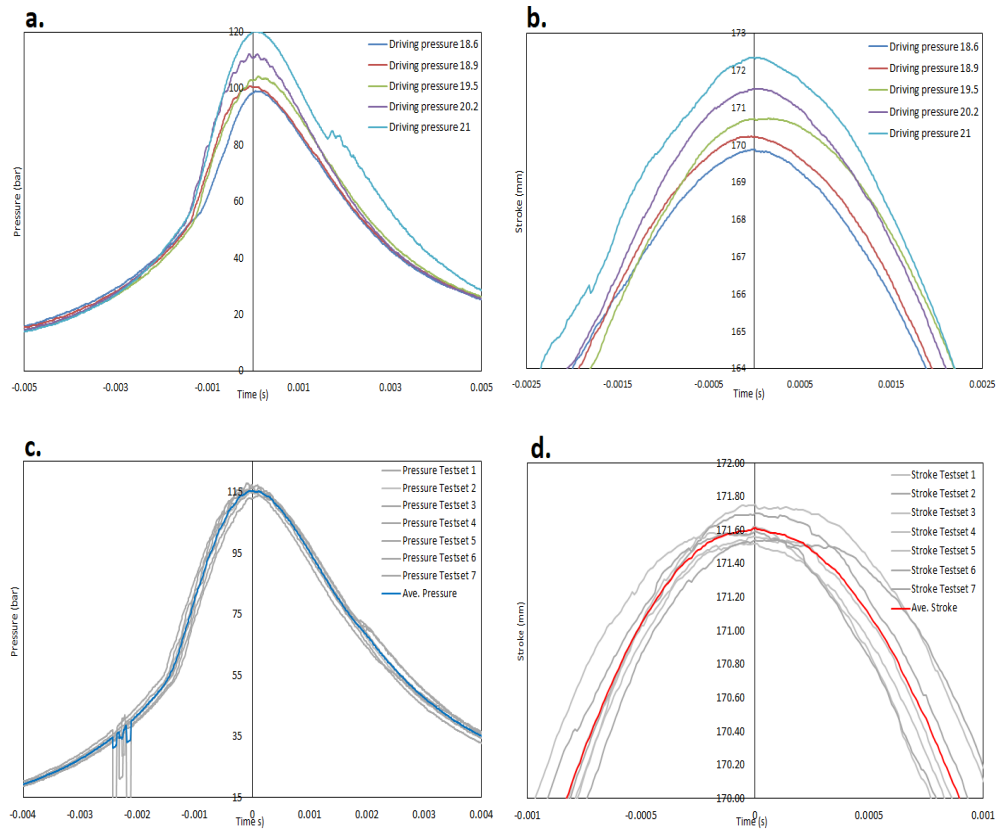


Figure 6-7 Study the mixture containing of 97% methane plus 3% n-pentane; a. approaching to the knock threshold operating condition by adjusting the driving pressure b. piston motion closed to TDC with adjusting the driving pressure c. pressure repeatability investigation at knock threshold condition d. stroke repeatability investigation at knock threshold condition

To obtain the knock threshold operating condition of the mixtures in the RCM, the driving pressure needed to be increased; since either self-combustion or knocking occurs, then the highest driving pressure creates the normal pressure trace considered as the threshold operating point.

It is necessary to investigate the proportion of the driving pressure effects on the compression ratio for different mixtures of methane and n-pentane, to ensure that the

tests have been done in the same conditions. Figure 6.9 shows the compression ratio data measured in the RCM since the driving pressure is varied for various proportions of pentane blended into methane. Generally, compression ratio is proportionally changed with respect to the driving pressure at the almost constant decreasing gradient between 1.3 and 1.7. To be more precise; compression ratio and driving pressure of all mixtures reduce, compression ratio reduces from 23.1 to 14 and driving pressure reduces from 22 bar to 18.6 bar, since the pentane content increases from 0.5% to 8% (by vol.) in the methane at knock threshold operating conditions of the mixtures, respectively.

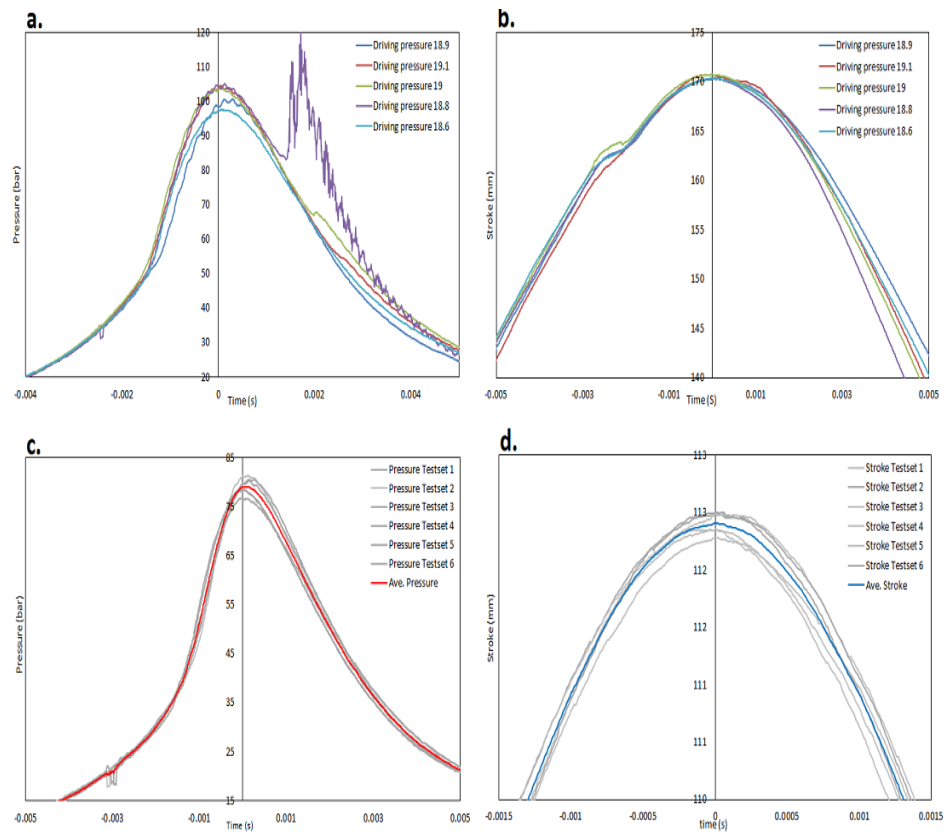


Figure 6-8 Study the mixture containing of 92% methane plus 8% n-pentane;
a. approaching to the knock threshold operating condition by adjusting the driving pressure
b. piston motion closed to TDC with adjusting the driving pressure
c. pressure repeatability investigation at knock threshold condition
d. stroke repeatability investigation at knock threshold condition

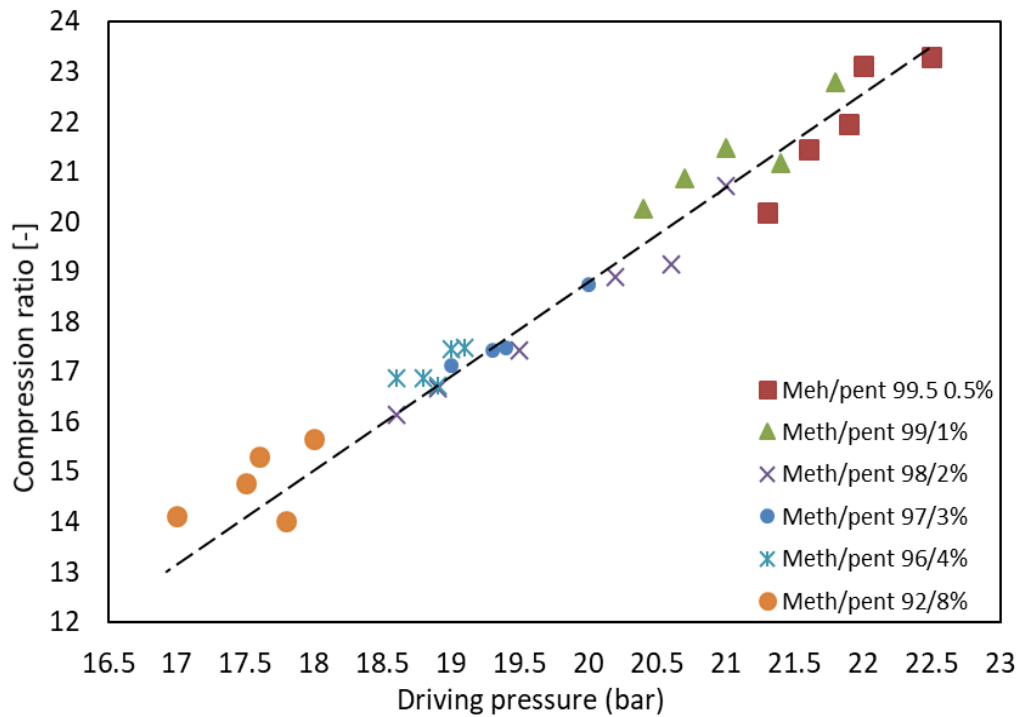


Figure 6-9 Influences of driving pressure on the compression ratio variation for different mixtures of methane-pentane, approaching to the threshold operating conditions

The RCM facility has been used to study the ignition delay behaviour, while it is equipped with a spark plug. The influences of the different proportions of pentane, while the methane content proportionally reduces on the ignition delay of the mixtures have been investigated. It is exhibited that the mixtures with a content of 0.5% pentane plus 99.5% methane and 1% pentane plus 99% methane have a constant ignition delay of around 70-80 ms. However, the temperature of the mixtures reduces by 2.5% from 810 K to 790 K, when the pentane content increases from 0.5% to 1% pentane at knock threshold operating condition. This small variation might be due to several concerns, such as inhomogeneity of the mixture, variation in temperature, initial charged mixture, or compression ratio. It is interesting to see that since the pentane content increases to 2%, 3% and 4%, the ignition delay remains in the range of 80 ms to 110

ms, while the temperature slightly reduces to 780 K, 760 K, 740 K and 730 K, respectively. Ignition delay for 8% pentane blended into 92% methane fluctuates wildly due to the presence of the higher amount of pentane in the mixture. The ignition delay of 92% methane plus 8% pentane is around 180 ms (on average) for the knock threshold operating point.

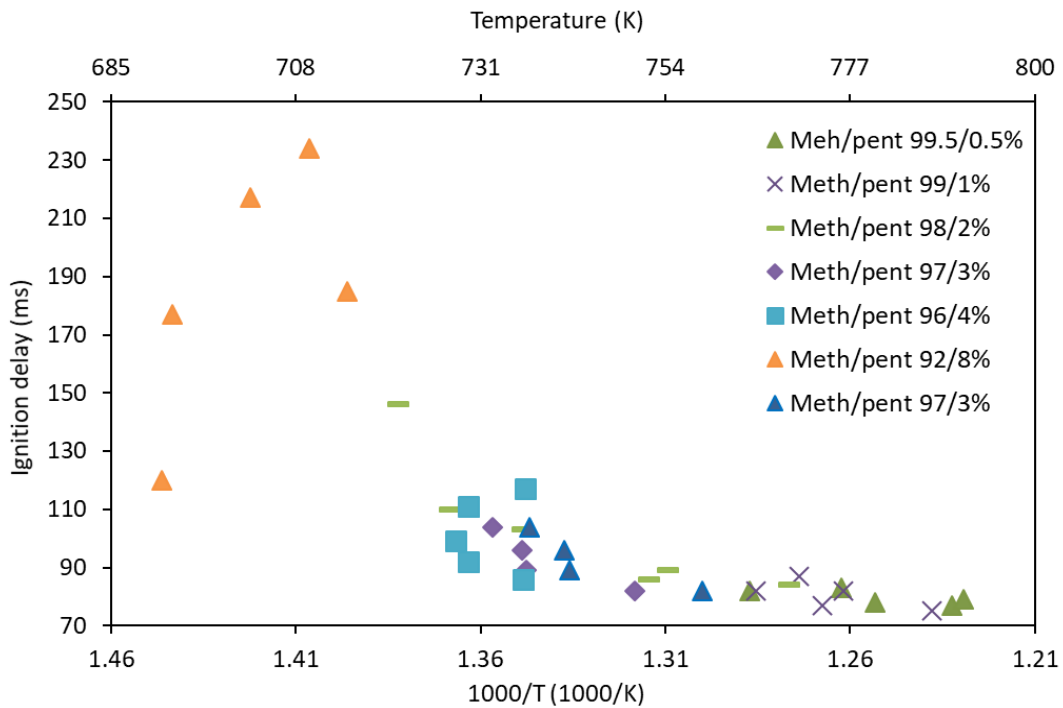


Figure 6-10 Influences of the blending of pentane into methane on ignition delay and temperature for different mixtures of methane and pentane

Figure 6.11 shows the peak pressures and compression ratios of measured data in the RCM for different proportions of pentane blended into methane. It expresses that the resistance of the mixture against knocking is affected since the pentane proportions increase from 0.5% to 8% (in vol.). It shows that only 0.5% pentane blended into 99.5% methane drops the peak pressure and compression ratio by 8% and 6.6%, and they reach 130.7 bar and 23, respectively. Blending 1% pentane and 99% methane leads to 5% and 8% decline in peak pressure and compression ratio, showing 124 bar and 21, and 8% decline in peak pressure and compression ratio, showing 124 bar and 21,

correspondingly. Peak pressure and compression ratio continue to decrease by 6.5% and 7.5%, since the pentane content rises to 2%. Tolerance of the mixtures in terms of peak pressure and compression ratio approaches 116 bar and 19.5. For 3% pentane, peak pressure is 103 bar and the compression ratio is 17.5. It is interesting that the peak pressure and compression ratio suddenly drops around 10%. As the pentane is blended more into the methane, the error also increases, so that as the figure shows for 4% and 8% pentane the points are off the average dashed line. To be more precise, peak pressure drops to 97 and 77 bar, when the pentane increases from 4% to 8%, respectively. In the mixture, a 20% reduction in the tolerance of the mixture based on their peak pressure and compression ratio. Since the pentane content increases from 4% to 8%, then compression ratio also declines from 16 to 14; it also shows a lower reduction of 15% in comparison with peak pressure.

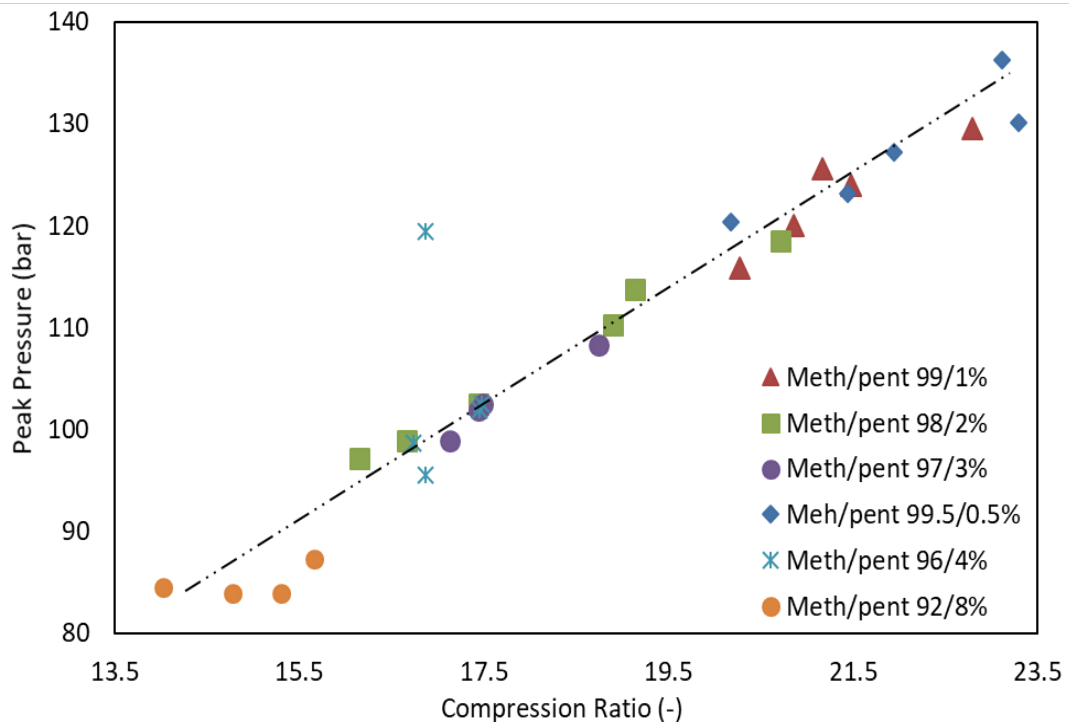


Figure 6-11 influences of the compression ratio on the peak pressure for different mixtures of methane-pentane

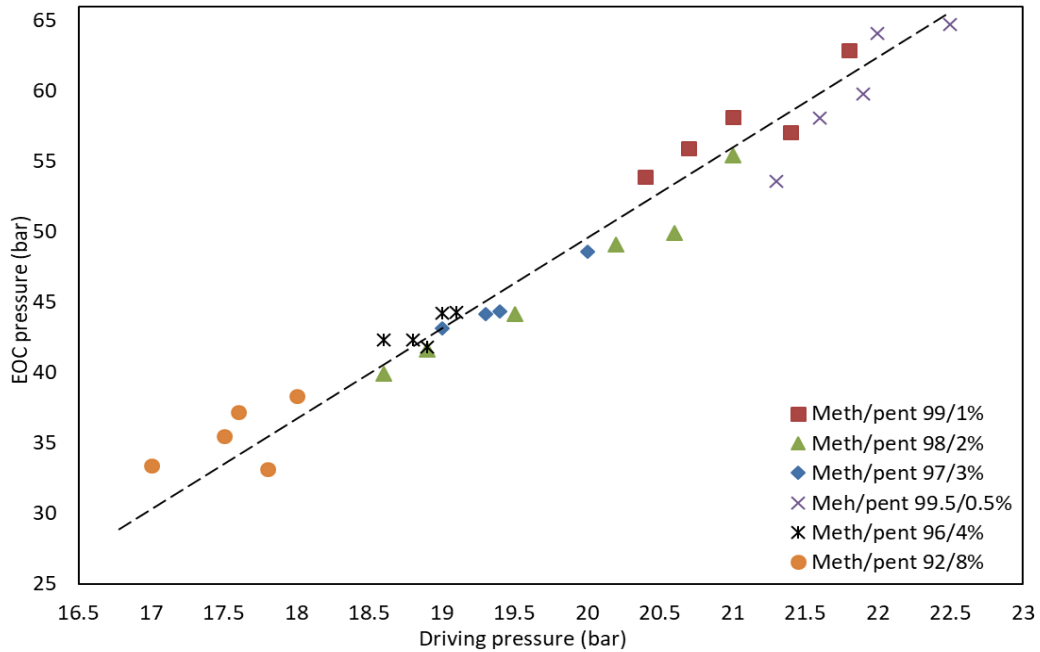


Figure 6-12 influences of driving pressure on the EOC stage for different methane-pentane mixtures, approaching to threshold operating condition

Figures 6.12 and 6.13 show the end of compression data measured in the RCM for both pressure and temperature, at the aforesaid conditions of various pentane and methane mixtures, and the compression ratio soared by increasing the driving pressure in the RCM. Figures 6.12 and 6.13 depict that as the n-pentane content increases the resistance of the compressed mixtures reduces. For instance, at the knock threshold conditions, EOC pressure and temperature reduce continuously by 11%, when the n-pentane content of the mixture increases from 0.5% to 3%, and they drop from 64 bar and 810 K to 44 bar and 740 K, correspondingly. The EOC pressure and temperature decline slightly by 5%, reaching to 42 bar and 730 K, when the pentane amount rises to 4% (and methane content reduces to 96%) in the mixture. There is a sharp decrease

in both EOC pressure and temperature when the amount of pentane in the mixture is doubled. The possible compressed conditions for the mixture with 8% n-pentane and 92% methane decreases to 33 bar in pressure and 690 K in temperature.

Figure 6.14 represents the ignition, combustion and peak pressure data measured in the RCM, separately at the threshold operating conditions of the various proportions of methane and n-pentane mixtures. As the n-pentane presence has established its influence on the mixture resistance against knocking, pressures have been analysed in more detail. The temperature field that develops during an actual RCM experiment is expected to depend strongly on the initial gas temperature and hence, wall boundary temperatures (Neuman 2015).

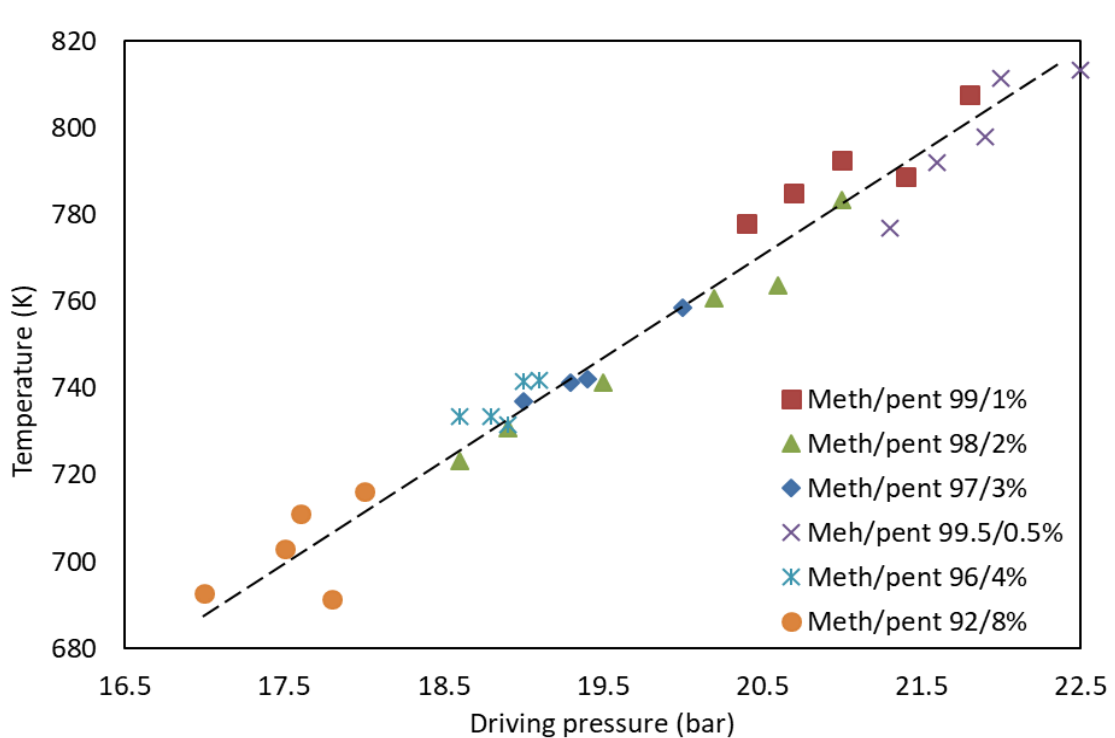


Figure 6-13 influences of driving pressure on the EOC stage for different methane-pentane mixtures, approaching to threshold operating condition

For knock threshold operating condition, an ignition pressure of 0.5% pentane plus 99.5% methane mixture is recorded as 41.5 bar. Since the pentane increases to 1%, the ignition pressure drops by 6%, and reaches 39 bar. It is interesting that the ignition pressure decreases to 35 bar, since the pentane content increases from 1% to 4% in volume and the methane content reduces from 99% to 96%. The ignition pressure of the mixture with 8% n-pentane is around 22 bar, which indicates a 36% reduction.

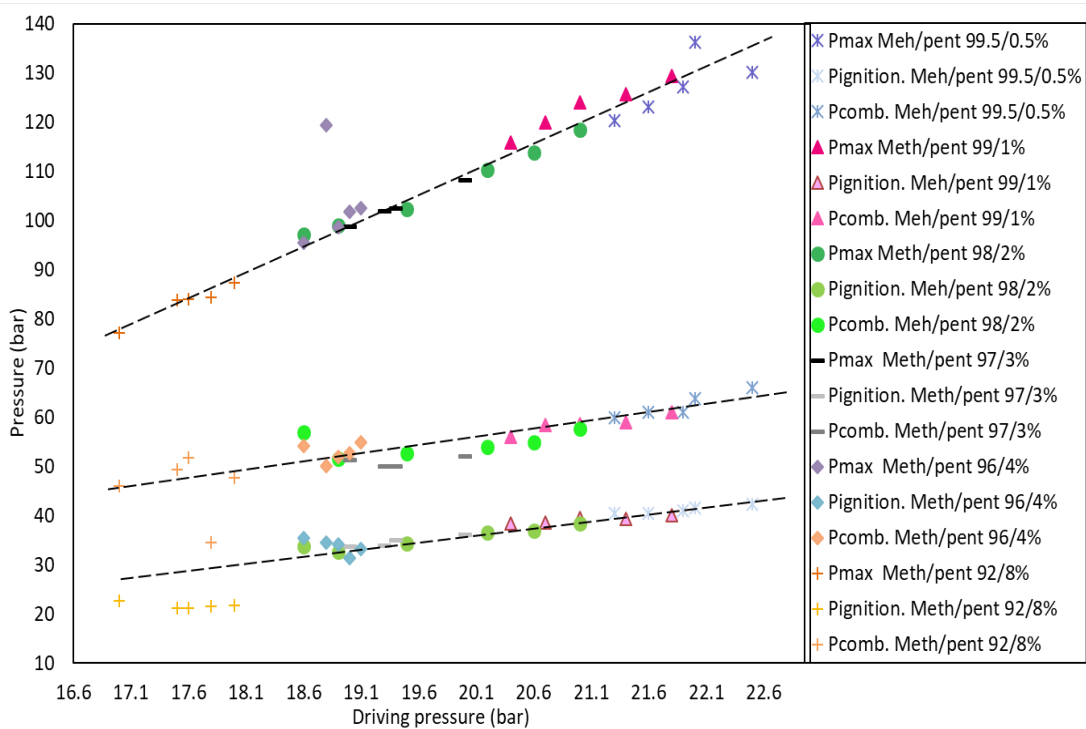


Figure 6-14 pressure analysis of different proportions of pentane blended into methane

The pressure of the condition in which the combustion starts is also of high importance, in order to categorise the pressure rise due to compression among different mixtures of methane and n-pentane. Thus, in Figure 6.14 pressure at the commencing point of combustion has been measured. According to the measured data, pressure reaches 64 bar and it continuously reduces to 59 bar, 55 bar, 50 bar and finally to 46

bar, for the mixtures containing 0.5%, 1%, 2%, 3% 4% and 8% n-pentane. From a theoretical point of view, the measured SOC pressure data have been compared with the EOC pressure which was calculated earlier in Figure 6.12. It expresses that the points are approximately at the same position, however, there are errors of 9% in some cases.

The peak pressure shows the maximum pressure can be achieved by the mixtures, since the combustion occurs at the knock threshold operating condition of the RCM. The resistance of the mixture reduces from 136 bar, 125 bar, 113 bar, 102 bar, 95 bar to 77 bar, since the pentane content increases from 0.5%, 1%, 2%, 3%, 4% and 8% in the methane, respectively.

Generally, by comparing the pressures of the different mixtures of methane and pentane, it is clear that ignition pressure steadily decreases by the rate of 2.3, since the pentane content increases from 0.5% to 8% in the mixture and the SOC pressure for all data measured show almost the same constant increasing trend as the ignition pressure; However, peak pressure data measured in the RCM reduces severely by the slope of almost 9.

6.4.1 Methane-pentane Reference Curve

Figure 6.15 exhibits the peak pressure and compression ratio data measured and determined in the RCM, operating at knock threshold operating condition for different proportions of methane plus pentane mixtures. Figure 6.15 summarises the influences

of blending n-pentane into the pure methane, while the RCM is run on the knock threshold point with respect to the charged mixture. To be more precise, for a mixture of 0.5% n-pentane and 99.5% methane, peak pressure and compression ratio show as 136 bar and 23, correspondingly. According to the results, peak pressure and compression ratio drop to 125 bar and 21, for the mixture containing of 99% methane and 1% pentane. For mixture of 2% pentane and 98% methane, peak pressure declines to around 114 bar and compression ratio stays at 19. When the mixtures contain 3% pentane plus 97% methane and 4% pentane plus 96% methane, peak pressure and compression ratio reduce to 102.5 bar, 95.5 bar, 17.5 bar, 16.8 bar, respectively. Peak pressure drops to 77 bar and compression ratio reduces to 14, with the mixture comprising 8% pentane and 92% methane. As a result, as the pentane has lower resistance to knocking, the mixture with the higher content of pentane has less resistance against abnormal combustion (knocking).

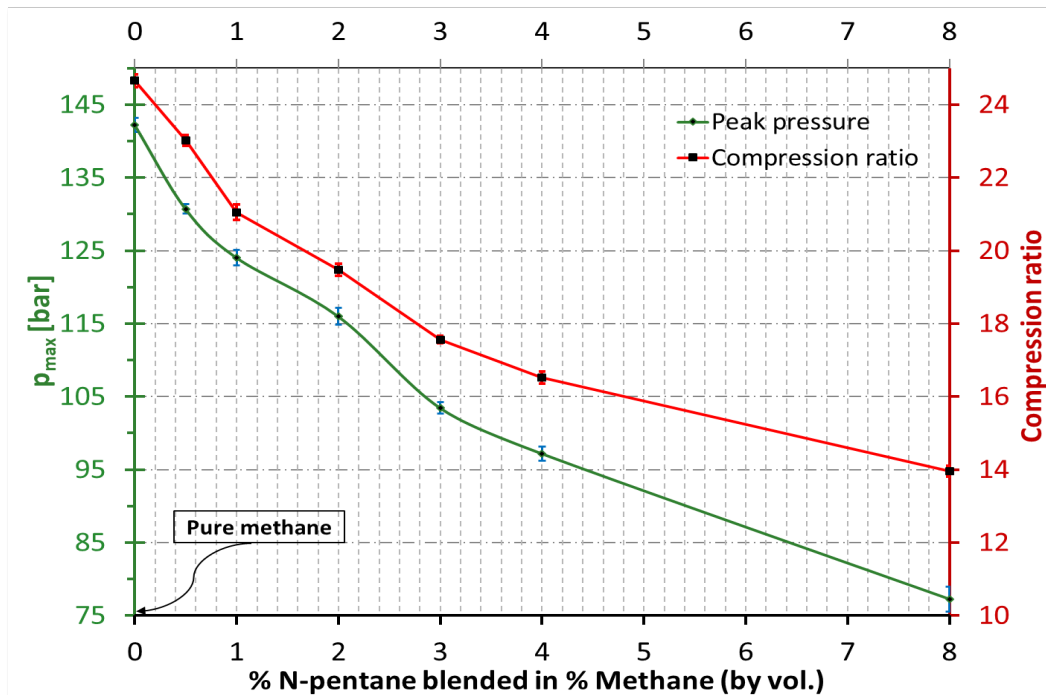


Figure 6-15 Summary of peak pressure and compression ratio of different proportions of methane plus n-pentane mixtures

6.4.2 Methane Number Reference Curves

Figure 6.16 shows the calculated methane number of the various mixtures of methane/pentane based on peak pressure data measured in the RCM. The methane numbers were calculated based on two different methods of Wartsila and the EN19625 standard, as described previously in section 2.3.

The highest MN is set for pure methane, which means it has the highest possible resistance against knocking among the gaseous fuels. Here, the influences of the different proportions of pentane blended into the methane have been investigated.

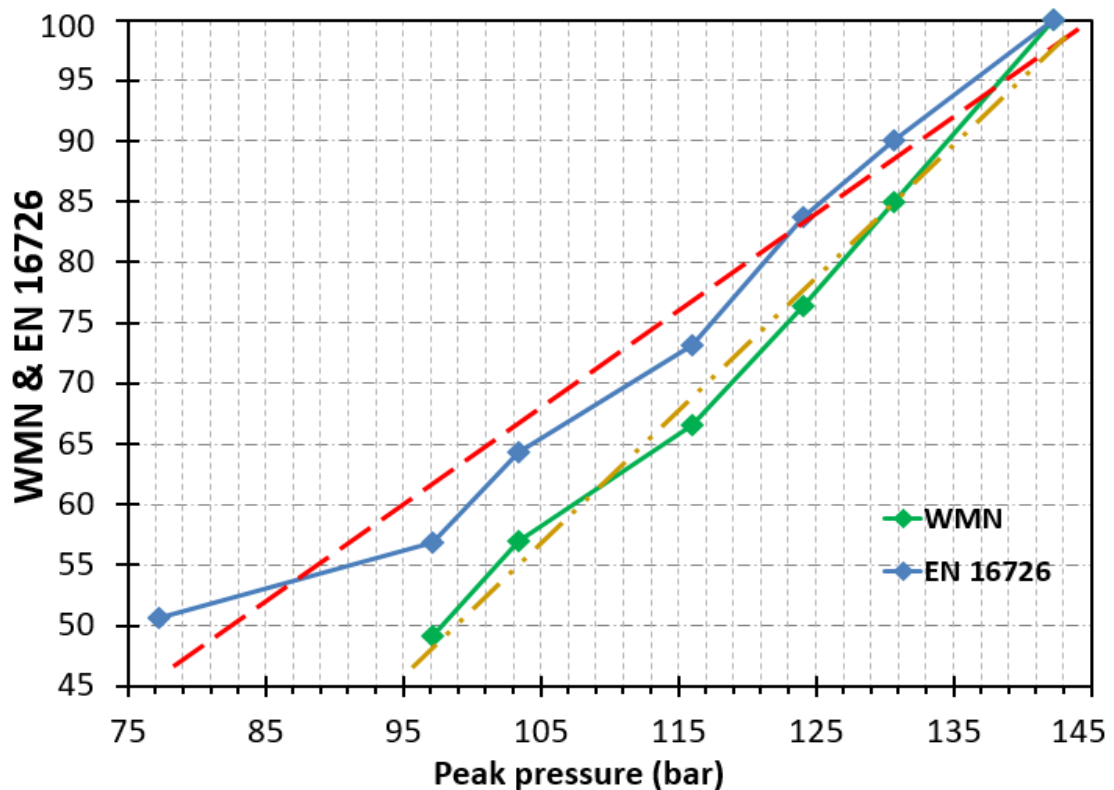


Figure 6-16 WMN and EN16726 methane number with respect to the peak pressure data measured in the RCM

According to both Wartsila and EN standard, in a mixture of 0.5% pentane plus 99.5% methane, the MN reduces to 85 and 90, respectively. The MN reduces to 76.4 based on Wartsila and 83.7 based on the EN Std., when the mixture is changed to 1% pentane plus 99% methane. When 2% n-pentane is blended into the 98% methane, the MN reduces to 66.6 from the Wartsila MN calculation and 73.2 from the EN std. The Wartsila methane number for the new mixture containing 3% n-pentane and 97% methane is 57; while methane number of the same mixture is higher with EN MN calculation and at 64.3. The WMN and EN Std. of 4% n-pentane blended into 96% methane is 49.2 and 56.9, respectively. For the mixture with 8% pentane content and 92% methane, the WMN is not able to calculate MN, but the EN Std MN shows 50.6 for the mixture.

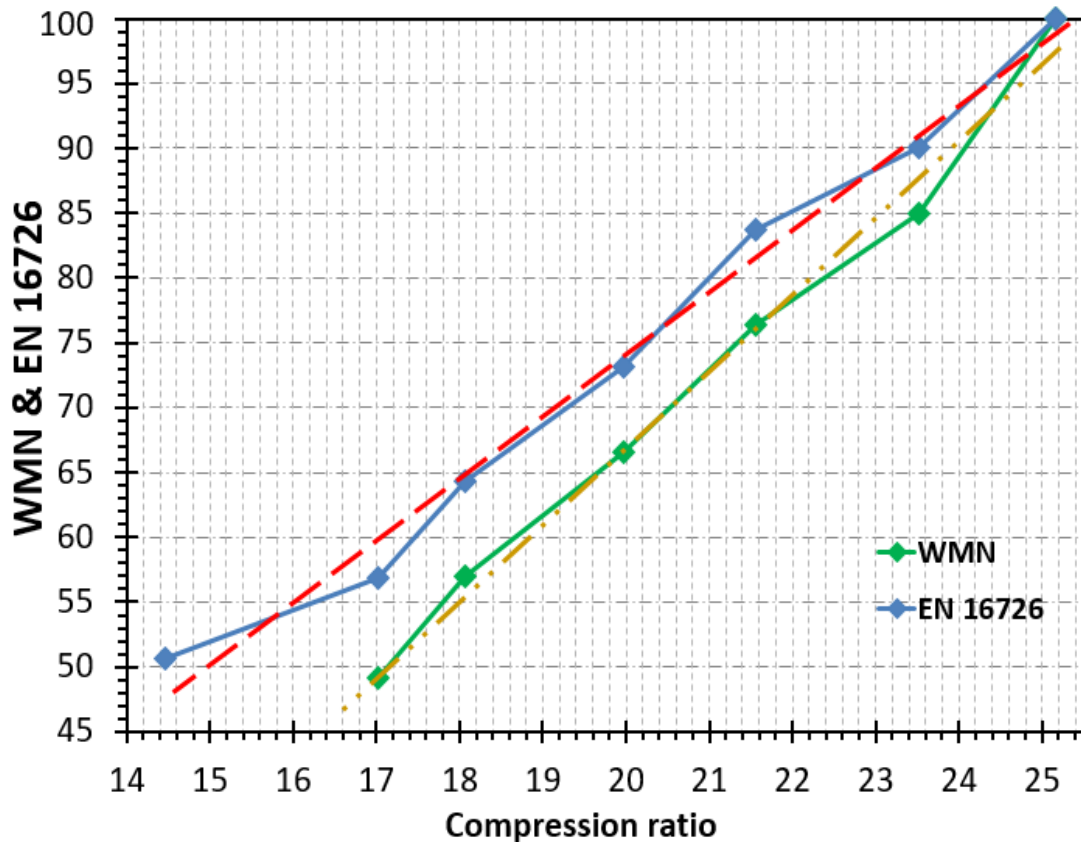


Figure 6-17 WMN and EN16726 methane number with respect to the compression ratio data measured in the RCM

Figure 6.17 shows the calculated WMN and EN std. MN of various proportions of the n-pentane blended into the methane based on the compression ratio data measured in the RCM. The compression ratio has been calculated based on the piston stroke recorded by the piston moving sensors. Figures 6.16 and 6.17 have been compared to investigate the reliability of the RCM sensors. According to the figures, the trends of both MN calculation methods prove the validity of the approaches; however, there are some inaccuracies in the mixtures, where these errors might be due to either the piston displacement sensor or pressure sensor and mixture inhomogeneity.

6.5 Conclusion

Combustion characteristics of different mixtures of n-pentane-methane for use in the future in reciprocating internal combustion engines have been investigated. The various mixtures of n-pentane and methane were used at knock threshold operating conditions. Tests were carried out at low temperature in order to obtain the effects of blending pentane into methane on combustion characteristics.

To run the tests based on the n-pentane-methane mixtures, a new check valve as well as a throttle valve were mounted between the main and auxiliary driving tanks in order to increase the damping effects, and so that the piston moves towards BDC after combustion and no longer hits the RCM piston tube.

It is believed that higher proportions of n-pentane in the methane increases the probability of the mixtures to knock. The EOC temperature of the mixture reduces since

the pentane content increases, so that the EOC temperature drops by 15%, as the mixture varies from 0.5% pentane plus 9.5% methane to 8% n-pentane plus 92% methane. Furthermore, the EOC pressure declines by around 48% from 64 bar to 31 bar. It is valid for the maximum allowable pressure achieved by the RCM for various mixtures of pentane and methane decreases. Since the resistance of the mixture reduces, compression ratio also reduces due to the lower driving pressure required to achieve the threshold operating point.

Although ignition delay of the mixtures with higher pentane proportion is shorter due to the higher activity of the pentane, it jumps twice when the pentane proportion increases from 4% to 8% n-pentane blended into the 92% methane.

CHAPTER 7 – CONCLUSION AND FUTURE WORKS

7.1 Conclusion

The main aim of this thesis was to study the effects of blending different fuels into pure methane in order to investigate the effects of the knock threshold operating conditions of these mixtures, as well as to study the possibility of generating reference curves from the measured data in the RCM to rank the unknown fuels. In particular, various mixtures of methane-ethane, methane-propane, methane-butane and finally methane-pentane have been studied, and the results and discussion for this research are shown in the preceding chapters. The aforementioned fuels were pre-mixed in a mixing reactor and then the mixtures were injected into the RCM cylinder according to each required test. The aim of this chapter is to present the summary and conclusions of this current investigation and to make suggestions for future work.

Three chapters of this study contain numerous results of the experimental data from the RCM, fuelled with various proportions of different fuels, with variable operating conditions. The most significant findings of the investigation are presented below according to the area of study from which they came.

It must be noted that stroke was varied for each test due to the charged driving pressure shooting the piston toward TDC. The initial conditions were held constant for all tests; however, two valves were installed on the driving section of the RCM, these valves help the piston to be decelerated by trapping the air in the driving section. It is necessary to install the valves when the driving charge air is very low to prevent collision of the piston and bottom frame of the RCM. Moreover, position sensors might

have shown inaccurate numbers in knocking combustion tests due to the vibrations occurring during either self-combustion or knocking.

- Investigation of combustion behaviour of blending propane in methane

In Chapter 4, first a systematic investigation was performed, to commence the main tests in stable, distributed temperature conditions. The heating elements were mounted inside the cylinder head as well as on piston wall to have a stabilized temperature in the cylinder. Moreover, mixtures were heated inside the reactor up to 50°C and to a heat exchanger tank was mounted just before the cylinder to increase the temperature of the mixture to 81°C.

As a spark plug was used in the tests, the timing was of high importance. According to the results, spark timing was selected as 10 mm bTDC due to the variation in the stroke occurring for each test. This advance spark timing was chosen due to adjusting the peak pressure at the TDC in order to make up the absence of connecting-rod.

Having considered the temperature and spark timing effects, the RCM was ready to investigate the combustion characteristics of the various methane-propane mixtures. This chapter focused on the effects of adding propane into the pure methane. Pure methane has the highest resistance against knocking so that peak pressure and compression ratio reach 142 bar and 24, respectively. By increasing the proportion of the propane into the methane, the peak pressure and compression ratio dropped;

however, the trend of reduction slowed down since the propane content increased up to 50%. The peak pressure and compression ratio stood at 96 bar and 16.7. Since the portion of the propane content in the mixture increased to more than 50%, the tendency of the mixtures to knock was not affected significantly.

- Investigation of combustion behaviour of blending ethane and butane into methane (separately)

In this chapter, two gaseous fuels were blended into pure methane, one was lighter (hydrocarbon) and the other was heavier than the propane. Mostly the peak pressure and compression ratio of various proportions of methane-ethane and methane-butane were investigated to generalise the effects of the different hydrocarbons on the pure methane operating in real engines.

As the ethane is lighter than butane, it is obvious that resistance of the mixtures containing butane is lower than the mixtures containing ethane with different portions. According to the results, the RCM was able to run the test under pure ethane, the peak pressure and compression ratio dropped to 120 bar and 21.5. Therefore, the RCM was not able to run the methane-butane with a higher proportion of than 10%.

The trend of the peak pressure and compression ratio were shown in the last section of each chapter. The ethane and butane addition into the pure methane and its influences on the combustion in the RCM were studied. It showed that the presence of small

proportions of butane in the pure methane, could affect the mixtures' tendency to knock.

- Investigation of combustion behaviour of blending n-pentane in methane

In Chapter six, the n-pentane was added into the pure methane to investigate the effects of adding heavier fuels in liquid form on the resistance of the mixtures against knocking. The pentane was injected into the mixing reactor and it vaporised in the 50°C temperature of the mixing reactor. Besides, a check valve and a throttle valve were installed in the driving section to prevent damage to the RCM operation, when the combustion occurs and the piston moves towards the BDC. According to the

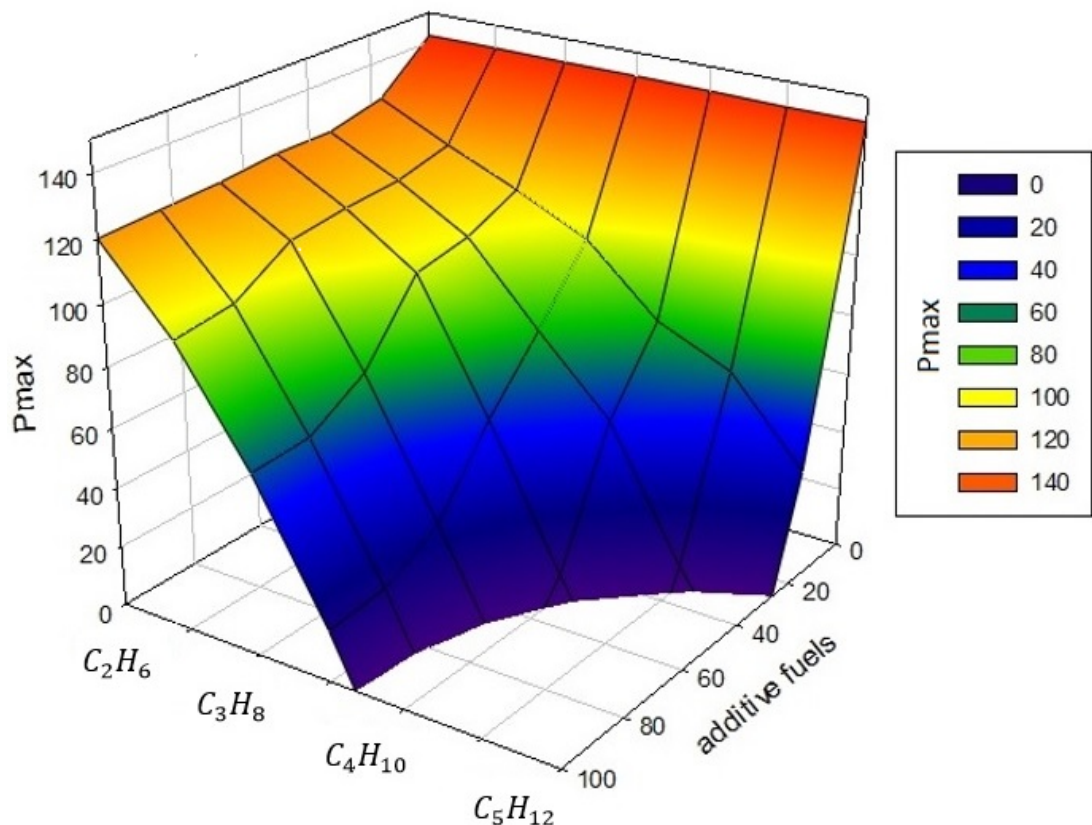


Figure 7-1 Summarised reference curve for all tested mixtures in chapters 4, 5 and 6 with respect to Pmax

results, it is clear that only small proportions of pentane could cause a substantial reduction in the resistance of the mixtures against knocking.

In fig. 7.1 and 7.2, the threshold operating conditions of the all investigated mixtures with different proportions are summarised. Fig. 7.1 and 7.2 show variations of the Pmax and WMN affected by adding different proportions of different gaseous fuels of ethane, propane, butane and pentane into the methane operating at threshold conditions, respectively. As the pure methane has the highest tolerance against knocking and as the methane content reduces by the other fuels in the mixtures, the resistance of the mixtures decreases. It should be noted that, resistance of the mixtures whose have heavier mixtures reduces more drastically.

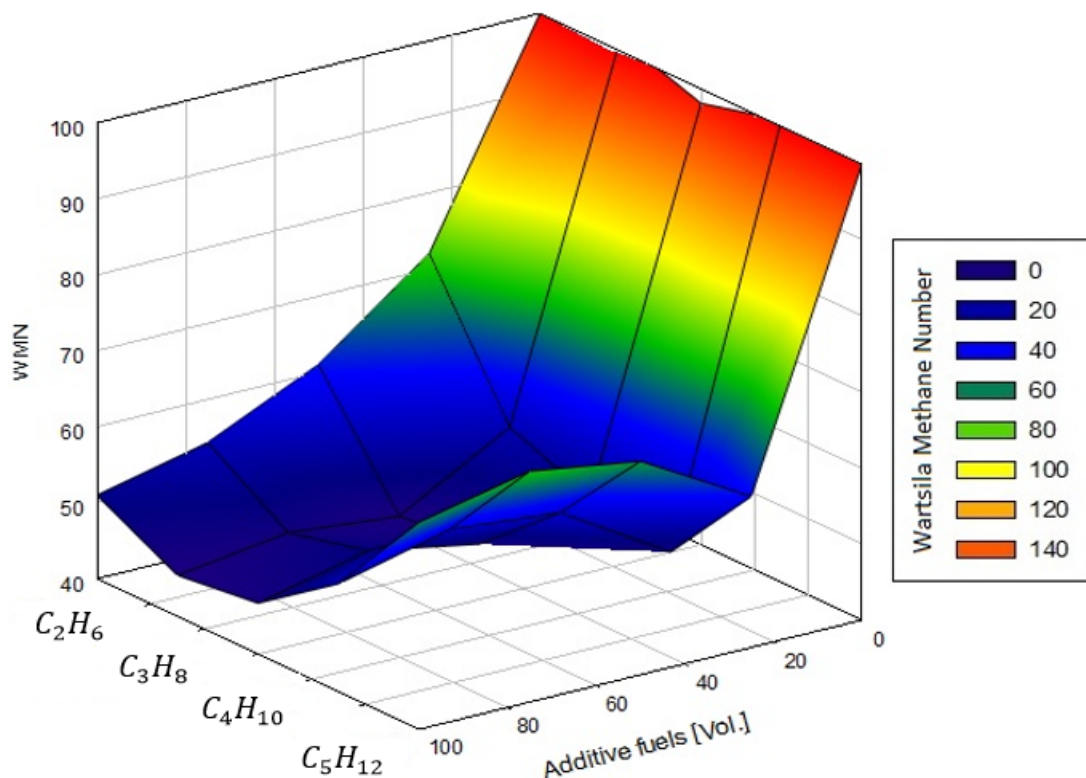


Figure 7-2 Summarised reference curve for all tested mixtures in chapters 4, 5 and 6 with respect to WMN

7.2 Recommendations for Future Works

Research performed during this work focused on the possible engine specification improvements and their effects on currently available RCMs. The author would like to recommend the following works for extension of the research on modelling and experimental investigations:

- More data, including in-cylinder pressure and piston motion with different gases and blends should be obtained. These new gases should be taken from those which are tested in real engines.
- Improving the lean-mixture combustion by installation of an injector in the pre-chamber section, so that the lambda increases to 2, the same as that used in the engines, since the stability of the data improves.
- Systematically study of the influences of the inert gases mixed into the methane and other gaseous hydrocarbons, to adjust the calculated WMN.
- Systematically study the piston speed, which is affected by charged driving pressure.
- Systematically study of the positioning sensor to verify the simulation results with the experimental results

- Systematically study of increasing temperature of the combustion chamber and initial conditions to achieve almost the same initial condition of the real engines.
- Investigation of the knock intensity for the ethane, butane, butane and pentane with different driving pressure and influences of the compression ratio on the combustion instability.

List of Publications

Shokrollahihassanbarough, Farzad, Ali Alqahtani, and Mirosław L. Wyszynski.
"Thermodynamic simulation comparison of opposed two-stroke and conventional four-stroke engines." *Combustion Engines* 54 (2015).

Alqahtani, Ali, Farzad Shokrollahihassanbarough, and Mirosław L. Wyszynski.
"Thermodynamic simulation comparison of AVL BOOST and Ricardo WAVE for HCCI and SI engines optimization." *Combustion Engines* 54 (2015).

Shokrollahi, F., Wyszynski, M. and Sundell, J.P., 2018. STUDY OF THE INFLUENCES OF BLENDING DIFFERENT PROPORTIONS OF PROPANE INTO METHANE ON COMBUSTION CHARACTERISTICS AT THE KNOCK THRESHOLD BY USING RCM. JOURNAL OF KONES POWERTRAIN AND TRANSPORT, 25(1).

References

Affleck, W. and A. Thomas (1968). "An opposed piston rapid compression machine for preflame reaction studies." Proceedings of the Institution of Mechanical Engineers **183**(1): 365-387.

Alexandrino, K., M. U. Alzueta and H. J. Curran (2018). "An experimental and modeling study of the ignition of dimethyl carbonate in shock tubes and rapid compression machine." Combustion and Flame **188**(Supplement C): 212-226.

Ali, S. A. and S. Saraswati (2014). Identification of flame development and rapid burning angle for SI engine. 2014 Students Conference on Engineering and Systems.

Allcott, H. and N. Wozny (2014). "Gasoline prices, fuel economy, and the energy paradox." Review of Economics and Statistics **96**(5): 779-795.

Allen, C. M. (2012). Advanced rapid compression machine test methods and surrogate fuel modeling for bio-derived jet and diesel fuel autoignition, Michigan State University. Mechanical Engineering.

Alqahtani, A., F. Shokrollahihassanbarough and M. L. Wyszynski (2015). "Thermodynamic simulation comparison of AVL BOOST and Ricardo WAVE for HCCI and SI engines optimization." Combustion Engines **54**.

Beeley, P., J. Griffiths and P. Gray (1980). "Rapid compression studies on spontaneous ignition of isopropyl nitrate art I: Nonexplosive decomposition, explosive oxidation and conditions for safe handling." Combustion and flame **39**(3): 255-268.

Beerer, D., V. McDonell, S. Samuelsen and L. Angello (2009). Interpretation of Flow Reactor Based Ignition Delay Measurements. ASME Turbo Expo 2009: Power for Land, Sea, and Air, American Society of Mechanical Engineers.

Bonatesta, F., B. Waters and P. Shayler (2010). "Burn angles and form factors for Wiebe function fits to mass fraction burned curves of a spark ignition engine with variable valve timing." International Journal of Engine Research **11**(2): 177-186.

Bradley, D., M. Lawes and M. Materego (2015). Interpretation of auto-ignition delay times measured in different rapid compression machines. 25th International Colloquium on the Dynamics of Explosions and Reactive systems, Leeds.

Campbell, M. F., S. Wang, C. S. Goldenstein, R. M. Spearrin, A. M. Tulgestke, L. T. Zaczek, D. F. Davidson and R. K. Hanson (2015). "Constrained reaction volume shock tube study of n-heptane oxidation: Ignition delay times and time-histories of multiple species and temperature." Proceedings of the Combustion Institute **35**(1): 231-239.

Chaos, M. and F. L. Dryer (2010). "Chemical-kinetic modeling of ignition delay: Considerations in interpreting shock tube data." International Journal of Chemical Kinetics **42**(3): 143-150.

Cho, G., D. Jeong, G. Moon and C. Bae (2010). "Controlled auto-ignition characteristics of methane–air mixture in a rapid intake compression and expansion machine." Energy **35**(10): 4184-4191.

Conti, J., P. Holtberg, J. Diefenderfer, A. LaRose, J. T. Turnure and L. Westfall (2016). International Energy Outlook 2016 With Projections to 2040, USDOE Energy Information Administration (EIA), Washington, DC (United States). Office of Energy Analysis.

Cox, A., J. Griffiths, C. Mohamed, H. Curran, W. Pitz and C. Westbrook (1996). Extents of alkane combustion during rapid compression leading to single-and two-stage ignition. Symposium (International) on Combustion, Elsevier.

Darcy, D., H. Nakamura, C. J. Tobin, M. Mehl, W. K. Metcalfe, W. J. Pitz, C. K. Westbrook and H. J. Curran (2014). "A high-pressure rapid compression machine study of n-propylbenzene ignition." Combustion and Flame **161**(1): 65-74.

Das, A. K., C.-J. Sung, Y. Zhang and G. Mittal (2012). "Ignition delay study of moist hydrogen/oxidizer mixtures using a rapid compression machine." International journal of hydrogen energy **37**(8): 6901-6911.

Davidson, D., D. Haylett and R. Hanson (2008). "Development of an aerosol shock tube for kinetic studies of low-vapor-pressure fuels." Combustion and Flame **155**(1-2): 108-117.

Desantes, J. M., J. J. Lopez, J. M. Garcia-Oliver and D. Lopez-Pintor (2017). A 5-Zone Model to Improve the Diagnosis Capabilities of a Rapid Compression-Expansion Machine (RCEM) in Autoignition Studies. SAE Technical Paper Series, 2017-01-0730, SAE International.

Desgroux, P., L. Gasnot and L. Sochet (1995). "Instantaneous temperature measurement in a rapid-compression machine using laser Rayleigh scattering." Applied Physics B: Lasers and Optics **61**(1): 69-72.

Di, H., X. He, P. Zhang, Z. Wang, M. S. Wooldridge, C. K. Law, C. Wang, S. Shuai and J. Wang (2014). "Effects of buffer gas composition on low temperature ignition of iso-octane and n-heptane." Combustion and Flame **161**(10): 2531-2538.

Dohring, K. (1986). The relative effects of intake and compression generated turbulence on IC engine combustion duration, University of British Columbia.

Donovan, M., X. He, B. Zigler, T. Palmer, M. Wooldridge and A. Atreya (2004). "Demonstration of a free-piston rapid compression facility for the study of high temperature combustion phenomena." Combustion and flame **137**(3): 351-365.

EIA, U. (2013). "Annual energy outlook 2013." US Energy Information Administration, Washington, DC: 60-62.

Falk, K. (1906). Journal of the American Chemical Society **28**(11): 1517-1534.

Falk, K. G. (1907). "THE IGNITION TEMPERATURES OF GASEOUS MIXTURES." Journal of the American Chemical Society **29**(11): 1536-1557.

Ferguson, C. R. and A. T. Kirkpatrick (2015). Internal combustion engines: applied thermosciences, John Wiley & Sons.

Fomin, N. (2010). "110 years of experiments on shock tubes." Journal of Engineering Physics and Thermophysics **83**(6): 1118-1135.

Galindo, J., H. Climent, B. Plá and V. D. Jiménez (2011). "Correlations for Wiebe function parameters for combustion simulation in two-stroke small engines." Applied Thermal Engineering **31**(6): 1190-1199.

Gersen, S., A. Mokhov, J. Darneveil and H. Levinsky (2010). "Ignition properties of n-butane and iso-butane in a rapid compression machine." Combustion and Flame **157**(2): 240-245.

Gersen, S., A. Mokhov, J. Darneveil, H. Levinsky and P. Glarborg (2011). "Ignition-promoting effect of NO₂ on methane, ethane and methane/ethane mixtures in a rapid compression machine." Proceedings of the Combustion Institute **33**(1): 433-440.

Goldsborough, S. S., C. Banyon and G. Mittal (2012). "A computationally efficient, physics-based model for simulating heat loss during compression and the delay period in RCM experiments." Combustion and Flame **159**(12): 3476-3492.

Goldsborough, S. S., S. Hochgreb, G. Vanhove, M. S. Wooldridge, H. J. Curran and C.-J. Sung (2017). "Advances in rapid compression machine studies of low-and intermediate-temperature autoignition phenomena." Progress in Energy and Combustion Science **63**: 1-78.

Griffiths, J., P. Halford-Maw and C. Mohamed (1997). "Spontaneous ignition delays as a diagnostic of the propensity of alkanes to cause engine knock." Combustion and flame **111**(4): 327-337.

Griffiths, J., P. Halford-Maw and D. Rose (1993). "Fundamental features of hydrocarbon autoignition in a rapid compression machine." Combustion and flame **95**(3): 291-306.

Griffiths, J. F., J. P. MacNamara, C. Mohamed, B. J. Whitaker, J. Pan and C. G. Sheppard (2002). "Temperature fields during the development of autoignition in a rapid compression machine." Faraday discussions **119**: 287-303.

Grogan, K. P., S. S. Goldsborough and M. Ihme (2015). "Ignition regimes in rapid compression machines." Combustion and Flame **162**(8): 3071-3080.

Han, D., S. Deng, W. Liang, P. Zhao, F. Wu, Z. Huang and C. K. Law (2017). "Laminar flame propagation and nonpremixed stagnation ignition of toluene and xylenes." Proceedings of the Combustion Institute **36**(1): 479-489.

Healy, D., H. J. Curran, S. Dooley, J. M. Simmie, D. M. Kalitan, E. L. Petersen and G. Bourque (2008). "Methane/propane mixture oxidation at high pressures and at high, intermediate and low temperatures." Combustion and Flame **155**(3): 451-461.

Heywood, J. B. (1988). Internal combustion engine fundamentals, McGraw-hill New York.

Huang, J., P. Hill, W. Bushe and S. Munshi (2004). "Shock-tube study of methane ignition under engine-relevant conditions: experiments and modeling." Combustion and flame **136**(1-2): 25-42.

Ihara, T., T. Tanaka and K. Wakai (2009). "Effects of octane number on autoignition and knocking phenomena in a stratified mixture." Combustion, Explosion, and Shock Waves **45**(4): 428.

Kitsopanidis, I. and W. Cheng (2006). "Soot formation study in a rapid compression machine." Journal of engineering for gas turbines and power **128**(4): 942-949.

Kobori, S. and T. Kamimoto (1995). Development of a rapid compression-expansion machine simulating diesel combustion, SAE Technical Paper.

Lapuerta, M., O. Armas and J. Hernández (1999). "Diagnosis of DI Diesel combustion from in-cylinder pressure signal by estimation of mean thermodynamic properties of the gas." Applied Thermal Engineering **19**(5): 513-529.

Lee, C., S. Vranckx, K. A. Heufer, S. V. Khomik, Y. Uygun, H. Olivier and R. X. Fernandez (2012). "On the chemical kinetics of ethanol oxidation: shock tube, rapid compression machine and detailed modeling study." Zeitschrift für Physikalische Chemie **226**(1): 1-28.

Lee, C., S. Vranckx, A. Heufer Karl, V. Khomik Sergey, Y. Uygun, H. Olivier and X. Fernandez Ravi (2012). On the Chemical Kinetics of Ethanol Oxidation: Shock Tube, Rapid Compression Machine and Detailed Modeling Study. Zeitschrift für Physikalische Chemie. **226**: 1.

Lee, D. and S. Hochgreb (1998). "Rapid Compression Machines: Heat Transfer and Suppression of Corner Vortex." Combustion and Flame **114**(3): 531-545.

Leiker, M., C. K. C. W, U. Pfeifer and M. Rankl (1972). Evaluation of antiknocking property of gaseous fuels by means of methane number and its practical application to gas engines. MECHANICAL ENGINEERING, ASME-AMER SOC MECHANICAL ENG 345 E 47TH ST, NEW YORK, NY 10017.

Libert, B., J. Spector and D. Tapscott (2007). We are smarter than me: how to unleash the power of crowds in your business, Pearson Prentice Hall.

Lindström, F., H.-E. Ångström, G. Kalghatgi and C. E. Möller (2005). An empirical SI combustion model using laminar burning velocity correlations, SAE Technical Paper.

Liu, C., H. Song, P. Zhang, Z. Wang, M. S. Wooldridge, X. He and G. Suo (2018). "A rapid compression machine study of autoignition, spark-ignition and flame propagation characteristics of H₂/CH₄/CO/air mixtures." Combustion and Flame **188**(Supplement C): 150-161.

Liu, H., H. Zhang, Z. Shi, H. Lu, G. Zhao and B. Yao (2014). "Performance characterization and auto-ignition performance of a rapid compression machine." Energies **7**(9): 6083-6104.

Lutz, A. E., R. J. Kee, J. A. Miller, H. A. Dwyer and A. K. Oppenheim (1989). "Dynamic effects of autoignition centers for hydrogen and C_{1,2}-hydrocarbon fuels." Symposium (International) on Combustion **22**(1): 1683-1693.

Malenshek, M. and D. B. Olsen (2009). "Methane number testing of alternative gaseous fuels." Fuel **88**(4): 650-656.

Mansfield, A., M. Wooldridge, H. Di and X. He (2015). "Low-temperature ignition behavior of iso-octane." Fuel **139**: 79-86.

Materego, M. C. (2015). Auto-ignition characterisation of synthetic fuels via Rapid Compression Machine, University of Leeds.

Mehl, M., H. Curran, W. Pitz and C. Westbrook (2009). Chemical kinetic modeling of component mixtures relevant to gasoline, Lawrence Livermore National Laboratory (LLNL), Livermore, CA.

Minetti, R., M. Carlier, M. Ribaucour, E. Therssen and L. Sochet (1996). Comparison of oxidation and autoignition of the two primary reference fuels by rapid compression. symposium (international) on combustion, Elsevier.

Mitakos, D. A. (2014). Experimental investigations for phenomenological modelling of two-stage auto-ignition under HCCI conditions, ETH Zurich.

Mittal, G. (2006). A rapid compression machine–design, characterization, and autoignition investigations, Case Western Reserve University.

Mittal, G., M. Chaos, C.-J. Sung and F. L. Dryer (2008). "Dimethyl ether autoignition in a rapid compression machine: Experiments and chemical kinetic modeling." Fuel Processing Technology **89**(12): 1244-1254.

Mittal, G. and M. Chomier (2014). "Interpretation of experimental data from rapid compression machines without creviced pistons." Combustion and Flame **161**(1): 75-83.

Mittal, G., M. P. Raju and C.-J. Sung (2008). "Computational fluid dynamics modeling of hydrogen ignition in a rapid compression machine." Combustion and Flame **155**(3): 417-428.

Mittal, G., M. P. Raju and C.-J. Sung (2010). "CFD modeling of two-stage ignition in a rapid compression machine: Assessment of zero-dimensional approach." Combustion and flame **157**(7): 1316-1324.

Mittal, G. and C.-J. Sung (2006). "Aerodynamics inside a rapid compression machine." Combustion and Flame **145**(1): 160-180.

Mittal, G. and C.-J. Sung (2007). "Autoignition of toluene and benzene at elevated pressures in a rapid compression machine." Combustion and Flame **150**(4): 355-368.

Mittal, G. and C. J. Sung (2007). "A rapid compression machine for chemical kinetics studies at elevated pressures and temperatures." Combustion Science and Technology **179**(3): 497-530.

Mohamed, C. (1998). "Suppression of reaction during rapid compression and its effect on ignition delay." Combustion and flame **112**(3): 438-444.

Moxey, B. (2014). A study of flame development with isooctane alcohol blended fuels in a optical spark ignition engine.

Muradov, N. Z. and T. N. Veziroğlu (2008). "'Green" path from fossil-based to hydrogen economy: An overview of carbon-neutral technologies." International Journal of Hydrogen Energy **33**(23): 6804-6839.

Nakamura, H., D. Darcy, M. Mehl, C. J. Tobin, W. K. Metcalfe, W. J. Pitz, C. K. Westbrook and H. J. Curran (2014). "An experimental and modeling study of shock tube and rapid compression machine ignition of n-butylbenzene/air mixtures." Combustion and Flame **161**(1): 49-64.

Nam, V. D., M. T. Lim and O. Lim (2017). "Study on Auto-Ignition Characteristics of Gasoline-Biodiesel Blend Fuel in a Rapid Compression Expansion Machine." Energy Procedia **105**(Supplement C): 1789-1795.

Neuman, J. (2015). Development of a rapid compression controlled-expansion machine for chemical ignition studies, Marquette University.

Park, J., K. Huh and K. Park (2000). "Experimental study on the combustion characteristics of emulsified diesel in a rapid compression and expansion machine." Proceedings of the Institution of Mechanical Engineers, Part D: Journal of Automobile Engineering **214**(5): 579-586.

Payman, W. and W. C. F. Shepherd (1946). "Explosion waves and shock waves VI. The disturbance produced by bursting diaphragms with compressed air." Proc. R. Soc. Lond. A **186**(1006): 293-321.

Payri, F., S. Molina, J. Martín and O. Armas (2006). "Influence of measurement errors and estimated parameters on combustion diagnosis." Applied Thermal Engineering **26**(2-3): 226-236.

Pepiot-Desjardins, P. and H. Pitsch (2008). "An efficient error-propagation-based reduction method for large chemical kinetic mechanisms." Combustion and Flame **154**(1-2): 67-81.

Petersen, E. L., D. M. Kalitan, A. B. Barrett, S. C. Reehal, J. D. Mertens, D. J. Beerer, R. L. Hack and V. G. McDonell (2007). "New syngas/air ignition data at lower

temperature and elevated pressure and comparison to current kinetics models." Combustion and Flame **149**(1): 244-247.

Pfahl, U., K. Fieweger and G. Adomeit (1996). Self-ignition of diesel-relevant hydrocarbon-air mixtures under engine conditions. Symposium (International) on Combustion, Elsevier.

Quinn, M. K. and K. Kontis (2013). "Pressure-sensitive paint measurements of transient shock phenomena." Sensors **13**(4): 4404-4427.

Ramalingam, A., K. Zhang, A. Dhongde, L. Virnich, H. Sankhla, H. Curran and A. Heufer (2017). "An RCM experimental and modeling study on CH₄ and CH₄/C₂H₆ oxidation at pressures up to 160bar." Fuel **206**(Supplement C): 325-333.

Ribaucour, M., R. Minetti, M. Carlier and L. Sochet (1992). "Autoinflammation à haute pression. Conception, réalisation et test d'une machine à compression rapide." Journal de chimie physique **89**: 2127-2152.

Ryan, T., T. Callahan and S. R. King (1993). "Engine Knock Rating of Natural Gases—Methane Number." Journal of engineering for gas turbines and Power **115**(4): 769-776.

Saharin, S. B. (2013). Vaporization and autoignition characteristics of ethanol and 1-propanol droplets: influence of water, Université de Bourgogne.

Schaub, F. and R. Hubbard (1985). "A procedure for calculating fuel gas blend knock rating for large-bore gas engines and predicting engine operation." Journal of engineering for gas turbines and power **107**(4): 922-930.

Shiga, S., S. Ozone, H. Machacon, T. Karasawa, H. Nakamura, T. Ueda, N. Jingu, Z. Huang, M. Tsue and M. Kono (2002). "A study of the combustion and emission characteristics of compressed-natural-gas direct-injection stratified combustion using a rapid-compression-machine." Combustion and Flame **129**(1): 1-10.

Sieminski, A. (2014). "International energy outlook." Energy information administration (EIA) **18**.

Spadaccini, L. and M. Colket Iii (1994). "Ignition delay characteristics of methane fuels." Progress in energy and combustion science **20**(5): 431-460.

Stone, R. (2012). Introduction to internal combustion engines, Palgrave Macmillan.

Sung, C.-J. and H. J. Curran (2014). "Using rapid compression machines for chemical kinetics studies." Progress in Energy and Combustion Science **44**: 1-18.

Szwaja, S. (2011). "Simplified calculation of combustion progress in the IC engine." Teka Komisji Motoryzacji i Energetyki Rolnictwa **11**.

Tanaka, S., F. Ayala and J. C. Keck (2003). "A reduced chemical kinetic model for HCCI combustion of primary reference fuels in a rapid compression machine." Combustion and flame **133**(4): 467-481.

Tanoue, K., T. Jimoto, T. Kimura, M. Yamamoto and J. Hashimoto (2017). "Effect of initial temperature and fuel properties on knock characteristics in a rapid compression and expansion machine." Proceedings of the Combustion Institute **36**(3): 3523-3531.

Tanoue, K., T. Kimura, T. Jimoto, J. Hashimoto and Y. Moriyoshi (2017). "Study of prechamber combustion characteristics in a rapid compression and expansion machine." Applied Thermal Engineering **115**: 64-71.

Version, A. B. (2010). "User guide." Edition **7**: 2010.

Vieille, P. (1899). "Sur les discontinuités produites par la détente brusque de gaz comprimés." Comptes Rendus **129**(1228): 68.

Westbrook, C., H. Curran, W. Pitz, J. Griffiths, C. Mohamed and S. Wo (1998). The effects of pressure, temperature, and concentration on the reactivity of alkanes: Experiments and modeling in a rapid compression machine. Symposium (international) on combustion, Elsevier.

Wiebe, I. (1956). "Halbempirische formel für die Verbrennungs-Geschwindigkeit." Academy of Sciences of the USSR, Moscow 1956.

Würmel, J. and J. Simmie (2005). "CFD studies of a twin-piston rapid compression machine." Combustion and flame **141**(4): 417-430.

Yeliana, C. Cooney, J. Worm and J. Naber (2008). "The Calculation of Mass Fraction Burn of Ethanol-Gasoline Blended Fuels Using Single and Two-Zone Models", SAE International.

Hudson, C., Gao, X. and Stone, R., 2001. "Knock measurement for fuel evaluation in spark ignition engines". *Fuel*, 80(3), pp.395-407.

Naber J.D., Blough J.R., Frankowski D., Goble M., Szpytman J.E.: Analysis of combustion knock metrics in spark-ignition engines, SAE Transactions Journal of Engines, V115, 2007, 223-243.

Szwaja S., Hydrogen Combustion Knock Analysis, 10th International Conference on Heat Engines and Environmental Protection. Proceedings. Balatonfüred, Hungary. 2011, pp. 197-202.

APPENDIX A

% This manuscript filters the pressure trace of the different methane-propane portions to obtain the high-pass pressure pulsations. Then, spectrum and power spectrum can be calculated from the pulsations.

```
%*****
```

```
clear all;
```

```
A=load('m90.dat'); % the pressure trace file is inputted here.
```

```
time=A(:,1);
```

```
p0=A(:,2);% sampling frequency = 100 kHz, T=10 us
```

```
%*****
```

```
Filtering
```

```
CutF = 3500/50000; %band
```

```
[x2,x1] = butter(4,CutF,'high'); %filter design
```

```
pf1=filtfilt(x2,x1,p0); %pressure pulsations
```

```
%lower and higher limits for time and pressure pulsations
```

```
a0=find(time>0);
```

```
a1=a0(1);
```

```
a2=a1+1023;
```

```
pf1=pf1(a1:a2);
```

```
time=time(a1:a2);
```

```

%*****

%CALCULATING SPECTRUM
y=pf1;

Y = fft(y,1024); % vector with fft - complex values

yy = Y.* conj(Y)/1024;

f = 100000*(0:512)/1024;% 100 kHz sampling frequency

[m,i]=max(abs(Y));

f_max=f(i)/1000;% frequency for max. peak in spectrum in kHz

%*****

%PLOTS
figure

plot(time,p0(a1:a2));

xlabel('time (seconds)')

ylabel('combustion pressure (MPa)')

figure

plot(time,pf1);

xlabel('time (seconds)')

ylabel('pressure pulsations (MPa)')

p_max=max(abs(pf1)); %maximal amplitude of the pulsation pressure from the test
in MPa

figure

```

```
plot(f,abs(Y(1:513)))  
  
title('Frequency content of y')  
  
xlabel('frequency (Hz)')  
  
ylabel('Amplitude')  
  
clear a0 a1 a2
```