Numerical investigation on the in-cylinder flow with SI and CAI valve timings

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Numerical investigation on the in-cylinder flow with SI and CAI valve timings

by

Julien Aymeric Beauquel

Doctoral thesis submitted in partial fulfilment of the requirements for the award of Doctor of Philosophy (Ph.D.) of Loughborough University

June 2016

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I would like to dedicate this thesis to my family and friends who supported me during the entire project.
Abstract

The principle of controlled auto-ignition (CAI) is to mix fuel and air homogeneously before compressing the mixture to the point of auto-ignition. As ignition occurs simultaneously, CAI engines operate with lean mixtures preventing high cylinder pressures. CAI engines produce small amounts of nitrogen oxides (NOx) due to low combustion temperatures while maintaining high compression ratios and engine efficiencies. Due to simultaneous combustion and lean mixtures, CAI engines are restricted between low and mid load operations. Various strategies have been studied to improve the load limit of CAI engines. The scope of the project is to investigate the consequences of varying valve timing, as a method to control the mixture temperature within the combustion chamber and therefore, controlling the mixture auto-ignition point. This study presents computational fluid dynamics (CFD) modelling results of transient flow, inside a 0.45 litre Lotus single cylinder engine. After a validation process, a chemical kinetics model is combined with the CFD code, in order to study in-cylinder temperatures, the mixture distribution during compression and to predict the auto-ignition timing. The first part of the study focuses on validating the calculated in-cylinder velocities. A mesh sensitivity study is performed as well as a comparison of different turbulence models. A method to reduce computational time of the calculations is presented. The effects of engine speed on charge delay and charge amount inside the cylinder, the development of the in-cylinder flow field and the variation of turbulence parameters during the intake and compression stroke, are studied. The second part of the study focuses on the gasoline mixture and the variation of the valve timing, to retain different ratios of residual gases within the cylinder. After validation of the model, a final set of CFD calculations is performed, to investigate the effects of valve timing on flow and the engine parameters. The results are then compared to a fully homogeneous mixture model to study the benefits of varying valve duration. New key findings and contributions to CAI knowledge were found in this investigation. Reducing the intake and exhaust valve durations created a mixture temperature stratification and a fuel concentration distribution, prior to auto-ignition. It resulted in extending the heat release rate duration, improving combustion. However, shorter valve timing durations also showed an increase in heat transfer, pumping work and friction power, with a decrease of cylinder indicated efficiency. Valve timing, as a method to control auto-ignition, should only be used when the load limit of CAI engines, is to be improved.
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Nomenclature, symbols and abbreviations

1D one-dimensional
2D two-dimensional
3D three-dimensional
A crankshaft radius
abs absolute
AFR air-fuel ratio
A_{in} wetted area of the entrance of the inlet port
ANN artificial neural network
Ar symbol for argon
ATDC after top dead centre
ATDCF after top dead centre firing
atm atmospheric
BDC bottom dead centre
BG Bai and Gosman spray/wall interaction model
BMEP brake mean effective pressure
BSFC brake specific fuel consumption
BTDC before top dead centre
BTDCF before top dead centre firing
C_{2}H_{4} molecular formula for ethylene
C_{2}H_{5}OH molecular formula for ethanol
C_{3}H_{6} molecular formula for cyclopropane
C_{4}H_{10} molecular formula for butane
C_{6}H_{6} molecular formula for benzene
C_{7}H_{14} molecular formula for heptene or cycloheptane
C_{7}H_{16} molecular formula for heptane
C_{7}H_{8} molecular formula for toluene
C_{8}H_{16} molecular formula for octene or cyclooctane
C_{8}H_{18} molecular formula for octane
CAD crankshaft angle degree
CAI controlled auto-ignition
CFD computational fluid dynamics
CH_{4} molecular formula for methane
CI compression-ignition
CIDI compression-ignition direct injection
C_{n}H_{2(n+1-g)} general molecular formula for cycloalkanes
C\(_n\)H\(_{2n}\) general molecular formula for alkenes
C\(_n\)H\(_{2n+2}\) general molecular formula for alkanes
CH\(_2\)O molecular formula for formaldehyde
CO molecular formula for carbon monoxide
CO\(_2\) molecular formula for carbon dioxide
CR compression ratio
D engine bore diameter
d\(_e\) hydraulic diameter of the inlet port surface
DEE diethyl ether
DI direct injection
DI-CAI direct injection controlled auto-ignition
DME dimethyl ether
DNS direct numerical simulation
DTBP di-tert-butyl peroxide
EGR exhaust gas re-circulation
EtOH ethanol
EVC exhaust valves close
EVO exhaust valves open
FMEP friction mean effective pressure
g number of carbon rings in the molecular structure
h current height of the cells for the dynamic mesh layering option
H symbol for hydrogen atom
H\(_2\) molecular formula for hydrogen gas (diatomic)
H\(_2\)O molecular formula for water
H\(_2\)O\(_2\) molecular formula for hydrogen peroxide
HC hydrocarbon emissions
HCCI homogeneous compression charge ignition
He symbol for helium
h\(_{ideal}\) normal height of cells for the dynamic mesh layering option
HO\(_2\) molecular formula for hydroperoxyl radical
HRR heat release rate
HTHR high-temperature heat release
HTR high-temperature reaction
HXT Han, Xu and Trigui (spray/wall interaction model)
I\(_2\) molecular formula for iodine
IC internal combustion
IEGR internal exhaust gas recirculation
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<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>IMEP</td>
<td>indicated mean effective pressure</td>
</tr>
<tr>
<td>IMEP360</td>
<td>gross indicated mean effective pressure</td>
</tr>
<tr>
<td>IMEP720</td>
<td>net indicated mean effective pressure</td>
</tr>
<tr>
<td>ISO</td>
<td>international organisation for standardisation</td>
</tr>
<tr>
<td>IVC</td>
<td>inlet valves close</td>
</tr>
<tr>
<td>IVO</td>
<td>inlet valves open</td>
</tr>
<tr>
<td>$k$</td>
<td>turbulent kinetic energy parameter for the turbulence model</td>
</tr>
<tr>
<td>Kr</td>
<td>symbol for krypton</td>
</tr>
<tr>
<td>L</td>
<td>connecting rod length</td>
</tr>
<tr>
<td>$L$</td>
<td>Global motion length scale</td>
</tr>
<tr>
<td>$l$</td>
<td>Macroscopic agitation scale</td>
</tr>
<tr>
<td>LDA</td>
<td>laser Doppler anemometry</td>
</tr>
<tr>
<td>LDV</td>
<td>laser Doppler velocimetry</td>
</tr>
<tr>
<td>LES</td>
<td>large eddy simulation</td>
</tr>
<tr>
<td>LPG</td>
<td>liquefied petroleum gas</td>
</tr>
<tr>
<td>LRR</td>
<td>Launder-Reece-Rodi turbulence model</td>
</tr>
<tr>
<td>LTHR</td>
<td>low-temperature heat release</td>
</tr>
<tr>
<td>LTR</td>
<td>low-temperature reaction</td>
</tr>
<tr>
<td>m</td>
<td>mass</td>
</tr>
<tr>
<td>M</td>
<td>molar mass</td>
</tr>
<tr>
<td>N</td>
<td>crankshaft rotational speed</td>
</tr>
<tr>
<td>$n$</td>
<td>number of carbon atoms</td>
</tr>
<tr>
<td>N</td>
<td>amount of substance of gas</td>
</tr>
<tr>
<td>$N_2$</td>
<td>molecular formula for nitrogen gas</td>
</tr>
<tr>
<td>$N_2O$</td>
<td>molecular formula for nitrous oxide</td>
</tr>
<tr>
<td>NA</td>
<td>naturally aspirated</td>
</tr>
<tr>
<td>Ne</td>
<td>symbol for neon</td>
</tr>
<tr>
<td>Ng</td>
<td>swirl ratio</td>
</tr>
<tr>
<td>$NO_2$</td>
<td>molecular formula for nitrogen dioxide</td>
</tr>
<tr>
<td>NOx</td>
<td>nitrogen oxides</td>
</tr>
<tr>
<td>O</td>
<td>symbol for oxygen atom</td>
</tr>
<tr>
<td>$O_2$</td>
<td>molecular formula for oxygen gas (diatomic)</td>
</tr>
<tr>
<td>$O_3$</td>
<td>molecular formula for ozone</td>
</tr>
<tr>
<td>OA</td>
<td>O'Rourke and Amsden spray/wall interaction model</td>
</tr>
<tr>
<td>OH</td>
<td>molecular formula for hydroxyl radical</td>
</tr>
<tr>
<td>p</td>
<td>perimeter of the entrance of the inlet port</td>
</tr>
<tr>
<td>P</td>
<td>pressure</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Full Form</td>
</tr>
<tr>
<td>--------------</td>
<td>-----------</td>
</tr>
<tr>
<td>Pair</td>
<td>partial pressure of dry air</td>
</tr>
<tr>
<td>PaSPFR</td>
<td>partially stirred plug flow reactor</td>
</tr>
<tr>
<td>P&lt;sub&gt;D&lt;/sub&gt;</td>
<td>piston displacement</td>
</tr>
<tr>
<td>PDA</td>
<td>particle Doppler anemometry</td>
</tr>
<tr>
<td>PDF</td>
<td>probability density function</td>
</tr>
<tr>
<td>PIV</td>
<td>particle image velocimetry</td>
</tr>
<tr>
<td>PM</td>
<td>particulate matter emissions</td>
</tr>
<tr>
<td>PMEP</td>
<td>pumping mean effective pressure</td>
</tr>
<tr>
<td>P&lt;sub&gt;P&lt;/sub&gt;</td>
<td>piston position</td>
</tr>
<tr>
<td>ppm</td>
<td>parts per million</td>
</tr>
<tr>
<td>ppmv</td>
<td>parts per million volume</td>
</tr>
<tr>
<td>PRF</td>
<td>primary referenced fuel</td>
</tr>
<tr>
<td>PTV</td>
<td>particle tracking velocimetry</td>
</tr>
<tr>
<td>P&lt;sub&gt;water&lt;/sub&gt;</td>
<td>partial pressure of water vapour</td>
</tr>
<tr>
<td>R</td>
<td>ideal gas constant</td>
</tr>
<tr>
<td>RANS</td>
<td>Reynolds average Navier-Stokes</td>
</tr>
<tr>
<td>RCF</td>
<td>rapid compression facility</td>
</tr>
<tr>
<td>RCM</td>
<td>rapid compression machine</td>
</tr>
<tr>
<td>Re</td>
<td>Reynolds number</td>
</tr>
<tr>
<td>REGR</td>
<td>reformed exhaust gas recirculation</td>
</tr>
<tr>
<td>RH</td>
<td>relative humidity in the air</td>
</tr>
<tr>
<td>RMS</td>
<td>root mean square</td>
</tr>
<tr>
<td>RNG</td>
<td>renormalisation group</td>
</tr>
<tr>
<td>RON</td>
<td>research octane number</td>
</tr>
<tr>
<td>rpm</td>
<td>rotation per minute</td>
</tr>
<tr>
<td>RSM</td>
<td>Reynolds stress model</td>
</tr>
<tr>
<td>S</td>
<td>engine stroke</td>
</tr>
<tr>
<td>S</td>
<td>symbol for sulphur atom</td>
</tr>
<tr>
<td>SCCI</td>
<td>stratified charge compression-ignition</td>
</tr>
<tr>
<td>SGS</td>
<td>sub-grid scale</td>
</tr>
<tr>
<td>SI</td>
<td>spark-ignition</td>
</tr>
<tr>
<td>SIDI</td>
<td>spark-ignition direct injection</td>
</tr>
<tr>
<td>SOC</td>
<td>start of combustion</td>
</tr>
<tr>
<td>SOI</td>
<td>start of ignition</td>
</tr>
<tr>
<td>SRM</td>
<td>stochastic reactor model</td>
</tr>
<tr>
<td>t</td>
<td>time</td>
</tr>
<tr>
<td>T</td>
<td>absolute temperature</td>
</tr>
<tr>
<td>Symbol</td>
<td>Definition</td>
</tr>
<tr>
<td>--------</td>
<td>------------------------------------------------</td>
</tr>
<tr>
<td>$T$</td>
<td>time scale</td>
</tr>
<tr>
<td>TDC</td>
<td>top dead centre</td>
</tr>
<tr>
<td>TDCF</td>
<td>top dead centre firing</td>
</tr>
<tr>
<td>TDR</td>
<td>turbulent dissipation rate</td>
</tr>
<tr>
<td>TI</td>
<td>turbulence intensity</td>
</tr>
<tr>
<td>TKE</td>
<td>turbulence kinetic energy</td>
</tr>
<tr>
<td>$T_{Turb}$</td>
<td>turbulence time scale</td>
</tr>
<tr>
<td>$u$</td>
<td>characteristic velocity</td>
</tr>
<tr>
<td>UDF</td>
<td>user defined functions</td>
</tr>
<tr>
<td>UHC</td>
<td>unburned hydrocarbons</td>
</tr>
<tr>
<td>$U_p$</td>
<td>instantaneous piston velocity</td>
</tr>
<tr>
<td>$V$</td>
<td>instantaneous cylinder volume</td>
</tr>
<tr>
<td>$V$</td>
<td>velocity</td>
</tr>
<tr>
<td>$V_{BDC}$</td>
<td>maximum cylinder volume</td>
</tr>
<tr>
<td>$V_D$</td>
<td>displacement volume</td>
</tr>
<tr>
<td>$V_{TDC}$</td>
<td>clearance volume</td>
</tr>
<tr>
<td>VVA</td>
<td>variable valve actuation</td>
</tr>
<tr>
<td>VVT</td>
<td>variable valve timing</td>
</tr>
<tr>
<td>$x$</td>
<td>horizontal axis</td>
</tr>
<tr>
<td>$X_e$</td>
<td>symbol for xenon</td>
</tr>
<tr>
<td>$y$</td>
<td>vertical axis</td>
</tr>
<tr>
<td>$Y^+$</td>
<td>dimensionless wall distance</td>
</tr>
<tr>
<td>$Y_1$</td>
<td>distance between the wall and the centre of the first cell</td>
</tr>
<tr>
<td>$\bar{U}_p$</td>
<td>average piston speed</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>inverse effective Prandtl number</td>
</tr>
<tr>
<td>$\alpha_c$</td>
<td>collapse factor for the cells for the dynamic mesh layering option</td>
</tr>
<tr>
<td>$\alpha_s$</td>
<td>split factor for the cells for the dynamic mesh layering option</td>
</tr>
<tr>
<td>$\beta$</td>
<td>boundary node relaxation for the dynamic mesh spring smoothing option</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>turbulent dissipation rate parameter for the turbulence model</td>
</tr>
<tr>
<td>$\theta$</td>
<td>crankshaft angle</td>
</tr>
<tr>
<td>$\mu$</td>
<td>dynamic viscosity of a fluid</td>
</tr>
<tr>
<td>$\mu_t$</td>
<td>turbulence viscosity</td>
</tr>
<tr>
<td>$\rho$</td>
<td>fluid density</td>
</tr>
<tr>
<td>$\Omega_k$</td>
<td>rotation vector</td>
</tr>
</tbody>
</table>
Conference and Journal publications generated from this study


Chapter 1: Introduction

The purpose of an internal combustion (IC) engine is to convert the chemical energy contained in the fuel into mechanical work. It uses an exothermic reaction to increase the pressure in a closed volume, which forces the piston to move downward and produce work. The linear movement of the piston is converted into rotational motion by the connecting rod at the crankshaft. A lot of attention is paid to vehicle engines in order to improve their power, torque and efficiency. Further, the fuel consumption and emissions have to be reduced, to meet environmental regulation standards. The two most popular forms of combustion used in IC engines are spark-ignition (SI) and compression-ignition (CI). In the SI principle, used in production gasoline engines, fuel is injected through the inlet port, when suction occurs inside the cylinder, during the intake stroke. Tumble and swirl flow motion inside the combustion chamber, are usually used to optimise the rate at which the air-fuel particles mix. The mixture is then compressed by the piston until it reaches top dead centre (TDC). The compression ratio in a gasoline engine is usually limited to 11:1, due to engine knocking; although compression ratios as high as 13:1 are seen for high-performance racing engines when high-octane gasoline is used. A spark from a spark plug ignites the compressed mixture, depending on the ignition timing, usually just before TDC, initiating combustion that spreads inside the combustion chamber. However, SI engines present a number of disadvantages:

- High carbon monoxide (CO) and hydrocarbon (HC) emissions
- High fuel consumption compared to CI engines
- Pre-ignition
- Engine knock

The emissions of SI engines depend on the air-fuel ratio (AFR) corresponding to the required engine mode. For instance, a rich mixture will be needed to compensate for poor fuel vaporisation at cold start, low load at idle or for the additional power required for full load and acceleration. A representation of the emissions concentration variation depending on the fuel/air equivalence ratio for spark-ignition engines was presented by Heywood (1988) [1] in Figure 1.1.
Pre-ignition is the phenomenon of the ignition of the air-fuel mixture in a SI engine prior to the spark plug firing. Engine knock is a different phenomenon defined after the spark plug has fired, as pockets of fuel/air mixture outside of the flame front, auto-ignite. It can be due to a low octane rating of the fuel, hot spots in the cylinder or incandescent residue from the previous cycle, like carbon deposits.

In CI engines, the fresh charge of air is induced during the intake stroke and then compressed during the compression stroke. Typical compression ratios for CI engines usually exceed 14:1 and ratios over 22:1 are common. The fuel is then injected when the piston approaches top dead centre firing (TDCF) and ignites due to the high air temperature within the cylinder. This method leads to higher engine fuel conversion efficiency and lower fuel consumption. However, it creates more pollutants like
Nitrogen Oxide emissions (NOx), due to the high temperatures of combustion and particulate matter (PM) emissions due to the incomplete combustion.

A combination of these two methods (SI and CI) is called controlled auto-ignition (CAI), which has recently attracted more attention from researchers. The principle is to mix fuel and air homogeneously, before compressing the mixture to the point of auto-ignition. There is no electric discharge from a spark plug to ignite the mixture; instead, the temperature of the mixture is raised by compression. Ignition occurs at several places at the same time inside the combustion chamber, which makes the air-fuel mixture burn almost simultaneously. Auto-ignition could be controlled to reduce engine emissions along with raising engine efficiency [2]. CAI engines achieve extremely low levels of NOx emissions without the use of catalytic aftertreatment, due to a lower temperature of combustion. The HC emissions are higher than in SI engines due to the incomplete oxidation during the simultaneous combustion. The CO emissions are also higher than in SI engines due to the gases trapped in the crevice, but both HC and CO emissions can be treated by catalytic aftertreatment, to meet automotive emission standards [3].

1.1 The importance of controlled auto-ignition

Limited fossil fuel resources and the impact of pollutant emissions on the environment and health have become urgent problems to solve. An internal combustion engine used for commercial vehicles usually produces nitrogen oxides (NOx), particulate matter (PM), hydrocarbons (HC) and carbon monoxide (CO) emissions. As a result, the emissions levels of new vehicle engines are constantly being reduced to match the revised European emission standards. The current emission standards for passenger vehicles are defined by the adaptation of the directive 88/77/EEC [4] and more recently the directive 2005/78/EC (Euro 5) of the European commission in 2009. Table 1.1 shows the list of directives applied to 88/77/EEC since December 1987.
Table 1.1 Adaptation of directive 88/77/EEC [4]

<table>
<thead>
<tr>
<th>Directive number</th>
<th>Euro 1</th>
<th>Euro 2</th>
<th>Euro 3</th>
<th>Euro 4</th>
<th>Euro 5</th>
<th>Euro 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Date</td>
<td>26.06.91</td>
<td>23.03.94</td>
<td>13.10.98</td>
<td>03.10.02</td>
<td>14.11.05</td>
<td></td>
</tr>
</tbody>
</table>

Tables 1.2 and 1.3 describe the changes of pollutant emission standards from 1992 to 2014 for diesel and gasoline engine passenger vehicles. All emission level limits have significantly reduced for both diesel and gasoline engines. For instance, the NOx emission level is reduced from 500 mg/km in 2000 to 80 mg/km in 2014 for diesel engines. The average passenger vehicle sold by 2008 produced 140g/km of CO₂. In 2012, the CO₂ emissions have been reduced to 120g/km (com/2007/0019, Commission of the European communities, 7.2.2007).

Table 1.2 Emissions standards for diesel engine passenger vehicles [4]

<table>
<thead>
<tr>
<th>Date</th>
<th>Name</th>
<th>Diesel CO (g/km)</th>
<th>Diesel HC (g/km)</th>
<th>Diesel NOx (g/km)</th>
<th>Diesel PM (g/km)</th>
<th>Diesel HC+NOx (g/km)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1992</td>
<td>Euro 1</td>
<td>2.72</td>
<td>-</td>
<td>-</td>
<td>0.14</td>
<td>0.97</td>
</tr>
<tr>
<td>1996</td>
<td>Euro 2</td>
<td>1</td>
<td>-</td>
<td>-</td>
<td>0.08</td>
<td>0.7</td>
</tr>
<tr>
<td>2000</td>
<td>Euro 3</td>
<td>0.64</td>
<td>-</td>
<td>0.5</td>
<td>0.05</td>
<td>0.56</td>
</tr>
<tr>
<td>2005</td>
<td>Euro 4</td>
<td>0.5</td>
<td>-</td>
<td>0.25</td>
<td>0.025</td>
<td>0.3</td>
</tr>
<tr>
<td>2009</td>
<td>Euro 5</td>
<td>0.5</td>
<td>-</td>
<td>0.18</td>
<td>0.005</td>
<td>0.23</td>
</tr>
<tr>
<td>2014</td>
<td>Euro 6</td>
<td>0.5</td>
<td>-</td>
<td>0.08</td>
<td>0.005</td>
<td>0.17</td>
</tr>
</tbody>
</table>

Table 1.3 Emissions standards for gasoline engine passenger vehicles [4]

<table>
<thead>
<tr>
<th>Date</th>
<th>Name</th>
<th>Gasoline CO (g/km)</th>
<th>Gasoline HC (g/km)</th>
<th>Gasoline NOx (g/km)</th>
<th>Gasoline PM (g/km)</th>
<th>Gasoline HC+NOx (g/km)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1992</td>
<td>Euro 1</td>
<td>2.72</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.97</td>
</tr>
<tr>
<td>1996</td>
<td>Euro 2</td>
<td>2.2</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.5</td>
</tr>
<tr>
<td>2000</td>
<td>Euro 3</td>
<td>2.3</td>
<td>0.2</td>
<td>0.15</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2005</td>
<td>Euro 4</td>
<td>1</td>
<td>0.1</td>
<td>0.08</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2009</td>
<td>Euro 5</td>
<td>1</td>
<td>0.1</td>
<td>0.06</td>
<td>0.005</td>
<td>-</td>
</tr>
<tr>
<td>2014</td>
<td>Euro 6</td>
<td>1</td>
<td>0.1</td>
<td>0.06</td>
<td>0.005</td>
<td>-</td>
</tr>
</tbody>
</table>
However, the current progress of research for SI and CI engines cannot match the emissions provisions. A three-way catalyst aftertreatment, can be used to reduce the three main pollutants (CO, HC and NOx) simultaneously and convert them into regular emissions (CO₂, H₂O and N₂) in the three-way conversion region [5]. An illustration of the catalyst conversion zones can be seen in Figure 1.2. As the mixture becomes leaner, the efficiency of NOx conversion drops significantly. The high conversion efficiency for the three pollutants is in the region between a stoichiometric mixture and a rich mixture with an air-fuel equivalence ratio of 0.995. This makes the three-way catalyst inefficient for CI and CAI engines due to their lean mixture operation. Nitric oxide (NOx) emissions can be reduced for SI engines but at the cost of fuel consumption. Standards like Euro 6, force gasoline and diesel engine manufacturers to significantly reduce NOx and PM emissions [4].

![Rich/Lean Catalyst Conversions](image)

**Figure 1.2 Efficiency of three-way catalyst conversion depending on the air-fuel ratio [5]**

1.2 **Characteristics of controlled auto-ignition engines**

In a CAI engine, there is no electric discharge from a spark plug to ignite the mixture of air and fuel. The piston movement during the compression stroke increases the cylinder pressure and the corresponding cylinder temperature until auto-ignition occurs. The auto-ignition temperature depends on the mixture properties. As the mixture ignites
simultaneously, CAI combustion occurs faster than in SI and CI engines. If a stoichiometric mixture is inducted into the cylinder, the high pressure created by the simultaneous auto-ignition could damage the engine. Hence, CAI engines are operating with lean mixtures, preventing very high pressures within the cylinder. The main advantages of CAI combustion are the reduction of pollutant emissions combined with lower fuel consumption. In fact, as the peak of temperature within the cylinder is greatly reduced compared to a SI engine, NOx emissions are almost non-existent. Lean mixtures lead to higher efficiency than SI engines and have the potential to create even higher efficiency than CI engines. CAI engines can run throttle-less which eliminates throttling losses which are present in other combustion systems such as SI engines. The main challenge of CAI engines is the difficulty in controlling the occurrence of auto-ignition. Due to the cylinder pressure limit, the mixture is lean, therefore restricting the engine power. The combustion also creates high CO and HC emissions prior to the catalyst aftertreatment. CAI engines could be designed for focused operating conditions to reduce the range of control, speed and load required, which is ideal for hybrid vehicles and power generation applications. However, most engines have to adapt their power output to the users continually changing requirements. In order to govern the operating conditions in a CAI engine, the control of the mixture temperature is key to achieving combustion. It can be obtained by controlling the compression ratio, by retaining or recirculating exhaust gases, pre-heating the intake charge or by increasing the intake charge pressure (using a turbocharger or a supercharger).

A method to control the compression ratio involves the use of a movable plunger within the cylinder head. An alternate method consists of controlling the position of the engine stroke using a varying crankshaft offset [6]. Alternatively, the temperature of the mixture can be regulated to control auto-ignition. One method consists of heating the intake charge prior to it entering the cylinder [7]. Another method consists of retaining residual gases from the previous combustion cycle by controlling the valve parameters, a method called variable valve actuation (VVA) [8, 9]. Depending on the amount of residual gas retained, the temperature of the mixture can be controlled. On the contrary, cooled exhaust gas recirculation (EGR) can be used to dilute the charge and postpone auto-ignition [10, 11].
In CI engines, air alone is compressed during the compression stroke. The fuel is then introduced by direct injection over a period of time. The slow release of the fuel during the injection stage results in a reduction of the pressure peak and the energy release rate during the expansion stroke. In SI engines, the air-fuel mixture is introduced during the intake stroke. As the spark starts the ignition process, the total amount of energy contained in the gasoline will be released slowly during the expansion stroke, due to the propagating flame. Again, this leads to a reduction of the cylinder pressure peak and energy release rate. In SI and CI engines, the working range is complete from low to high load. Adding more air-fuel mixture to the combustion chamber increases the engine output. As the heat release rate (HRR) is slow, the engines can withstand the excess of power provided by the additional fuel, during high load operations. In CAI engines, the entire mixture ignites almost simultaneously, which creates high peaks of cylinder pressure and energy release. The engine design must be robust to withstand higher pressures, and are therefore heavier, compared to SI and CI engines. Various strategies can be used to obtain a lower HRR and cylinder pressure peak. For example, using two different blends of fuel would change the ignition timings at different locations within the cylinder. Further, as the pressure and heat release peaks would be lower, a compressed charge would contain additional air-fuel mixture, which would increase the engine output. If the engine in CAI mode is restricted from low-load to mid-load conditions, a spark plug could be used for high load applications. As the mixture used in CAI engines is lean, the temperature peaks are lower than in SI and CI engines, which prevents the formation of NOx. However, low-temperature combustion also leads to incomplete burning of the fuel in near-wall regions within the cylinder, lowering the power output and producing high CO and HC emissions. An oxidising catalyst can be used to reduce the CO and HC emissions. In CAI engines, the mixture ignites almost simultaneously due to the cylinder pressure and corresponding temperature. The homogeneous mixture is isobaric, which reduces the chance of engine knock considerably. Engine knock may still occur in CAI engines at high load, due to the high air-fuel ratio.
1.3 Brief review of current progress on controlled auto-ignition

The U.S. Department of energy review shows that CAI combustion technology has the potential to be highly efficient and to produce low emissions [2]. CAI engines can have efficiencies as high as CI whilst producing very low NOx and PM emissions. CAI can operate on gasoline, diesel, gas and most alternative fuels. Therefore, it incorporates the best features of both SI and CI engines. It has the advantage of minimising particulate emissions like SI engines but without throttling losses and the advantage of the CI high efficiency. CAI is also applicable to other sectors such as power generation. CAI engines could also be used and optimised for hybrid vehicle applications where the range of loads and speeds is reduced compared to typical vehicle engines. In CAI engines, the combustion is governed by local chemical kinetic reaction rates unlike the SI and CI engines. The chemical kinetics modelling of CAI combustion has unveiled that the energy release is linked to hydrogen peroxide (H₂O₂) decomposition into two hydroxyl (OH) radicals [13]. H₂O₂ decomposition occurs at temperatures ranging from 1050 K to 1100 K. With high-octane fuels, little heat is released before the main ignition occurs, between 1050 K and 1100 K. However, with low-octane fuels, like diesel, some reactions begin at temperatures as low as 800 K. The energy release for low-temperature reactions is small but helps to rapidly increase the mixture temperature necessary for hydrogen peroxide decomposition and auto-ignition. Figure 1.3 illustrates the concentration of H₂O₂ and its radicals hydrogen (H), OH, and hydroperoxyl (HO₂) during auto-ignition. The combustion occurs when H₂O₂ decomposes releasing a high quantity of OH, which in turn reacts with the fuel molecules, releasing more heat and starting a chain reaction. It is this effect that causes CAI to be sensitive to fuel type.
Another illustration of fuel sensitivity in CAI is shown in Figure 1.4. A chemical kinetics model is used by Kelly-Zion and Dec (2000) [13] to calculate the auto-ignition variables for (a) n-heptane and (b) iso-octane fuels. In this study, the fuel equivalence ratio, defined as the fuel to oxidiser ratio, divided by the stoichiometric fuel to oxidiser ratio, is varied for both fuels. The results demonstrated that a change of the fuel equivalence ratio shows a variation of the ignition timing for the two fuels as seen in the figure. Also, the ignition for n-heptane occurs in two stages, the first stage starting at around 800 K. For the iso-octane, a single-stage ignition is seen starting at around 1100 K. The auto-ignition timing shows a high sensitivity to the fuel type. Fuels with single-stage ignition, like octane, have shown superior ignition control over two-stage ignition fuels, like heptane.
One of the main restrictions of CAI is a high combustion rate, which decreases the attainable indicated mean effective pressure (IMEP). Hence, CAI combustion shows reduced load limits and engine speeds. Some studies aim to increase the heat release duration in order to extend the CAI load range [14, 15, 16, 17, 18, 19, 20]. The first
method that can be used is a charge stratification. Using a two-stage injection process, where the first injection of fuel is at an early stage and the second injection of a different fuel is later, can create a stratification charge which will advance ignition and improve the load limit [14]. An alternate method is the use of in-cylinder turbulence to thermally stratify the charge. The effects of turbulence rapidly increase the temperature gradients. Turbulence has a great effect on initial hot spots for lean hydrogen combustion [15]. Another method used to extend the heat release duration, is the injection of water inside the cylinder [16, 17]. Water injection has demonstrated a greater effect on the ignition timing when higher inlet temperatures are used. Although the NOx values recorded were very low, the studies showed that the use of water during the combustion can reduce NOx emissions further. In the case of dual-timing fuel injection, water can still be injected between the two fuel injections. The HRR can be doubled in some cases, with reduced NOx and HC emissions. The quantity of water injected should not exceed the quantity of fuel injected, which would cause an excessive deterioration of combustion. When the quantity of injected water reaches 20% of the fuel content, it significantly reduces the available load range of the engine. The last method consists of using various fuels, or additives, to control the ignition postponement and burn rate [18].

Various studies have demonstrated the benefits of supercharging, turbocharging and increasing the inlet temperature [19, 20, 21, 22]. This would improve CAI combustion efficiency and lead to a further reduction in emissions. Also, by elevating the pressure with low oxygen concentration, the NOx mass is shown to decrease. Overall, the load limit for CAI can be extended, when using supercharging combined with exhaust gas recirculation (EGR), without increasing the maximum cylinder pressure. The HC emissions decrease with higher EGR rates and a high engine load. The maximum load and brake efficiencies are higher with a turbocharger, compared to a mechanical supercharger. Further, high boost superchargers can increase the fuel consumption. It is shown that it would be preferable to use a smaller supercharger with a moderate pressure boost.
Many of the CAI studies involve the use of cooled EGR or residual gases to increase the control of auto-ignition. A fraction of the burnt gas is retained within the cylinder from the previous combustion cycle by using shorter exhaust valve durations. The residual gases contained in the cylinder increase the overall mixture temperature which advances ignition [23, 24, 25]. On the contrary, cooled EGR can be used to dilute the charge and postpone ignition [12, 19, 26]. However, ignition postponement has been shown to be dependent on fuel type [27].

Numerous studies conducted on CAI engines have used chemical kinetics software packages in order to understand, predict and improve auto-ignition and the corresponding after-combustion emissions. The first approach, called the single-zone model, considers the combustion chamber as a unique zone of reaction and temperature [13]. A different approach, used to predict the emissions levels is called the multi-zone model [28], where the combustion chamber is divided into multiple zones, for defining the reactions and temperatures. It can be used to efficiently simulate charge stratification, piston crevice and near-wall treatment. For instance, the accuracy of the predictions for HC and CO emissions near the piston-ring crevice can be increased using the multiple-zone model. Due to the poor combustion quality near the piston bowl region and the vicinity of the cylinder, a significant portion of CO is found in these regions. However, where computer restrictions apply, the computational time can be considerably reduced by simplifying the detailed chemical kinetics mechanism [29]. Another approach to monitor and to understand the combustion in CAI engines is the use of laser-induced fluorescence [30, 31, 32]. Usually, the measurements can be made very close to the cylinder wall. The occurrence of multiple isolated ignition spots shows that CAI combustion relies on distributed reactions rather than flame propagation.

The use of in-cylinder turbulences to improve the load range and HRR of CAI engines was also investigated [33, 34, 35, 36]. Controversial results are reported on the effect of turbulence on CAI combustion. Longer combustion duration and a longer HRR are reported when using a square bowl piston compared to a flat piston [33, 34, 35]. The combustion chamber geometry is found to affect CAI operation and therefore, the design of the chamber could be used as a tool for increasing the load range of a CAI
engine. The temperature distribution is also found to significantly affect CAI combustion [36]. However, swirl enhancement is found to have little effect on combustion duration [33].

### 1.4 Technological questions and specific objectives of this study

From the various investigation conclusions, it is clear that CAI engines have the potential to replace conventional combustion engines such as SI and CI, due to the revised European emission regulation standards. Low NOx and PM emissions along with CI-like efficiencies are the main features of CAI engines. However, the main drawbacks of CAI engines are auto-ignition control and the high energy release rate which restricts CAI load range and speed. Researchers have been investigating ways to extend CAI load range and speed by creating mixture temperature and fuel concentration stratifications, using fuel injection with different timings and the injection of fuels with different properties. Various investigations have been conducted to improve the control of CAI engines, such as controlling the compression ratio, retaining or recirculating exhaust gases, pre-heating the intake charge or increasing the intake charge pressure with a turbocharger or a supercharger.

The scope of this project is to investigate the consequences of varying the valve timing as a means to control the mixture temperature and therefore, the mixture auto-ignition. After a validation of the model, the use of computational fluid dynamics (CFD) code, combined with a chemical kinetics model, can allow monitoring of the generation of cylinder flow fields and turbulence variables during the intake and compression stroke and the prediction of auto-ignition. The effects of valve timing, used as a method of controlling auto-ignition, on the flow fields and turbulences and their effects on the mixture quality and cylinder temperature distribution, could be of great value to engine designers and researchers. A list of technological questions to aid new research direction can be summarised as follows:

- What is the effect of varying the valve timing on the fresh charge amount entering the cylinder, during the intake stroke?
What is the effect of varying the valve timing on the residual gases amount retained within the cylinder, after the exhaust valves close?

What is the effect of valve timing on the mixture ignition timing?

What is the effect of engine speed on the intake charge velocity entering the cylinder of a CAI engine, during the intake stroke?

Does the valve timing affect the intake charge velocity, entering the cylinder of a CAI engine during the intake stroke?

What is the effect of CAI valve timing on the fuel concentration in the mixture within the cylinder, during the intake and compression stroke?

What is the effect of using CAI valve timing on the temperature distribution within the cylinder, during the intake and compression stroke?

What is the consequence of using CAI valve timing on the combustion duration, compared to a fully homogeneous mixture case?

What is the effect of the fuel and temperature stratification on indicated work in a CAI engine, compared to a fully homogeneous mixture case?

What is the effect of using CAI valve timing on the cylinder indicated efficiency?

The main steps of this study are summarised as follows:

1. Develop a CFD model for SI and CAI engine configurations.

2. Analyse the available experimental data conducted and provided by Pitcher *et al.* (2003) [37].
3. Validate the calculated results against available experimental measurements supplied by Pitcher et al. (2003) [37].

4. Monitor the effects of valve timing and engine speed on the intake charge velocity during the intake stroke.

5. Study the effects of valve timing and engine speed on the turbulence parameters during the intake and compression stroke.

6. Investigate the effects of valve timing on temperature distribution and mixture fuel concentration within the cylinder.


1.5 Structure of the thesis
The current thesis is structured as follows:

In chapter 2, a fully detailed literature review is presented. The first part focuses on experimental work conducted on IC engines. The second part describes the numerical calculations on IC engines. Then, CAI principles and research directions are described. Chapter 3 displays the turbulence phenomena in IC engines, the difference between turbulence models and mesh generation. Chapter 4 presents the available laser Doppler anemometry (LDA) data and thermodynamic data for a single cylinder engine conducted and provided by Pitcher et al. (2003) [37]. The HRR is calculated from the experimental cylinder pressure obtained by Pitcher et al. (2003) [37]. Chapter 5 presents the numerical modelling methodology for SI and CAI valve timings. Then, a sensitivity and a mesh quality study are conducted, before the boundary conditions applied to the models are defined. Chapter 6 describes the validation of SI valve timings by comparing the numerical simulations with LDA measurements published by Pitcher et al. (2003) [37]. The in-cylinder velocity vectors are presented on the symmetrical axial plane to depict the tumble phenomenon. Further, the turbulence parameters such as turbulence intensity (TI), turbulence kinetic energy (TKE) and the turbulence dissipation rate...
(TDR) are revealed at different locations within the clearance volume. Chapter 7 validates the CFD simulations against LDA experimental work provided by Pitcher et al. (2003) [37] for CAI valve timings at two engine speeds, 1500 revolutions per minute (rpm) and 2000 rpm. The tumble phenomenon is compared between the two engine speeds as well as the turbulence parameters TI, TKE and TDR for different locations within the clearance volume. The charge delay for each speed is also calculated. Chapter 8 describes the numerical work conducted using the CFD code, combined with a chemical kinetics model, to be compared with the results obtained from the thermodynamic single cylinder engine published by Pitcher et al. (2003) [37]. A new set of numerical calculations is launched to obtain the effects of valve timing on the charge delay, temperature distribution and charge fuel stratification with a constant fuel quantity. The results are then compared to a fully homogeneous model. Chapter 9 presents the conclusions of this study and the recommendations for further work.
References


Chapter 2: Current status of computational fluid dynamics modelling of flow inside internal combustion engines

The flow inside an internal combustion (IC) engine is usually characterised by parameters such as fuel type, mixture density and concentration, velocity, pressure, heat and mass transfer. Generally, an average prediction of the flow is sufficient to allow optimisation of the combustion process. However, a detailed prediction with computational fluid dynamics (CFD) modelling techniques, allows an in-depth insight into the internal cylinder flow, so that emission reduction and suppression of unstable states during combustion, can be obtained. At present, CFD modelling techniques are widely used for investigations of the flow inside a wide range of IC engines. This can lead to a significant reduction in design lead time for development and validation of new IC engines.

This chapter briefly reviews previous studies using experimental and CFD modelling techniques and their validation for IC engines. In the first part of this chapter, experimental investigations are reviewed. The modelling techniques are described and discussed, together with their experimental validations. The second part of this chapter describes the studies conducted on controlled auto-ignition (CAI), to understand the auto-ignition characteristics and properties, to improve auto-ignition control, extend the load limit and reduce exhaust emissions.

2.1 Experimental investigation and computational fluid dynamics modelling on flow within internal combustion engines

2.1.1 Experimental tests and validations on turbulent flow inside internal combustion engines

A lot of attention has been paid to vehicle engines, in order to improve their power, torque and efficiency. Further, fuel economy and emissions have to be reduced to match environmental standards. To achieve these objectives many experimental investigations and validations of flow inside IC engines, have been conducted in the last two decades. One of the main effective methods of extracting experimental data on the flow inside IC engines is the use of laser Doppler velocimetry (LDV) or laser Doppler anemometry (LDA). In the experimental study conducted by Arcoumanis et al. (1990) [1] on a two
valve spark-ignition (SI) engine, the inlet port was inclined at 45° and 90°, to enhance the swirl and tumble motions. The LDV results have shown an improvement of the swirl ratio and tumbling vortex ratio for both cases when compared to the original configuration. To improve the combustion of SI engines, Hadded and Denbratt (1991) [2] investigated the turbulences inside a four-valve, optically accessible single cylinder, under motored conditions at a speed of 1500 rpm. LDA measurements revealed the turbulences before top dead centre firing (TDCF) for four different cylinder head geometries with different tumble magnitudes. After reviewing the turbulent flow motions inside a combustion chamber, and the effects of swirl and tumble motion, Hill and Zhang (1994) [3] combined the conclusions drawn from previous studies on flow inside IC engines. Researchers have used methods such as blades, deflectors, shrouds and various intake port and valve angles, to increase the turbulences. The experimental results (obtained using photometry during the combustion process) and the LDA measurements show that turbulence enhancement increases the flame propagation speed, reduces the cyclic variations and extends the lean limit. Hong and Chen (1997) [4] also obtained LDV measurements, within a single optical cylinder, in order to measure the in-cylinder length scale of the flow. Results show that the measurements of separated cylinder axial and radial components can be used to characterise the flow accurately. Kent et al. (1988) [5] obtained LDA measurements inside a four stroke engine running at 1500 rpm. The study examined the effects of two different inlet port designs and four different valve lifts, on the flow behaviour inside the cylinder. The combustion experimental work conducted on the same engine geometry revealed a decrease of the burn duration as the swirl ratio increased.

Again, Omori et al. (1991) [6] carried out LDV measurements to determine the in-cylinder flow characteristics during the intake and compression stroke, for three different piston shapes and three different inlet port types. The results clearly show the development of the tumble motion during the intake and compression processes, for all cases, as shown in Figures 2.1 and 2.2. Higher tumble levels are reported for the tumble port with shroud compared with other port designs.
Figure 2.1 Influence of piston shape on tumble [6]

Figure 2.2 Tumble for different port geometries [6]
Another experimental method used to study IC engine flow is called particle tracking velocimetry (PTV). This method is less common, but still gives some valuable results. An example of using this method is the investigation conducted by Choi (1998) [7] on a four stroke engine with 4 valves, to visualise the turbulences inside an engine cylinder as shown in Figure 2.3. Experimental measurements of the water flow inside an engine running at 600 rpm and 1200 rpm are obtained to calculate both the swirl and tumble ratios and demonstrate the suitability of using such a method, as a fast cylinder flow evaluation tool.

![Three-dimensional velocity vector field inside the cylinder for an engine motored at 600 rpm](image)

Figure 2.3 Three-dimensional velocity vector field inside the cylinder for an engine motored at 600 rpm [7]

Another example of using such technology is the study conducted by Khalighi (1990) [8]. The study uses PTV and water flow visualisation, to improve the in-cylinder flow behaviour inside a four stroke engine with 4 valves, as shown in Figures 2.4, 2.5 and 2.6 for various crank angle degrees (CAD) after TDC and different cycles. Different intake configurations were trialled, such as one or two valves operating or the use of a shroud of
different angles on one valve. Results have shown a very low cyclic variation of the large-scale motions, as well as a stronger tumble motion in the case of the inlet valve with the shroud configuration.

Figure 2.4 Swirl at 90 CAD after top dead centre [8]

(a) 55° after TDC

(b) 45° after TDC

(c) 60° after TDC

Figure 2.5 Tumble development [8]
Figure 2.6 Tumble variations for different cycles [8]

The experiment conducted by Reeves et al. (1999) [9] also used PTV to monitor the difference in tumble motion inside a transparent cylinder, while the engine was rotating at 1000 rpm for cases with low and high swirl ratios. Stansfield et al. (2007) [10] used particle image velocimetry (PIV) measurements to investigate the in-cylinder flow field, inside a four-valve, single, optical, SI cylinder, motored at speeds of 750 rpm, 2000 rpm and 3500 rpm. The study monitored the radial velocities, tumble ratio and intake manifold pressure fluctuation development, for the three engine speeds. At part-load, the results recorded a high level of cycle-to-cycle variation. The results also show a change in the flow tumble motion structure, between 2000 rpm and 3500 rpm. Pitcher et al. (2008) [11] investigated the effect of early inlet valve closing for a spark-ignition direct injection (SIDI) engine. Using an optical and thermodynamic engine, the optimum results show a
13% decrease in fuel consumption. Pitcher et al. (2008) [12] also investigated the flow field of an optical engine at 3500 rpm using PIV. The flow was found to have high cyclic variability. Results show a non-symmetrical swirl motion and the formation of a strong reverse tumble flow.

2.1.2 Computational fluid dynamics modelling of turbulent flow inside internal combustion engines

Although the experimental studies on flow inside IC engines, using LDA, PTV and PIV discussed in the previous section, can provide details of the internal flow field, the use of such experimental technologies is usually expensive and gives limited flow details for IC engines in practice. As an alternative, the use of computer-aided design and CFD has become popular in recent years for optimising the design of IC engines. The enhanced performance of computers further raises the capabilities of dealing with and predicting turbulent flows inside engine cylinders. However, the results of CFD modelling have to be validated against relevant experiments, such as those mentioned in the previous section. One of the main advantages of CFD modelling is that once the model is validated, it can reveal the whole flow pattern of the engine, even for parts which are usually inaccessible using experimental work. The results can be fully investigated so that the model can be modified and optimised, without the need for a costly prototype or a further validation process. Further, the settings of the simulation can be recorded to provide the basis for further studies. For instance, Affes et al. (1998) [13] described a combined computer-aided design and CFD method, for the optimisation of the inlet port angle and shape, of a four stroke engine. The method coupled computer-aided design and CFD software, to obtain the optimal bend, length and diameter of the inlet port as shown in Figure 2.7.
Figure 2.7 Optimisation history of the inlet port geometry [13]

Arcoumanis et al. (1988) [14] predicted the swirl motion inside a combustion chamber using CFD modelling. A steady flow engine test rig, with a single centred valve, was used to take measurements inside the open cylinder, to validate their CFD predictions. A CFD model of an internal combustion engine was also used by Chen and Shih (1997) [15] to validate the design of the inlet port. A computational mesh was generated to study three different inlet port curvature angles and lengths. The simulations were then compared to the experimental flow bench results. The results of the CFD model predicted similar flow rates to the experiments. Isshiki et al. (1985) [16] presented a single-port model, with one valve, using a method of rectangular prisms as shown in Figure 2.8. The study aimed to predict numerically, the effects of the valve as well as the angle and height of the inlet port, on volumetric efficiency and swirl intensity for the four different configurations.
Lebrere et al. (1996) [17] also used a CFD model to predict turbulent flow inside an engine cylinder. A comparison of two turbulence models is presented. The flow for different arrangements, from a centred to an off centred inlet port position as shown in Figure 2.9, was simulated. The study has shown that the turbulence model has a strong influence on the flow results, particularly at the end of the compression stroke.

The results obtained from using the standard k-ε and the Launder-Reece-Rodi (LRR) turbulence models are compared, as shown in Figure 2.10.
Figure 2.10 Velocity field comparisons for the k-ε and the Launder-Reece-Rodi models [17]

Le Coz et al. (1990) [18] investigated the velocity vector distribution inside a combustion chamber, of a four stroke engine, with two inlet valves. Three intake configurations were studied and compared, using LDV measurements. Using the KIVA engine code developed by Amsden et al. (1985) [19], a three-dimensional (3D) model was developed to extend the investigation of flow motion, prior to top dead centre (TDC). The results show a reduction of tumble strength during the compression stroke for all cases. Li et al. (2001) [20] investigated the in-cylinder tumbling flow motion inside a four valve SI engine. LDA measurements were obtained to validate the CFD calculations. CFD results clearly show the development of two counter-rotating vortices in the cylinder, during the intake stroke, as shown in Figures 2.11 and 2.12. During the compression stroke, the tumble motion still exists in the central region of the cylinder, while the anti-clockwise motion declined into smaller vortices and eddies.
Figure 2.11 Two-dimensional simulation of the velocity on the valve symmetry plane [20]

Figure 2.12 Three-dimensional tumble simulation on the valve symmetry plane for various crankshaft angles [20]
Wakisaka et al. (1986) [21] presented a model for numerical analysis, of in-cylinder turbulent flow of reciprocating engines. The study presented the swirl and tumble motions at different cross-sections of the combustion chamber, as shown in Figure 2.13. Various cases were investigated, with a centred and off-centred inlet valve, a flat piston and a piston with a cavity.

![Figure 2.13 Tumble and swirl motion for different planes [21]](image)

The development of the swirl ratio during the intake stroke was also monitored, as shown in Figure 2.14. The results compared the decay of the swirl motion for all cases. A faster decay of swirl was reported for non-symmetrical piston cavities when compared to symmetrical cavities.
Yavuz and Celik (1999) [22] compared various turbulence models for their applicability to the CFD modelling of flow inside IC engines. The CFD calculations show, that the use of the Lam-Bremhorst (low Reynolds number) turbulence model, gives better results for the turbulent flow inside an engine. The standard k-ε model was found to perform better than the renormalisation group (RNG) k-ε model. Zhu (1995) [23] conducted CFD calculations of a four stroke engine running at 2000 rpm. The calculations covered the full four stroke cycle, simulating the inlet valve movement, the piston movement and the exhaust valve movement. The computer simulation predicted the emission of carbon dioxide (CO₂) at the exhaust port, after combustion.
2.2 Research directions on controlled auto-ignition engines

The increasing price of fuel and constant revision of the emission standards has led the vehicle industry to search for alternatives to SI and compression-ignition (CI) engines. CAI engines have recently received increased attention from researchers. Compressing a homogeneous mixture of air and fuel to the point of auto-ignition can reduce engine emissions and increase engine efficiency. CAI engines have the potential to replace conventional combustion variants such as SI and CI, to match the revised European emission standards. Low nitrogen oxides (NOx) and particulate matter (PM) emissions along with CI-like efficiencies are the main features of CAI engines. However, the main drawbacks of CAI engines are auto-ignition control and the high energy release rate, which restricts CAI operation, range and speed. Many investigations conducted on CAI engines have aimed to understand the mechanisms of auto-ignition, using experiments or computational models to study the different variables, which can affect ignition and combustion. Other studies have investigated methods to improve the control, emissions and load and speed limits of CAI engines.

2.2.1 Experimental work conducted on controlled auto-ignition engines

Numerous experiments conducted on CAI engines aimed to study different variables, principles and combustion mechanisms, in order to understand auto-ignition further. Studies have utilised the use of fluorescent additives in fuel, to reveal additional findings during combustion. For instance, Kim and Ghandhi (2005) [24] reported laser-induced fluorescence results, for CAI combustion under light-load, using formaldehyde for n-heptane fuel. The experimental work utilised an optically accessible single-cylinder running at 600 rpm and 1200 rpm. The third harmonic of a laser excites the fluorescence of formaldehyde. The formaldehyde is shown to be dependent on local thermodynamic conditions but reaches a stable value at high temperature and pressure. At low equivalence ratios, the fluorescence persists late into the expansion stroke, after the entire heat release rate (HRR) is completed. The same results are demonstrated by Schrewe and Ghandhi (2007) [25]. They conducted a study on near-wall, formaldehyde planar laser-induced fluorescence measurement of CAI combustion. The measurements are made within 400 μm of the wall. Nygren et al. (2002) [26] studied the fluorescence of fuel distribution inside a CAI engine using a three-dimensional laser. A high-speed detection system
allowed the collection of images before combustion. The occurrence of multiple isolated ignition locations shows that CAI combustion relies on distributed reactions, rather than flame propagation. Griffiths et al. (2002) [27, 28] conducted some experiments using a rapid compression machine (RCM), to investigate the origins of engine knock for CAI engines. High-resolution pressure records, combined with an image intensifier, allowed the chemiluminescence to reveal knock occurrence. The study showed inhomogeneities prevail in the non-knocking reaction. In the case of engine knock, the image recording shows the formation of a blue flame, rather than a normal incandescent hot flame.

Measurement techniques such as LDA and PIV, are sometimes used to analyse the flow field or combustion inside engine cylinders. For instance, Pitcher et al. (2003) [29] carried out an experimental comparison of the flow fields in SI and CAI using LDA, to understand the differences between engine modes. Using the same experimental optical engine, for the SI and CAI modes, the valve strategy used for both cases was different; an early closing of the valves retained the exhaust gases for the next cycle in CAI mode while standard valve timing was used in SI mode. The study examined the vector fields, turbulence kinetic energy (TKE), vorticity and tumble ratio differences, between the two valve strategies. The results highlight the difference of tumble motion behaviour and motion centres, caused by a smaller valve lift magnitude, hence, higher velocities. Panao and Moreira (2007) [30] investigated the influence of the fuel spray characteristics, on the quality of the air-fuel mixture, for fuel-port injected engines. Using particle Doppler anemometry (PDA) measurements of droplet dynamics, the experimental work managed to quantify the fuel evaporation depending on the heat transfer. The results show that to obtain an improved fuel evaporation and mixture quality, the heat transfer regime needed to be close to the overall critical heat flux. Above this critical point, the interaction between successive injections deteriorated the mixture quality.

Other techniques have been used in various investigations, in order to increase the knowledge database of auto-ignition. For example, Mattison et al. (2007) [31] developed a diode laser absorption sensor, to measure in-cylinder parameters in CAI engines. The range of the sensor used, allowed the measurement of temperature from 300 K to 1700 K and pressure from 1 bar to 55 bar, for both motored and fired engine modes. It can
measure microsecond time-resolved data with a maximum error of 5 %, and also has the ability to sense the water concentration changes during the combustion process. The same technique can be applied to measure additional cylinder parameters such as temperature distribution, CO\textsubscript{2} emissions or carbon monoxide (CO) concentrations. Mehresh et al. (2005) [32] developed an ion-sensor, to study the combustion timing of a CAI engine running on propane. The sensor measurements were also able to capture the cyclic variations. Using the experimental data, a numerical model with a detailed chemical kinetic was developed, to further analyse the effects of the equivalence ratio and intake temperature, on the ion signal. A stronger ion signal was recorded for higher inlet temperatures or an increased equivalence ratio. The results show that due to the low temperature and high pressure of the CAI combustion, the nitrous oxide (N\textsubscript{2}O) mechanism contributes significantly, to the total production of NO\textsubscript{x}. Kim et al. (2002) [33] conducted a spectral analysis of a typical homogeneous charge compression-ignition (HCCI), compared to a stratified charge compression-ignition (SCCI) and a standard SI at an engine speed of 1000 rpm. In order to demonstrate the differences in the combustion processes, a detailed spectrum was obtained for each case. Compared to the SI, a cool flame region was measured for the HCCI. The SCCI demonstrated two cool flame regions. For HCCI, the cool flame region was found to be 12 CAD in front of the main hot flame, while being 10 and 5 CAD for the SCCI two cool flame regions. Using combustion measurements, Shibata et al. (2004) [34] studied the effect of the research octane number (RON) on auto-ignition of a supercharged CAI engine. The RON of the fuel mixture was obtained by adding n-heptane to the base fuel blend. The results have shown that the low-temperature heat release depends on the fuel characteristics. Despite fuels with a high RON being resistant to engine knock and appropriate for HCCI operations, the study shows misfires are produced at higher engine speeds, due to the late high-temperature heat release. The study was later extended by Shibata et al. (2005) [35] to 12 different blends of gasoline. It was found that n-paraffin and isoparaffin resulted in a large low-temperature heat release (LTHR) value. On the other hand, benzene, naphthenes and olefins have been found to reduce the LTHR. The measurements of two fuels with different blends, but the same RON, can have significant differences in the heat release pattern. It is mainly due to the effect of some of the species of the blend of gasoline on the LTHR. Again, the work was extended by Shibata and Urushihara (2006) [36] for
23 experimental blends of fuel, under heated air intake conditions, at an engine speed of 1000 rpm. The results show that peroxide (H₂O₂) was produced and accumulated during the LTHR reactions. The high-temperature heat release (HTHR) starts earlier with rich n-paraffin fuel, which improves performance comparative to other fuels. Also, the heating of the intake air has shown to reduce the intake charge mass, and hence, the injected fuel quantity, which reduced the indicated mean effective pressure (IMEP). Mack et al. (2007) [37] prepared an experimental method to gain further knowledge of the combustion characteristics of fuel blends, using ¹⁴C isotope tracers. Results show that ethanol (EtOH) burns faster with the addition of diethyl ether (DEE) or di-tert-butyl peroxide (DTBP). The temperature required for auto-ignition is shown to decrease significantly, with the addition of DTBP for all fuel blends. Dayma et al. (2007) [38] investigated the oxidation of methanol. The study concluded that the oxidation of methanol is due to the nitric oxide (NO) being converted to nitrogen dioxide (NO₂) by hydroperoxyl (HO₂). The additional production of hydroxyl (OH) from the oxidation of NO by HO₂ promotes the oxidation of the fuel. A detailed kinetic model was conducted and demonstrated reasonable agreement with the experimental data. Based on experimental measurements, Aichlmayr et al. (2003) [39] validated a detailed chemical kinetics model, to increase the knowledge of small scale HCCI engines. The minimum engine bore and stroke, for CAI operations, were found. Ando et al. (2003) [40] investigated the auto-ignition characteristics of natural gas mixtures, using a rapid compression and expansion machine. A chemical kinetics model was combined with CFD code to further support the findings. The results show that initial temperature and density, influence auto-ignition timing. For natural gas mixtures, a temperature higher than 1000 K is needed for a complete combustion. Lu et al. (2005) [41] investigated the differences of ignition timing, burn duration, cyclic variations and emissions, between the primary-referenced fuels (PRFs). Four blends with different concentrations of iso-octane and n-heptane were studied. For the first-stage combustion (at low-temperature reactions (LTR)), an increase in the mixture octane number will delay the ignition, reduce the peak of the HRR and increase the cylinder pressure and temperature. The experimental results show that the first stage combustion characteristics are highly dependent on the concentration of n-heptane in the mixture. For the second stage combustion, the combustion duration decreased with higher equivalence ratios and a lower octane number. The cyclic variations decreased with higher octane
number mixtures. The NOx emissions increased significantly when the equivalence ratio exceeded a critical value of 0.3. Lu et al. (2005) [42] also investigated the effects of cooled exhaust gas re-circulation (EGR), intake charge temperature, coolant temperature and engine speed on CAI combustion of an iso-octane and n-heptane mixture. The results demonstrated that an increase of EGR delayed the first-stage and second-stage combustions while extending the combustion duration. EGR has shown lower effects on the CO and hydrocarbons (HC) emissions with low RON mixtures. For mixture above RON25, the CO and HC emissions were significantly increased. The ignition timing was advanced and the combustion duration shortened with an increase of the intake charge temperature, an increase of the coolant outlet temperature or a decrease of the engine speed. The intake charge temperature has shown the highest influence on combustion characteristics.

2.2.2 Numerical work conducted on controlled auto-ignition engines
On the other hand, when the use of experimental work is not practical or is time-consuming, computational calculations can be conducted on CAI engines to study the combustion mechanisms, processes and engine parameter influences in a reduced amount of time, when compared to the experimental equivalence. Some of the numerical studies aimed to predict the emission levels, using chemical kinetics software packages. To achieve this goal, several methods can be used. The single zone model considers a unique zone of temperature and species concentration for the calculations. For instance, Sandia National Laboratories (2003) [43] used a single zone model to visualise the rise of emissions in the case of incomplete combustion. Using a very lean mixture, as the equivalence ratio is decreased from 0.26 to 0.1, the combustion efficiency reduces from 95 % to 51 %. The results show that it was caused by insufficient temperature to initiate the CO to CO\textsubscript{2} reactions before expansion. This study showed that the combustion efficiency at low-load could be improved by stratifying the charge with a higher concentration of fuel in the centre of the cylinder. In practice, this can be achieved by injecting the fuel later during the cycle, so that it reduces the mixing duration prior to combustion. Using a late injection of - 70 CAD before TDC firing (BTDCF), the combustion efficiency was improved from 51 % to 78 % with very low NOx emission of 1 g per kg of fuel. Yamasaki and Iida (2001) [44] conducted a study on CAI engines using
butane. Butane has shown a two-stage auto-ignition like heptane, an LTR and a high-temperature reaction (HTR). Different parameters are varied to demonstrate their influence on the LTR and HTR. The calculations used a detailed chemical kinetics model of 161 species and 461 reactions to predict the rate of heat release with LTR and HTR accurately. It was demonstrated that the timing is advanced and the combustion duration is shorter by increasing the initial temperature, pressure, or reducing the CO₂ concentration. For high combustion efficiency, the maximum temperature inside the cylinder was kept above 1500 K. Similar results for the low and high-temperature rates were found with the chemical kinetics model of hydrocarbon developed by Westbrook (2000) [45].

Another method to increase the accuracy of the emission level, or the auto-ignition calculations, is called the multi-zone model. It considers multiples zones of mixture and temperature for the calculations. For example, Aceves et al. (2002) [46] developed a multi-zone chemical kinetic model to calculate the CO and HC emissions. Different piston crevice geometries were studied using a removable piston crown. Using a 4-cylinder turbocharged direct injection (TDI) Volkswagen engine converted to HCCI mode, the multi-zone model was validated with exhaust emission measurements. Komninos et al. (2007) [47] also developed a multi-zone model to examine the effects of various engine parameters on performance and emission levels. Parameters such as the compression ratio, the equivalence ratio, the initial temperature, the initial pressure and the engine speed have shown variations of the hydrogen auto-ignition timing. The study showed that an increase of the compression ratio (CR) or the initial mixture temperature advanced the hydrogen auto-ignition timing and increased the NOₓ emissions. These parameters were adjusted to delay the ignition after TDC and therefore, improve the efficiency as it increased the work during the expansion stroke. Increasing the equivalence ratio and initial pressure have been found to increase the engine load, as the indicated mean effective pressure was increased linearly. In this work, increasing the engine speed has been found to increase the efficiency, as it delayed the ignition of hydrogen. Flowers et al. (2002) [48] calculated the CO and HC emissions for iso-octane CAI combustion by conducting multi-zone simulations. Three cases have been studied for a different number of chemical kinetic zones of 10, 20 and 40 using a fully detailed chemical kinetic
mechanism of 859 species and 3606 reactions. For an iso-octane fuelled CAI engine, the study concluded that 10 zones are enough to resolve the HC emissions but 40 zones are required to solve CO emissions. Zheng and Yao (2006) [49] studied the chemical kinetics reaction of n-heptane for CAI combustion. Using a detailed chemical kinetics model with 544 species and 2446 reactions, the study investigated the two-stage auto-ignition of n-heptane: the heat release at the LTR at 750 K and the HTR at 1000 K. HTR can be separated into a blue flame reaction stage followed by a hot flame reaction stage. Four regions for CAI combustion were identified: a complete combustion region, a high CO emissions region, where low-temperature reaction and blue flame reaction occur, a high formaldehyde (CH$_2$O) emissions region, where only low-temperature reactions occur, and a misfire region. Cook et al. (2007) [50] developed a multi-zone model, which considers different zones of enthalpy. The model was developed to calculate the auto-ignition of HCCI engines when thermal inhomogeneities are used to reduce the maximum heat release rate. The model was found to be able to detect spontaneous ignitions and deflagrations.

Other methods consist of coupling software packages such as the chemical kinetics model, surface treatment and CFD to obtain a more detailed multi-zone model. For instance, Zeng et al. (2007) [51] conducted a computational study on CAI combustion by coupling two software packages. A detailed chemical kinetics model of 53 species and 325 reactions was considered for the oxidation mechanism of methane. CHEMKIN was used as a chemistry solver and DETCHEM as a surface reaction solver. The two software packages were integrated into the KIVA-3V code for CFD simulations. The study focused on the differences between the two-dimensional (2D) single-zone model, a 2D six-zone model and a three-dimensional (3D) model. Because of the uniform temperature, pressure and composition assumptions, the 2D single-zone model over-predicted the temperature and NOx emissions. The 2D six-zone model was found to predict accurately the HC, CO, and NOx emissions but did not take into account the flow field. In this study, the 3D model was found to be more accurate for emission calculations while considering the flow field but took the longest computing time. Fiveland et al. (2000) [52] studied the coupling of a CFD software package with a chemical kinetics model for natural gas and hydrogen combustion in a CAI engine, using 11 species and 23 reactions, and 53 species
325 reactions, respectively. The study concluded on the importance of coupling the chemical kinetics model with CFD to increase the accuracy of the calculation for the gas exchange and turbulent heat transfer. Song-Chaung et al. (2003) [53] implemented a chemical kinetics code into the CFD calculations to study. The computational time was found to be highly dependent of the mesh size. The study found that a coarse mesh could predict a premixed HCCI combustion in the main volume of the cylinder with the same level of accuracy as a fine mesh. However, the piston ring crevice in the model needed to be defined with a fine mesh for an accurate calculation of the emissions. The study found high levels of HC and CO emission near the piston bowl region and the vicinity of the cylinder, mainly due to the poor combustion quality. Colin et al. (2005) [54] developed a new auto-ignition model coupling a detailed chemical kinetics model to a CFD model to include the low-temperature phenomena. Hence, the cool flame ignition delay, the cool flame fuel consumption and the reactions between the cool flame and the main ignition were studied for n-heptane. Soylu (2005) [55] examined the combustion characteristics of natural gas using detailed chemical kinetics. The study highlighted that if the mixture energy was released for a short duration at TDCF, the cylinder pressure may exceed the design limit due to the cylinder volume being at its minimum. The author suggested multiple methods to control auto-ignition, while maintaining a high efficiency, such as variable valve timing, variable compression ratio, using a varying mixture of natural gas and propane. Increasing the equivalence ratio using a supercharger has shown to increase the IMEP. However, the study has shown that increasing the EGR fraction reduces the efficiency and the IMEP. Ryu et al. (2005) [56] conducted a CFD study of spray structure and evaporation characteristics of high-pressure injectors for CAI. The VECTIS commercial engine CFD code is used and the results are compared to the experiments. The study revealed the uniform distribution of fuel when using early injection. However, when injected later during the stroke, the fuel concentrates in the bowl zone. The fuel evaporation is sensitive to the influence of intake temperature and pressure. Choi and Chen (2005) [57] proposed a fast prediction model to predict the start of combustion for CAI engines. The computed ignition delay data by SENKIN code is used for the training of artificial neural networks (ANN). A typical run of the ANN takes around 30 ms and gives an average error of 5 %. Jia et al. (2008) [58] studied the effect of early injection on wall spray. After reviewing all the spray/wall interaction models available, the study
described three well-developed models: Bai and Gosman (BG), O'Rourke and Amsden (OA), Han, Xu and Trigui (HXT). Using the KIVA-3V code with a gas pressure of 15 bar, the three models were compared for wall spray radius, mean diameters and droplet tangential velocity. While all three models under-predicted the wall spray radius, the HXT predictions were found to be in better agreement with the experiments than the other two models, mainly due to the gas density consideration. Good results were shown for the BG and HXT models for droplet tangential velocity.

Numerous investigations studied the reduction of the amount of species and reactions considered in the chemical kinetics model, to reduce the computational time necessary for the calculations. Developed from a fully detailed chemical kinetics model, the reduced chemical kinetics model takes into account the main species and reactions for the given fuel oxidation mechanism. For instance, Su and Huang (2005) [59] worked on the development of a reduced chemical kinetic model of n-heptane. The model contains 40 species and 62 reactions and shows the well-known two-stage ignition characteristics for n-heptane. Compared to the expanded model including 544 species and 2446 reactions, the computational time is reduced to 1/1000th of the time with the use of the reduced model. He et al. (2005) [60] conducted a study on iso-octane auto-ignition and ignition delay. A rapid compression facility (RCF) was used to obtain the experimental data over a range of pressures, temperatures, EGR, equivalence ratio and oxygen fraction. The equivalence ratio was found to have a strong effect on ignition delay. Using those results, a new formula for ignition delay of iso-octane was presented. For the numerical work, three chemical kinetics models were compared to the measurements to evaluate the performance of a detailed, reduced and skeleton mechanism. It was found that the detailed chemical kinetics model reproduced the experimental results when the oxygen fraction was close 0.22. The reduced chemical kinetics model performed well when the oxygen fraction was close 0.13. Jia and Xie (2006) [61] proposed a new reduced chemical kinetics model for the auto-ignition of iso-octane. Reduced to 38 species and 69 reactions, the model has been shown to calculate HC, CO and NOx emissions accurately. The model was reduced to a single zone, which reduced the computational time considerably. Maroteaux and Noel (2006) [62] proposed a further reduction of n-heptane oxidation mechanism. From a detailed mechanism of 130 reactions, a reduced mechanism with 37
species and 61 reactions was proposed. The model was then further reduced to 25 species and 26 reactions using sensitivity analysis and steady state approximations. Lova et al. (2002) [63] developed an automatic method to reduce chemical mechanisms. The method used quasi-steady-state assumptions and computed the steady-state species concentration by algebra rather than differential equations. A full mechanism with 53 species was reduced to 14 non-steady state species. Shaver et al. (2006) [64] simulated the transition of a CAI engine to a conventional SI engine mode. Using exhaust re-induction and variable valves actuation (VVA) for controlling auto-ignition, the simulations show good results when compared to the experimental engine results. The model calculates the combustion timing, in-cylinder pressure and exhaust temperature at steady and transient states. The model could be used to develop controllers for CAI transition modes. Tanaka et al. (2003) [65] proposed a reduced chemical kinetics model for CAI of PRF. With 32 species and 55 reactions, the model was validated against the experimental cylinder pressures. However, the study demonstrated that the combustion was highly dependent on the octane number and initial pressure. The second oxygen addition and the olefin formation reactions determine the energy release and the ignition delay during the first stage. The temperature at the end of the first stage reactions was found to increase as the octane number decreases. Hernandez et al. (2007) [66] developed a diesel fuel surrogate model for CAI engines by merging the kinetics mechanisms of n-heptane and toluene. The model was validated by experimental data and found to be composed of 50 % of n-heptane for 50 % of toluene. High EGR quantities have shown to decrease the n-heptane/toluene reactivity.

Finally, less common types of combustion models are the stochastic reactor model (SRM) and the partially stirred plug flow reactor (PaSPFR) model, which considers local quantities such as mass fractions and temperatures to be variables. The PaSPFR model also accounts for the fluctuations of the local quantities. For instance, Bhave et al. (2006) [67] carried out a numerical analysis for the source of CO emissions. Using a probability density function (PDF) in an SRM, the calculations have shown that the CO emissions were dependent on the fluid-wall interactions, the mixing of hot and cold air-fuel particles and the wall temperature. The inhomogeneities during the compression stroke have been found to alter the ignition timing and the rate of formation of CO. Su et al. (2006) [68]
presented a new SRM based on a PDF for CAI engines with direct injection (DI). The study found that the computational time increased rapidly when considering all the gas exchange processes. A method was proposed to reduce the amount of particle studied using a sample procedure, which reduced the computational time by a factor of eight. The study also investigated the error of using such a method. The calculations demonstrated that no error was accumulated for multiple cycles. Maigaard et al. (2000) [69] studied the effects of inhomogeneities in CAI engines. The authors developed a new PaSPFR model, with a detailed chemical model for natural gas of 53 species and 590 reactions, by defining crevices and thermal boundary layers, colder zones have been found close to the crevices. The model has shown a better agreement than the previous models when compared to the experimental work. The results revealed that the ignition delay is a function of the turbulent mixing of the hot bulk and a colder boundary layer. Kraft et al. (2000) [70] validated a PaSPFR model with interaction by exchange with the mean mixing model (IEM). The model was found to be capable of simulating inhomogeneities and showed good results for CO and HC emission calculations. However, the calculations were found to under-predict the results by 40 % when compared to the experimental values.

2.2.3 Improving the control of auto-ignition for controlled auto-ignition engines

Most of the experimental and computational studies conducted on CAI engines aim to understand the variation of the auto-ignition timing, depending on the properties of different fuels, when compressed to the point of auto-ignition. Changing the engine variables, such as the inlet pressure, intake temperature and CR can increase the database of the fuels properties in order to extend auto-ignition control. In addition, cooled EGR can be added to the mixture to dilute the charge and postpone auto-ignition. This method was used by Yap et al. (2006) [71] to study the effect of adding hydrogen to natural gas for CAI combustion. An electric air heater was used to preheat the air charge prior to the methane entry port. In addition, a reformed exhaust gas recirculation (REGR) loop mixing fresh charge and part of the EGR was implemented to the intake of the system. Hydrogen addition was found to advance the start of auto-ignition for a given intake temperature. This implies that the intake temperature required for stable CAI operation could be lowered to obtain the same auto-ignition timing. Aichlmayr et al. (2002) [72] modelled a
10 W miniature free-piston CAI engine using detailed chemical kinetics. The investigation aimed to find the conditions necessary for auto-ignition inside small-scale engines, as the current knowledge based on CAI conventional size engines is not applicable to miniature engines. Small-size engines generally run at much higher speeds, can have compression ratios up to 30:1 and have large surface area to volume ratios which will affect heat transfer rates. The study generated new operational maps for small-scale engines in CAI mode for variables such as the compression ratio, the aspect ratio of the cylinder (bore/stroke ratio), the intake and combustion peak temperatures. Kelly-Zion and Dec (2000) [73] conducted a computational study on CAI engines for two fuel types, n-heptane and iso-octane. The study used a single-zone chemical kinetics model, which treats the air-fuel charge as a single-zone with uniform composition. The study investigated the effects of varying the fuel equivalence ratio (defined as fuel to oxidiser ratio divided by the stoichiometric fuel to oxidiser ratio), the CR, the engine speed and the amount of cooled EGR on the auto-ignition timing. An illustration of the CR effects on auto-ignition timing for n-heptane and iso-octane is presented in Figure 2.15. The ignition of n-heptane is seen to occur in two stages, the first stage starting at a temperature of around 800 K. For the iso-octane, a single-stage ignition is starting at a temperature of around 1100 K. The CR has shown a high variation of the auto-ignition timing for both fuels.
Figure 2.15 Effects of the compression ratio on cylinder gas temperature for
(a) n-heptane and (b) iso-octane [73]

High variations of the auto-ignition timing have also been demonstrated between six engine speeds ranging from 600 rpm to 3600 rpm for both fuels as shown in Figure 2.16.
Figure 2.16 Effects of the engine speed on cylinder gas temperature for
(a) n-heptane and (b) iso-octane [73]

The effect of EGR was also investigated in this study. The amount of cooled EGR has
been found to have less effect on iso-octane than on n-heptane as shown in Figure 2.17.
For both fuels, when 50 % EGR is contained within the mixture, the CR or the intake
temperature needs to be increased to obtain the same auto-ignition conditions when compared to the mixture without EGR.

Figure 2.17 Effects of the exhaust gas recirculation on cylinder gas temperature for (a) n-heptane and (b) iso-octane [73]
The fuel equivalence ratio has also demonstrated fewer variations of the auto-ignition timing on iso-octane than on n-heptane as shown in Figure 1.4 of Chapter 1. The study has demonstrated that the auto-ignition timing is highly sensitive to the fuel type. Fuels with a single-stage ignition, like octane, have shown advantages for control over two-stage ignition fuels, like heptane. Further, iso-octane presents the advantage of using a higher CR limit, which provides the potential for a high, diesel-like, engine efficiency.

Other studies retain residual gases, also called internal exhaust gas recirculation (IEGR), from the previous cycle to the next, to control auto-ignition by using shorter valve lift durations. Milovanovic et al. (2004) [74] investigated the influence of valve timing on the control of CAI engines. Different values of residual gases were obtained by varying the valve timings. The experimental cylinder pressure, temperature, IMEP and brake specific fuel consumption (BSFC) were obtained using a variable valve train system. The study showed that the variable valve timing strategy had a strong influence on auto-ignition. EVC and IVO have shown the strongest effect on auto-ignition while EVO and IVC have been found to have minor effects. A study conducted by Chen and Milovanovic (2002) [75] investigated the effects of the residual gases on CAI engines fuelled with methane (CH\(_4\)). CH\(_4\) has a very high octane number of 120, which makes it resistant to auto-ignition. Furthermore, methane is the most stable hydrocarbon fuel and its chemical kinetics is well developed, with only 53 species and 325 reactions, it made the computational cost acceptable. It was found that the overall effect of increasing the retained residual gases within the cylinder advanced the auto-ignition, as shown in Figures 2.18, due to the overall temperature increase of the mixture.
Figure 2.18 Cylinder pressure trace data for controlled auto-ignition with different quantities of retained residual gases [75]

Studying the isolated effect of the main species contained in the residual gases, it was found that increasing the nitrogen (N$_2$) amount within the mixture has a small effect on delaying auto-ignition, but had a moderate effect on reducing the HRR peak and extending the HRR duration due to the dilution effect, as shown in Figure 2.19.

Figure 2.19 Isolated effect of nitrogen on the heat release rate [75]
Increasing oxygen (O₂) was found to have a small effect on advancing the auto-ignition and had no effect on the HRR peak or duration as seen in Figure 2.20.

Figure 2.20 Isolated effect of oxygen on the heat release rate [75]

Increasing the quantity of CO₂ or water (H₂O) in the mixture greatly delayed the auto-ignition, but had small effects on reducing the HRR peak and extending the HRR duration as shown in Figures 2.21 and 2.22.
Osei-Owusu et al. (2007) [76] conducted a numerical investigation on the auto-ignition of gasoline for CAI engines. The study investigated the effects of engine speed on auto-ignition for various quantities of residual gases retained in the mixture. Considering the full operating range of the engine (all engine speeds), the study identified three distinct zones for ignition of the residual gases ranges. In zone 1, auto-ignition occurs for residual gases ranging from 36 % to 41 %. In zone 2, with residual gases ranging from 41 % to
46 %, auto-ignition can occur. It signifies that ignition assistance is preferred for this zone. For zone 3, with residual gases higher than 46 %, pure auto-ignition occurs without the need of any ignition assistance. Babajimopoulos et al. (2003) [77] demonstrated the dominance of the temperature factor for the ignition timing using a KIVA-3V single-zone model. The study concluded that at high residual gases levels, the mixture composition is not homogeneous. This leads to a composition stratification that has significant effects at TDCF. Yap et al. (2005) [78] investigated the residual gases trapping method for CAI operations fuelled with propane. Due to the high RON of propane (112), the application required an increase of the compression ratio combined with inlet charge heating and residual gases trapping to achieve auto-ignition. It was found that increasing the compression ratio decreased the charge temperature requirements, but led to higher pressure rise rates. Varying the inlet valve timing has been shown to help reduce the maximum pressure rise rates. The results demonstrated low NOx emissions due to the nature of CAI combustion.

Some studies investigated methods to improve the control of CAI engines by supercharging, turbocharging and controlling the intake charge temperature. For instance, Canakci (2007) [79] conducted experiments on the effects of boost pressure on the performance and the emissions of a direct injection controlled auto-ignition (DI-CAI) engine. A heavy duty diesel engine was converted into CAI mode with gasoline direct injection. For the same equivalence ratio and intake charge temperature, three different intake charge pressures were tested for different speeds. To keep the same equivalence ratio for all intake pressures, the quantity of fuel injected was increased for higher intake pressures, as more air was present in the charge. The results have shown that the engine torque increased with higher boost pressure but decreased as the engine speed increased. The exhaust temperature increased with higher engine speeds but decreased with higher boost as the start of ignition (SOI) was advanced. The combustion efficiency increased with engine speed. However, CO and NOx emissions increased with higher engine speeds for each pressure tested. HC emissions have shown to decrease with engine speed. Christensen and Johansson (2000) [80] studied a supercharged CAI single cylinder engine fuelled with natural gas and iso-octane as a pilot fuel. High quantities of EGR were used to extend the combustion duration. The authors demonstrated that the load limit for
auto-ignition can be extended when using supercharging combined with EGR without increasing the maximum cylinder pressure. The highest gross IMEP was found to be 16 bar with an inlet boost pressure of 1.5 bar, 48 % EGR, a near-stoichiometric mixture and a CR of 17.2:1. For this case, the gross indicated efficiency was found to be 46 %. The highest gross efficiency was found to be 51 % with a boost pressure of 1.1 bar, a CR of 23.8:1 and 62 % EGR. However, the cylinder peak pressure rose from 170 bar to 190 bar between the two cases. The HC emissions were decreasing with increased EGR rate and engine load. The NOx emissions were under 0.04 g/kWh for a gross IMEP of 16 bar. Gharahbaghi et al. (2006) [81] compared the emissions and the fuel economy between a supercharged and a naturally aspirated (NA) CAI engine at 1500 rpm with retained residual gases. The supercharger has shown to be efficient in producing the excess of air needed for lean combustion. Delaying the exhaust valve timing has shown an improvement of the load limit but also an increase of NOx emissions. Furthermore, supercharging the engine has shown to increase the fuel consumption. A smaller supercharger with a moderate boost should be used to reduce the fuel consumption penalty. Hyvönen et al. (2003) [82] investigated the different boosting strategies for a multi-cylinder CAI engine to extend the operating load limit at 2000 rpm. A comparison between NA, mechanical supercharger and turbocharger was conducted. When the engine was running without any load, it was found that throttling the intake air increased the combustion efficiency from 70 % to 90 % and decreased the fuel consumption. Hence, the additional pumping loss created by the throttle valve was compensated by the improvement of the combustion efficiency. High maximum loads and brake efficiencies were found with a turbocharger when compared to a mechanical supercharger. This was mainly due to the large amount of parasitic losses of the supercharger. The maximum load achieved with the turbocharger, was found to be a brake mean effective pressure (BMEP) of 10 bar.

Other studies investigated the variation of the intake charge temperature to control auto-ignition. For example, Hyvönen et al. (2006) [83] conducted experimental comparisons of three multi-cylinder CAI engines with different cylinder displacements: a 5-cylinder 1.6 L engine, a 4-cylinder 2 L engine and a 6-cylinder 11.7 L truck engine. The comparisons were conducted at an engine speed of 2000 rpm, with all engines
running on RON91 gasoline. An additional engine speed of 1000 rpm was tested for the truck engine. The auto-ignition timing was controlled by varying the intake charge temperature. The 6-cylinder truck engine has shown to have the highest combustion efficiency (93 – 96 %) compared to the other two engines (90 %). At a BMEP of 2 bar, the highest brake efficiency was found to be 32.3 % for the engine running at 1000 rpm.

2.2.4 Improving the load limit of controlled auto-ignition engines

Numerous studies evaluated methods and strategies to extend the heat release duration in order to improve the CAI load limit. For instance, Huang et al. (2004) [84] investigated the use of a spark plug to extend the operation limits of a CAI engine fuelled with highly diluted n-butane mixtures. The diluted charge was able to support the propagating flame for most of the operating conditions. The study found that the dilution was too high at light load or idle conditions for the spark to have an effect on combustion, but it could still be used to prevent misfires from occurring. Other studies investigated techniques to create a stratification of the charge by using a dual-fuel injection. For instance, Wang et al. (2006) [85] combined a CFD software package to a chemical kinetics code for iso-octane, which considered 89 species. The model was developed to study the injection strategy and has been found to successfully predict the turbulences, emissions and combustion. Using a three-stage calculation, the chemical reactions were coupled to the CFD code only between 320 CAD and 390 CAD as shown in Figure 2.23, TDCF occurring at 360 CAD. The rest of the CFD calculation was computed without the use of the chemical kinetics mechanism. The investigation demonstrated that a homogeneous charge can be realised by using single fuel injection. Hence, by adding a different fuel in the middle of the compression stroke as second fuel injection, a stratification charge can be obtained, which improved the load level and advanced the ignition.
Sjoberg and Dec (2007) [86] conducted a study on late-cycle combustion stability for a single and a two-stage ignition. The single-stage ignition fuel was 100 % iso-octane while the two-stage ignition fuel blend was composed of 80 % iso-octane and 20 % n-heptane. The results demonstrated a decrease of the cylinder pressure peak and an increase of the heat release duration when the combustion was delayed after TDCF, which would increase the load limit for CAI operations. However, the cyclic variation has shown to increase as the auto-ignition was delayed into the early stage of the expansion stroke for the two fuel blends. When compared to the fuel blend composed of 80 % iso-octane and 20 % n-heptane, the 100 % iso-octane blend demonstrated higher cyclic variation. An excessive auto-ignition delay has shown an increased risk of partial-burn or misfires. The partial-burn had different effects on the two fuel blends. The 100 % iso-octane blend demonstrated an increased reactivity for the next cycle. However, the PRF80 did not show an increase of reactivity due to the blend being already more reactive than the 100 % iso-octane blend.
Numerous studies have been carried out to investigate the improvement of CAI load range by using fuel additives. For instance, Tanaka et al. (2003) [87] investigated the auto-ignition timing and the heat release rate for pure hydrocarbon fuels with additives using an RCM. A two-stage ignition with a short ignition delay was found for fuels with a \(-\text{CH}_2\text{-CH}_2\text{-CH}_2\)- structure. For these fuels, the auto-ignition was highly dependent on the energy release during the first stage ignition. For fuel blends with n-heptane and iso-octane, the auto-ignition was found to be a function of the ratio of oxygen to n-heptane and was independent of the RON. A reduction of the ignition delay was found with additives without any effect on the heat release rate. The study concluded that the ignition delay and the heat release rate can be independently controlled by selecting the fuel blend and the additive. Yamada et al. (2005) [88] studied the effects of methanol and ozone when used as additives for combustion of dimethyl ether (DME). The investigation revealed that methanol delayed the ignition by up to 15 CAD at an 8 % addition to DME. Ozone addition advanced the ignition timing by up to 20 CAD at only 0.015 % to DME. The temperature of the flame has been shown to reduce by 70 K and the reaction chain duration was extended. Shudo and Yamada (2007) [89] also conducted a study on the addition of hydrogen to delay the auto-ignition of DME. In this study, hydrogen was demonstrated to be an effective way of controlling combustion. Hydrogen addition increased the heat release duration and delayed the temperature rise during the oxidation of DME. Hydrogen addition has been shown to prevent early ignition and could be used to allow higher load operations for CAI. Dubreuil et al. (2007) [90] performed experiments for mixtures of pure n-heptane, n-heptane and iso-octane, and n-heptane and toluene. The study investigated the effects on the ignition timing of adding nitric oxide (NO) to the EGR. The EGR quantity in the mixture was varied from 0 % to 50 % with the addition of NO between 0 and 500 parts per million volume (ppmv). The intake temperature was maintained at 350 K and the equivalence ratio kept at 0.3. A single zone model with detailed kinetic was developed to confirm and rationalise the experimental results. EGR has been shown to delay the cool flame and main flame timings. The results showed that the addition of 100 ppmv of NO has a maximum effect on the cool flame timing, which had an equivalent effect as 50 % of EGR. In this case, the cool flame timing was delayed by 2 CAD. For an addition of 100 ppmv of NO, the EGR has been found to have twice the effect on the main flame delay than NO addition. Yeom et al. (2007) [91]
conducted experiments on liquefied petroleum gas (LPG) and gasoline for CAI exhaust emissions. Using variable valve timing (VVT) and DME addition, the study investigated the effects of intake valve timing and fuel injection quantity on the exhaust emissions. The CO$_2$ emissions were found to be reduced when using LPG when compared to gasoline. The CO$_2$ emissions were further reduced as the inlet valve opening (IVO) was delayed. However, CO and HC emissions have shown to increase as the IVO was delayed. Due to a later combustion, the CO and HC emissions were found to be higher for LPG when compared to gasoline. Xingcai et al. (2006) [92] conducted an experimental study on the auto-ignition of a mixture of n-heptane with the addition of ethanol. The ethanol concentrations in n-heptane were ranged from 0 % to 50 %. The experiments were conducted on a single-cylinder CAI engine at a constant speed of 1800 rpm with port injection. The addition of ethanol demonstrated an increase of IMEP from 3.38 bar to 5.1 bar. The thermal efficiency has also shown to increase at high engine load but deteriorated at light load. With the addition of 20 % to 50 % of ethanol in the mixture, the ignition was gradually delayed due to the high RON. Very low HC emissions were recorded for mixtures containing between 0 % and 30 % of ethanol. However, the HC emissions increased significantly for mixtures containing between 40 % and 50 % of ethanol. For both fuels, the CO emissions were both high for moderate engine loads but decreased for high and low load operations. The n-heptane mixtures have shown low cyclic variations, which increased with the addition of ethanol. Kong (2007) [93] studied the CAI combustion of natural gas and dimethyl ether mixtures using CFD calculations with detailed kinetics. The chemical kinetics model contained 83 species and 360 reactions and produced good results for the combustion and the NOx emissions. The study demonstrated that ignition was achieved by DME oxidation, which in turn led to the combustion of the natural gas. Also, a larger amount of DME in the mixture reduced the peak of heat release. Mack et al. (2005) [94] conducted a study using a mixture of ethanol (EtOH) and DEE for CAI combustion. The study involved numerical simulations and experimental carbon 14 tracing. For a mixture of DEE and EtOH, the DEE was found to be more reactive than the EtOH. However, as the two blends of fuel were similar, no large elongation of energy release was observed. Wong and Karim (2000) [95] studied the effects of hydrogen addition to mixtures of methane or propane on the cyclic variation and the ignition timing. The hydrogen has been found to reduce the cycle-to-cycle
variations while increasing the load limit. The results highlighted the benefits of using hydrogen as an additive rather than the main fuel. Yao et al. (2006) [96] conducted a study on control strategies for CAI engines with port injection, using methanol and DME mixtures. A diesel single cylinder engine was modified for dual-fuel port injection. The results showed that EGR and DME percentage are two important parameters needed to control thermal efficiency and emissions. A control of the auto-ignition timing can be achieved by adjusting the DME quantity and EGR rate. An optimal combustion region was found with high quantities of DME and EGR. CO emissions have shown to decrease with an increase of the IMEP, but HC emissions were increased. Lü et al. (2007) [97] studied mixtures of n-heptane with the addition of methanol, ethanol, isopropanol and methyl-tert-butyl ether. It was found that ethanol was the best additive considering the load limit, the emissions and the thermal efficiency. The CO emissions have shown to be dependent on the maximum combustion temperature, while the HC emissions were determined by the ratio of ethanol to total fuel. Morsy (2007) [98] studied the addition of DME, CH₂O and H₂O₂ to methane for a CAI engine with a CR of 18:1 and a volume displacement of 1132 cm³. A single-zone model was incorporated into the SENKIN code. The chemical kinetic mechanism included 79 species and 351 reactions. It was found that a mixture with an initial temperature of 400 K and without any additives would fail to auto-ignite. The results show that H₂O₂ is more effective than the other two additives in advancing ignition timing. The addition of a volume fraction of 7 % of H₂O₂ was able to generate auto-ignition for an initial mixture temperature of 350 K, while a minimum of 12.5 % and 35 % by volume were needed for DME and CH₂O, respectively. However, the addition of CH₃O to the mixture has shown to produce fewer NO emissions than the H₂O₂ additive. A near TDC ignition resulted in the same NO quantity produced for both additives H₂O₂ and CH₂O.
Another method employed to extend the heat release duration is the use of water addition. The first method consists of injecting water within the cylinder. One of the studies conducted by Christensen et al. (1999) [99] reduced the rate of combustion by injecting water into the cylinder for three different fuels: ethanol, iso-octane and natural gas. The experimental work was carried out at 1000 rpm with a compression ratio of 18:1 for both naturally aspirated (NA) and supercharged engines. The water was injected using a conventional fuel injector. The water injection delayed the ignition and increased the load limit for CAI engines, as the water slowed down the combustion rate and reduced the cylinder pressure peaks. The NOx emissions recorded were reduced further with the use of water. However, higher emissions of HC and CO were produced due to the degradation of combustion quality.

The second method is the use of water blending with the fuel prior to the mixture being injected within the cylinder. Megaritis et al. (2007) [100, 101] studied the effect of water addition to a bio-ethanol fuel blend. Low concentrations of water in the fuel appeared to have minimal effects on combustion. On the contrary, when the water was increased to 20% of the fuel content, it significantly reduced the available load range of the engine. It was found that moderate quantities of water contained in the fuel reduced the cylinder temperature. However, the fuel quantity was increased in order to maintain a stable combustion, which resulted in obtaining the initial cylinder temperature and NOx emissions without water blending. The results showed that contrary to the variable rate direct water injection, the fixed rate water blending with ethanol is counterproductive to reduce the cylinder pressure peaks at high loads.

Some studies investigated the effects of engine turbulence on the mixture properties to improve the load limit of CAI engines. For instance, Chen et al. (2006) [102] proposed a direct numerical simulation (DNS) on CAI engines to demonstrate the influence of temperature inhomogeneities on ignition. One-dimensional (1D) and 2D DNS simulations were carried out for lean hydrogen reduced reaction mechanism. A PDF was created and a multi-zone model was compared to the 1D and 2D models. The results demonstrated the behaviour and speed of the ignition front, illustrating the importance of the initial temperature gradient. Using the validated model to conduct additional
investigations, Hawkes et al. (2006) [103] investigated the variation of the length scale of temperature fluctuation on thermally stratified lean hydrogen combustion. The simulations concluded that the effects of turbulence were found to rapidly increase the temperature gradients. The multi-zone model produced excellent predictions on large length scale models without turbulence. It was found that turbulences have a strong effect on the initial hot spots. However, the multi-zone model performed worse with turbulence than without turbulence. Controversial results were reported on the effect of turbulence on CAI combustion between the swirl and tumble phenomenon. Christensen and Johansson (2002) [104, 105] demonstrated a longer combustion duration and a longer heat release rate by using a square bowl piston instead of a flat piston. The gross indicated efficiency was higher with the squared bowl piston, except for very late combustion timing. A moderate change in swirl ratio from 2 to 2.8 showed a small reduction in heat release rate. The combustion chamber geometry was found to affect CAI operations. On the other hand, Kong et al (2003) [106] demonstrated that the swirl enhancement had little effect on combustion duration. Sankaran et al. (2005) [107] performed calculations for different initial temperature distributions in a CAI engine fuelled with a lean hydrogen mixture. Three initial random temperature fields were simulated. The simulations revealed that the mixing and turbulence had significant influences on the initial location and development of ignition. The temperature field defined the temperature of the core, early ignition for the hot core and slow combustion of dormant gas for the cold core. Two different ignition cases were specified: the spontaneous propagation and the deflagration regime.

2.2.5 Reduction of the emissions of controlled auto-ignition engines

Some investigations developed various methods and strategies to improve the emissions levels of CAI engines. For instance, Kim and Lee (2006) [108] improved the emissions characteristics of CAI combustion by premixing various combinations of fuel (gasoline, diesel and n-heptane) with cooled EGR. The use of EGR with intake port fuel premixing produced NOx levels lower than 1/10th of the one of a conventional diesel engine. High levels of EGR are however limited by soot formation. Premixing of gasoline provided the most significant reduction of NOx and soot emissions. Kim and Lee (2007) [109] also experimentally investigated the effect of injection strategy using a narrow spray cone.
angle injector on the exhaust emissions of a single cylinder direct injection diesel engine in CAI mode. The work included three injection strategies: a conventional 156 ° large angle diesel injection with a piston bowl matching this angle, an early injection and piston bowl with a narrow angle of 60 ° and finally, a dual injection and piston bowl with a narrow angle of 60 °. Results showed that the NOx emissions were reduced, for a single injection timing from 30 CAD BTDCF, for both conventional diesel engine injection angle and narrow injection angle as shown in Figure 2.24.

![Figure 2.24 Effects of single injection timing](image)

Figure 2.24 Effects of single injection timing [109]

However, dual injection strategy appeared to be the best method to decrease the emissions significantly as shown in Figure 2.25. For this case, a very early timing was used for the first injection (from 50 to 70 CAD BTDCF) while the second injection timing was delayed (from 0 to 20 CAD after TDC firing (ATDCF)).
Figure 2.25 Effects of dual injection timing [109]
Shi et al. (2006) [110] studied the emission levels using a combination of cooled EGR and residual gases for CAI of diesel. The results have shown that high negative valve overlap benefited the fuel evaporation. Higher levels of residual gases also reduced the NOx emissions further but lowered the load limits of CAI operation due to the advance of the start of combustion (SOC). Cooled EGR delayed the start of LTR and HTR, which in turn helped to avoid engine knock at high load. It means that EGR could be used as a method to expand the load limit of CAI operations. EGR has also been found to decrease the NOx emissions at high load. However, EGR has shown to increase the CO emissions due to the incomplete combustion and low oxygen concentration. Zeng and Xie (2007) [111] proposed a new approach to further decrease the hydrocarbon emissions using in-cylinder catalysts. The combustion and emission characteristics were numerically simulated for three cases, including the baseline engine with an uncoated piston crown, a partial platinum coating (side surfaces of the piston crown), and a full platinum coating (top and side surfaces of the piston crown). A chemistry solver with a detailed mechanism of methane oxidation on the platinum catalyst and a surface reaction solver were coupled to a CFD code to calculate the exhaust emissions. The results showed that the level of the unburned hydrocarbons (UHC) was mainly produced near the combustion chamber walls and piston crevice volume. Results have shown that the full platinum coating reduced the UHC by up to 15%. It was found that the partial platinum coating gave the best results with a reduction of UHC by up to 20%. Papagiannakis and Hountalas (2004) [112] investigated a dual-fuel solution (diesel and natural gas) to reduce the exhaust emissions of CAI engines. The natural gas was used as a partial supplement for the diesel fuel. A compression-ignition direct injection (CIDI) engine was modified to operate under dual-fuel conditions. The study showed that the use of dual-fuel operation resulted in lower cylinder pressure peaks. At low load conditions, the combustion duration was found to be longer and the BSFC was lower compared to normal diesel operations. At high load, the combustion duration was found to be shorter with the BSFC being equal to normal diesel operations. Natural gas use for dual-fuel operations has shown to decrease the NOx emissions. However, HC and CO emissions were found significantly higher. Sjoberg and Dec (2005) [113] also investigated the lowest acceptable combustion temperatures for hydrocarbon fuels in CAI engines. The study regrouped experimental and computational investigations using different hydrocarbon classes such as iso-octane, n-heptane, toluene
and methylcyclohexane. The results showed that a minimum temperature of 1500 K was needed for the CO to CO\(_2\) reactions. CO oxidation did not achieve completion for temperatures below 1500 K. The combustion temperature peak was found to be independent of the fuel type. However, the study revealed the existence of in-cylinder thermal distribution caused by crevices and the thermal boundary layer. Kong and Reitz (2002) [114] carried out CFD simulations with detailed chemistry for predicting DI CAI engine combustion and emissions. The model predictions were in good agreement with the experiments and provided good results for the unburned HC, NOx and CO emissions. The engine configuration was found to produce low NOx due to a low gas temperature with a peak of 2000 K. When the overall equivalence ratio was reduced to 0.15, the degradation of the combustion produced higher unburned HC and CO emissions.
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Chapter 3: Turbulence modelling in vehicle engines

The three-dimensional turbulent flow inside an internal combustion (IC) vehicle engine is composed of a combination of phenomena. They can be explained separately by simple motions for a better description of the flow. This chapter briefly reviews the nature of flow turbulence inside the cylinder of vehicle engines and presents a description of turbulence models, which are widely used in computational fluid dynamics (CFD) modelling applied to engines. Suitable boundary conditions for such models are also presented and discussed.

3.1 Turbulence phenomena inside IC engines

Various flow scales that may exist inside the cylinder of a vehicle engine are sketched in Figure 3.1. The global motion over the length scale \( L \) represents a main or average motion scale over a time scale \( T \). The macroscopic agitation has a smaller scale \( l \) than the one for the global motion. The third scale is a microscopic scale which is strongly associated with turbulence.

The time of transport for the phenomenal turbulence at scale \( l \) is approximately described by:

\[
T_{\text{Turb}} \approx \frac{l}{u}
\]  

(3-1)
Such large-scale turbulence is usually characterised by the presence of coherent structures. The turbulence viscosity for such phenomenal turbulence with a time scale $T_{Turb}$ can be approximated by:

$$\mu_T \approx \frac{l^2}{T_{Turb}} \quad (3-2)$$

or

$$\mu_T \approx l u \quad (3-3)$$

The variation of the turbulence viscosity depends on the characteristic length scale $l$ and characteristic velocity $u$. Turbulence phenomena found inside a cylinder can be characterised by the occurrence of swirling and tumbling flow motions. Such swirling and tumbling flow motions usually exhibit strong shear flow instability which induces real turbulence embedded in phenomenal turbulence. A representation of the cascaded eddies within an engine cylinder is shown in Figure 3.2. The largest flow eddies have a low frequency until they are cascaded into smaller eddies, whose frequency is higher. The smallest flow eddies correspond to high-frequency fluctuations and will dissipate into heat due to the viscosity of the fluid. This energy cascade process carries on until the eddy size is down to the smallest eddies with scale known as the Kolmogorov length scale. At this scale, the occurrence of turbulence results in a transformation of the turbulence kinetic energy into thermal energy.

Figure 3.2 Visualisation of the energy dissipation
Figure 3.3 further shows two turbulence phenomena that can be found in an engine cylinder. It should be noted that the inside engine turbulence phenomena are usually a combination of these two motions, namely tumble and swirl. However, they are defined separately for a better description of flow inside a cylinder.

Tumbling is defined as a rotational flow around an axis perpendicular to the cylinder axis while swirling is defined as a rotating flow around an axis parallel to the cylinder axis. Figure 3.4 depicts the tumbling in a two-dimensional cutting-plane of the cylinder. It can be seen that the axis of rotation of the tumble motion will be altered as the piston is moving upwards and downwards. In this figure, the axis is moving up as the piston is rising during a compression stroke.
Figure 3.4 Representation of tumble on a 2D cylinder valve symmetry plane

Figure 3.5 shows the development of a swirl and tumble at the end of a compression stroke. The compression has no major impact on swirl motion, as it just compresses the rotational motion without affecting the velocity. However, the tumbling is strongly affected by the compression, as represented in the figure. The engine efficiency will be reduced when tumbling changes, from a relatively circular tumble, into an oval motion due to a loss in momentum.

Figure 3.5 Variation of swirl and tumble during the compression stroke

The difference of swirling between two and four ports cylinders is shown in Figure 3.6. It has been revealed already that the allocation of ports has less influence on the tumble motion but has a much stronger effect on the directions of the swirl motion. As there is only one inlet port in a two port cylinder, the swirl motion is rotating around the centre axis of the cylinder. For a four port cylinder, the cylinder has two inlet valves and two
axes of rotation. Thus, two swirl motions are merging in the symmetry plane of the cylinder.

![Diagram showing exhaust and inlet valves for two and four valves per cylinder]

Figure 3.6 Swirl difference for two valves and four valves per cylinder

3.2 Turbulence models

To model the flows inside an engine cylinder using CFD, the difficulty resides in choosing the turbulence models and the near-wall flow models, to obtain the best compromise between time and reliability for the application. Turbulence models can, generally, be classified as the classical Reynolds average Navier-Stokes (RANS), the direct numerical simulation (DNS) and the large eddy simulation (LES) models. The DNS is the most accurate approach solving the Navier-Stokes equations without averaging or approximation, other than numerical discretisations whose errors can be estimated and controlled. In the DNS, the Navier-Stokes equations are solved on a very fine mesh to capture all significant structures of the turbulence. Although the DNS has been used successfully to study transitional and turbulent flow in simple flows in the past few years, the DNS requires a high computational time and is therefore too expensive to be used as a design tool for vehicle engines [1]. The LES are also three-dimensional turbulent models, where the time-dependent flow equations are solved for the mean flow and the large-scale eddies, while the small-scale eddies are averaged by the sub-grid scale (SGS) models. This approach is much less time-consuming than the DNS. However, the LES are still too costly for large-scale computations.
The RANS approaches have extensively been used for investigations of internal flow inside cylinders, due to their low computational cost and good convergence. In the RANS, the governing equations are averaged over a time period much larger than the time scales of the turbulent fluctuations, and the resulting equations are numerically integrated. The RANS models include the mixing length models, the one-equation models, the two-equation models and the Reynolds stress model (RSM) [2]. In this approach, all unsteadiness is averaged out, which means all the unsteadiness is regarded as part of the turbulence. As a result, the conservation equations include extra terms called the Reynolds stresses. The presence of the Reynolds stresses in the conservation equations means the RANS models are not closed. Some model coefficients have to be introduced for the closure correlation. These model coefficients are obtained using experimental data based on some simple shear flows, as discussed in the previous section. Hence, all RANS based models are empirical approximations of the actual equations. In other words, the derivation of these models has been largely based on intuitive, empirical correlation and, to some extent, constrained by physical possibilities. With careful applications, they can provide reasonably good results for internal flows inside cylinders.

Since the flow inside an engine cylinder includes curvature, swirling, impingement, strongly-accelerated, and recirculation flows, the internal fluid-dynamic behaviour is very complex. It is impractical to use the DNS or the LES for such complex flows. Hence, most previous CFD studies on vehicle engines are based on the RANS modelling technique, where the focus was on the practical use in industrial flows. The difficulties associated with solving transport equations, in complex flow configurations, are a result of the high degree of coupling between the momentum equations due to flow curvature, that are absent in simple flows in which the models are tuned and validated. A true modelling of the small scales in a fully developed turbulent flow requires an experimental construction of turbulent strain rate and stress tensors. It becomes challenging since available experimental techniques cannot reveal such information for three-dimensional complex flows. To date, experimental data is still rather limited to being used for the formulation of the three-dimensional industrial turbulence with complex geometries. The turbulent flow inside a cylinder is also greatly affected by the presence of solid wall boundaries (e.g. cylinder wall, cylinder head,
valves). It is in the near-wall region that the solution variables change with large gradients, momentum and scalar transports. Therefore, the turbulent models must also be suitable for the wall-bounded flows. Over the past decades, many near-wall treatments have been developed and validated as an extension of turbulence model closure to fit low Reynolds number flows and describe the flow close to a solid wall [3]. All the near-wall modelling is then filled with empirical information. The non-universality of the empirical information may result in deviations of the solutions from the actual behaviour. For internal flows inside vehicle engines, few attempts have been performed for an assessment. The three widely applied turbulence models are the standard \( k-\varepsilon \) eddy viscosity, the renormalisation group (RNG) \( k-\varepsilon \) and the RSM models, which have been used in many previous studies on CFD modelling of internal flow inside engine cylinders [3].

3.2.1 The standard two-equation \( k-\varepsilon \) turbulence model [6]

In this model, the turbulent kinetic energy \( k \) and its dissipation rate \( \varepsilon \) are calculated from the following transport equations:

\[
\frac{Dk}{Dt} = \frac{\partial}{\partial x_i} \left( \left[ \mu + \frac{\mu_t}{\sigma_k} \right] \frac{\partial k}{\partial x_i} \right) - \frac{\rho u_i u_j}{\partial x_j} \frac{\partial u_i}{\partial x_j} + \beta g \frac{\partial}{\partial x_i} \frac{\partial T}{\partial x_j} - \rho \varepsilon - 2 \rho \varepsilon \frac{k}{\gamma RT} \quad (3-4)
\]

\[
\frac{D\varepsilon}{Dt} = \frac{\partial}{\partial x_i} \left( \left[ \mu + \frac{\mu_t}{\sigma_\varepsilon} \right] \frac{\partial \varepsilon}{\partial x_i} \right) + C_1 \varepsilon \left( - \frac{\rho u_i u_j}{\partial x_j} \frac{\partial u_i}{\partial x_j} + C_2 \beta g \frac{\partial T}{\partial x_i} \right) - C_2 \rho \varepsilon \frac{\varepsilon^2}{k} \quad (3-5)
\]

where the terms:

\[
\frac{\partial}{\partial x_i} \left( \left[ \mu + \frac{\mu_t}{\sigma_k} \right] \frac{\partial k}{\partial x_i} \right) \]

represents diffusion,
\( \frac{\rho_{ij} \frac{\partial u_j}{\partial x_i}}{} \) is the Reynolds stress transportation due to inertia,

\( \beta g_i \frac{\mu_i}{\text{Pr}_i} \frac{\partial T}{\partial x_i} \) is the turbulent \( k\varepsilon \) production due to the temperature gradient,

\( \rho \varepsilon \) represents pure dissipation

\( 2\rho \varepsilon \frac{k}{\gamma RT} \) is the dissipation due to the internal state.

The turbulent viscosity is related to \( k \) and \( \varepsilon \) by:

\[
\mu_t = \rho C_{\mu} \frac{k^2}{\varepsilon} \quad (3-6)
\]

The above equations contain six adjustable coefficients \( C_{\mu}, C_1, C_2, C_3, \sigma_k \) and \( \sigma_\varepsilon \). The standard values of these coefficients in the standard \( k-\varepsilon \) model are 0.09, 1.44, 1.92, 2.0, 1.0 and 1.3 respectively.

### 3.2.2 The renormalisation group \( k-\varepsilon \) turbulence model [8]

The renormalisation group (RNG) \( k-\varepsilon \) model has a similar form to the standard \( k-\varepsilon \) model except for their coefficients. Hence, the RNG \( k-\varepsilon \) model can be solved in exactly the same way as the standard \( k-\varepsilon \) model. Two main coefficients of Equations (3-4) and (3-5) have been modified in the RNG \( k-\varepsilon \) model: the coefficient \( C_2 \) in the dissipation term and the eddy viscosity \( \mu_t \). \( C_2 \) in Equation (3-5) is replaced by \( C^*_2 \), defined as

\[
C^*_2 = C_2 + \frac{C_{\mu} \rho \eta^3 (1 - \eta / \eta_0)}{1 + \beta \eta^5} \quad (3-7)
\]

where \( \eta_0 = 4.38 \), \( \eta = Sk / \varepsilon \) and \( \beta = 0.012 \). The standard values of the RNG \( k-\varepsilon \) model coefficient are \( C_{\mu} = 0.0845 \), \( C_1 = 1.42 \), and \( C_2 = 1.68 \). When \( \eta < \eta_0 \), the correction term in Equation (3-7) makes a positive contribution, and \( C^*_2 \) becomes larger than \( C_2 \). When \( \eta > \eta_0 \), the correction term makes a negative contribution, and \( C^*_2 \) becomes less than \( C_2 \).
The eddy viscosity in the RNG $k$-$\varepsilon$ model is replaced with an effective eddy viscosity based on the equation below for low Reynolds number:

$$\mu_t = \sigma (\alpha \mu_{eff} - \mu) \quad (3-8)$$

where $\alpha$ is the inverse effective Prandtl number, and $\mu_{eff}$ is calculated from the following differential equation which is based on the RNG theory:

$$d \left( \frac{\rho^2 k}{\sqrt{\sigma t}} \right) = 1.72 \frac{\hat{v}}{\sqrt{\hat{v}^3 - 1 + C_v}} d \hat{v} \quad (3-9)$$

where $\hat{v} = \mu_{eff} / \mu$, $C_v \approx 100$. For high Reynolds number equation (3-9) is reduced to Equation (3-6).

### 3.2.3 The Reynolds stress turbulence model [9]

The Reynolds stress model (RSM) solves seven partial differential equations. Six of them are for the six independent Reynolds stresses and one is for the dissipation of turbulent kinetic energy. The standard RSM conservation equations can be written as follows:

$$\frac{D}{Dt} \left( \rho \overline{u_i u_j} \right) = \frac{\partial}{\partial x_k} \left( \mu \frac{\partial \overline{u_i u_j}}{\partial x_k} \right) + \frac{\partial}{\partial x_k} \left( \mu \frac{\partial \overline{u_i u_j}}{\partial x_k} \right) + P_{ij} + \phi_j - \frac{2}{3} \rho \varepsilon \delta_{ij} + F_{ij} \quad (3-10)$$

where

$$P_{ij} = -\rho \left( \overline{u_i u_j} \frac{\partial U_j}{\partial x_k} + \overline{u_j u_i} \frac{\partial U_i}{\partial x_k} \right) \quad (3-11)$$

$$\mu_t = \rho C_{\mu} \frac{k^2}{\varepsilon} \quad (3-12)$$
\[
\phi_j = -C_1 \rho \frac{\varepsilon}{k} \left( \overline{u_i u_j} - \frac{2}{3} k \delta_{ij} \right) - C_2 \left( P_{ij} + F_{ij} - \frac{2}{3} P_j \delta_{ij} \right)
\]

(3-13)

\[
F_{ij} = -2 \rho \Omega_k \left( \overline{u_i u_m e_{ikm}} + \overline{u_i u_m e_{jlm}} \right)
\]

(3-14)

where \( \Omega_k \) is the rotation vector and \( e_{ijk} \) is the alternating symbol; \( e_{ijk} = 1 \) if \( i, j \) and \( k \) are different and in cyclic order, \( e_{ijk} = -1 \) if \( i, j \) and \( k \) are different and in anti-cyclic order, and \( e_{ijk} = 0 \) if any two indices are the same. The transport equation of the scalar dissipation rate \( \varepsilon \) is identical to Equation (3-5). The above equations contain seven adjustable constants \( C_\mu, C_1, C_2, C_{1\varepsilon}, C_{2\varepsilon}, \sigma_k \) and \( \sigma_\varepsilon \). The standard values of the model coefficients in the RSM model are 0.09, 1.8, 0.6, 1.44, 1.92, 1.0 and 1.0, respectively.

3.2.4 The Reynolds-averaged Navier-Stokes equations

To solve the Navier-Stokes equations, a simplification can be applied by using the Reynolds decomposition. This technique can decompose an instantaneous turbulent flow into its time-averaged value and its fluctuating quantities. Hence, the Reynolds-averaged Navier–Stokes equations (RANS) can be expressed as follows:

\[
\rho \frac{\partial \overline{u_i}}{\partial t} + \rho \frac{\partial \overline{u_i u_j}}{\partial x_j} = \rho \overline{f_i} + \rho \frac{\partial}{\partial x_j} \left[ -\overline{p \delta_{ij}} + \mu \left( \frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} \right) - \rho \overline{u_i' u_j'} \right]
\]

(3-15)

where \( \rho \frac{\partial \overline{u_i}}{\partial t} + \rho \frac{\partial \overline{u_i u_j}}{\partial x_j} \) represents the change in mean momentum of the fluid element due to the unsteadiness in the mean flow and the convection by the mean flow. \( \rho \overline{f_i} \) is the mean body force, \( \overline{p \delta_{ij}} \) the isotropic stress due to the mean pressure field, \( \mu \left( \frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} \right) \) the viscous stresses, \( \rho \overline{u_i' u_j'} \) is the apparent stress due to the fluctuating velocity field usually referred to as Reynolds stress.
On the right part of the equation, the Reynolds stress, which is a non-linear term, needs additional assumptions to solve the RANS equations, which leads to many turbulence models variations depending on the turbulent flow properties.

3.3 The near-wall treatments
The turbulence models are primarily valid for turbulent core flows. Consideration, therefore, needs to be given of how to make these models suitable for near-wall flows. The commonly used near-wall treatments are the standard wall functions [2], the non-equilibrium wall functions [10] and the two-layer zonal model [11].

3.3.1 The standard wall functions
The standard wall functions do not resolve the viscosity affected inner region (viscous sub-layer and buffer layer). Instead, semi-empirical formulas are used to bridge the viscosity-affected region between the wall and the fully turbulent region as shown in Figure 3.7.

![Figure 3.7 Velocity distribution near a solid wall [5]](image)

The-law-of-the-wall for mean velocity yields [7]:

\[ U^* = \frac{1}{k} \ln(Ey^*) \]  

(3-16)
where

\[ U^* = \frac{U_p C_{\mu}^{1/4} k_p^{1/2}}{\tau_w / \rho} \]  
\[ y^* = \frac{\rho C_{\mu}^{1/4} k_p^{1/2} y_p}{\mu} \]  

(3-17)

(3-18)

and \( k (=0.4187) \) is the von Karman constant, \( U_p \) the mean velocity of the fluid at point \( p \), \( E (=9.793) \) an empirical constant, \( k_p \) represents turbulent kinetic energy at point \( p \) and \( y_p \) the distance from point \( p \) to the wall.

In Fluent, when \( y^* > 11.225 \) the log-law is employed and at the wall-adjacent cells, the laminar stress-strain relationship \( U^* = y^* \).

### 3.3.2 The non-equilibrium wall function

The non-equilibrium wall function [10] assumes that the wall-neighbouring cells consist of a viscous sub-layer, and a fully turbulent layer, and need to resolve the \( k \) equation at the wall-neighbouring cells. Thus, the non-equilibrium wall functions partly account for non-equilibrium effects neglected in the standard wall function. The log-law for mean velocity sensitised to pressure gradients is:

\[ \frac{\tilde{U} C_{\mu}^{1/4} k^{1/2}}{\tau_w / \rho} = \frac{1}{k} \ln \left( E \frac{\rho C_{\mu}^{1/4} k^{1/2} y}{\mu} \right) \]  

(3-19)

where

\[ \tilde{U} = U - \frac{1}{2} \frac{dp}{dx} \left[ \frac{y_v}{\rho k^{3/2}} \ln \left( \frac{y}{y_v} \right) + \frac{y - y_v}{\rho k^{3/2}} \frac{y_v^2}{\mu} \right] \]  

(3-20)

and

\[ y_v = \frac{\mu y_v^*}{\rho C_{\mu}^{1/4} k_p^{1/2}} \]  

(3-21)
where $y_v$ is physical viscous sub-layer thickness, and $y_v^* = 11.225$. Thus, the profile assumption made for turbulence quantities are:

$$\tau_w = \begin{cases} 0 & y < y_v \\ \tau_w & y > y_v \end{cases}$$ (3-22)

$$k = \begin{cases} \left( \frac{y}{y_v} \right)^2 k_p & y < y_v \\ k_p & y > y_v \end{cases}$$ (3-23)

$$\varepsilon = \begin{cases} \frac{2
\nu k}{y^2} & y < y_v \\ \frac{k^{3/2}}{\kappa \mu^{3/4}} y & y > y_v \end{cases}$$ (3-24)

### 3.3.3 The two layer near-wall model

The two layer near-wall model [11] divide the whole domain into two regions, a viscosity-affected region and a fully turbulent region. The turbulent model is modified to enable the viscosity-affected region to be resolved. The two regions are determined by a wall-distance-based turbulent Reynolds number, as $Re_y = \frac{\rho y \sqrt{k}}{\mu}$, where $y$ is the normal distance from the wall at the cell centres. Thus, in the fully developed turbulent region where $Re_y > Re_y^*$ and $Re_y^* = 200$, the turbulence model is employed. In the viscosity-affected near-wall region, where $Re_y < Re_y^*$, the one-equation model [12] is applied. The momentum equations and the $k$ equation are same as those in the turbulence models. The turbulent viscosity $\mu_t$ is computed from:

$$\mu_{t, \text{2layer}} = \rho C_{\mu_t} l_{\mu} \sqrt{k}$$ (3-25)

where the length scale, $l_{\mu}$, is calculated [13].
When using the k-ε model together with the use of the standard wall function, the value of $y+$ has to be set between 30 and 500. This ensures that the first nodal point measured from the wall would fall into the logarithmic zone as it is considered to be fully turbulent, as shown in Figure 3.8.

![Figure 3.8 Distance $Y_1$ between a wall and the centre of the first cell](image)

**3.4 Boundary conditions**

Numerical CFD modelling of internal flow inside vehicle engines is defined in terms of initial and boundary conditions. It is important that the boundary conditions are specified correctly to ensure the model will approximate the real flow conditions. Although boundary conditions for internal flow inside a cylinder may change from one case to another, most common boundary conditions used in CFD simulations are inlet, outlet, wall, pressure and symmetry. *Velocity inlet* boundary defines the velocity and direction of the inlet flow while *Pressure inlet* and *Pressure outlet* are used to define the total or static pressure at the inlet and outlet when the velocity is unknown. *Mass flow inlet* defines a flow rate and directions for compressible flow. *Outflow* is used to approximate the flow at an exit where the flow has become fully developed. The use of this boundary condition is restricted by many practical problems and it will be applied with particular care. Specification of *Wall* is relatively simple but the near-wall treatment is crucial when applying turbulence models as discussed in the previous section. *Symmetry* can be used to describe the flow with a symmetric axis or plane.

When turbulence models are employed in CFD calculations of internal flow in IC engines, they give rise to the need for the following boundary conditions:

- **Inlet:** distributions of $k$ and $\varepsilon$ must be given
- **Outlet or symmetry axis:** $\partial k/\partial n = 0$ and $\partial \varepsilon/\partial n = 0$
- **Cylinder walls:** approach depends on Reynolds number
For in-cylinder turbulence simulations, the detailed boundary condition information for \( k \) and \( \varepsilon \) is usually unavailable. Simple approximations for the inlet distributions for \( k \) and \( \varepsilon \) in internal flows can be obtained from the turbulence intensity \( T_i \) and a characteristic length \( L \) of the engine by means of the following simple assumed forms [4]:

\[
k = \frac{3}{2} (U_{ref} T_i) \text{;} \quad \varepsilon = C_{\mu}^\text{3/4} \frac{k^{3/2}}{\ell} \quad \text{;} \quad \ell = 0.07L \tag{3-26}
\]

where the characteristic length \( L \) will be either the inlet port diameter or cylinder diameter.

### 3.5 Mesh generation

For all CFD modelling, the first step is to set up a mesh. In Fluent CFD code used in this study, the mesh setup is realised through Gambit, computer-aided design software linked to Fluent.

The mesh is generated using TGrid. The flow problem with a complex geometry is simulated using unstructured mesh. The different types of mesh are represented in Figure 3.9. For a two-dimensional geometry, the mesh type can be triangular or quadrilateral. For a three-dimensional grid, the options are various. The cells can be tetrahedrons, hexahedrons, prisms and pyramids. When the geometry is too complex, a mix of the mesh types can be used and is called mixed mesh or hybrid mesh. The cells of the mesh can be refined or coarsened for the needs of CFD modelling. The type of grid can be defined as structured or unstructured depending on the complexity of the geometry in two or three dimensions. A structured grid means the geometry is separated by regular grid lines that do not cross each other more than once for the whole
geometry. A block-structured grid still contains grid lines that do not cross each other more than once, but the whole geometry does not have the same number of grid lines. Thus, it contains one or more interfaces to separate the different parts of the geometry. An unstructured grid is the most flexible solution, used mainly for very complex three-dimensional geometries. The volume cells may have any shape to fit an arbitrary solution domain boundary. Usually, a combination of tetrahedron and hexahedron for three-dimensional geometries is adopted. The advantage of using such a mesh generation is time-saving for the mesh creation and geometry flexibility. However, the disadvantage of this method is the irregularity of the cell structure, which causes numerical diffusion and results in a slower convergence of simulation than the use of a regular grid. The quadrilateral and hexahedral cells mesh are preferred over the use of triangular and tetrahedral cells due to mesh quality. In Gambit, the quality of mesh generated can also be accessed. For a two-dimensional mesh, the value of the mesh elements concerning “Equiangle Skew” should fall between 0 and 0.2. For a three-dimensional mesh, the value of the mesh elements concerning the “Equiangle Skew” and the “Equisize Skew” should be between 0 and 0.4, which ensures a better result. The aspect ratio is also important for the accuracy of the results since it decides the level of numerical diffusion. As a general guide, the ratio of the length of cells to the height of cells should not exceed 10.

![Figure 3.9 Types of mesh in 2D and 3D](image-url)
References


Chapter 4: Experimental work

The first part of the chapter describes the optical engine cylinder experimental data conducted and provided by Pitcher et al. (2003) [1]. The second part of the chapter presents the thermodynamic single cylinder engine experimental pressure trace also provided by Pitcher et al.

4.1 Optical engine cylinder data
Laser Doppler anemometry (LDA) and particle Doppler anemometry (PDA) are methods of measuring fluid velocities by detecting the Doppler frequency shift of laser light that has been scattered by small particles moving with the fluid. These measuring techniques enable instantaneous and time-averaged measurements of the velocities to be obtained with a high spatial resolution. In LDA, the principle of Doppler effect is used, which relates the interaction of light waves with a moving observer or light waves received by a stationary observer from a moving emitter [2].

The use of LDA for measuring the flow inside the cylinder is quite accurate and allows a measurement of three-dimensional components at high frequency. The disadvantage of using this technology for measurement of velocity distribution in a combustion engine is the need of a transparent window. Also, optical modification for circumventing the effect of deflection has to be taken into account. However, measurements can be conducted in the region of the cylinder stroked by the moving piston for both the inlet and the compression stroke, a region that is out of bounds when using thermal anemometry. Also, this technique allows measurements to be taken at high temperatures, enabling its use for monitoring exhaust and combustion processes. The LDA technique is employed in many studies for investigating the flow behaviour inside a cylinder or inlet ports [1, 2, 3, 4, 5, 6, 7 and 8]. Despite success in applying LDA for assessing the flow field inside the cylinder, its application is still limited by the cost of employing such technique.

Many LDA measurements have been conducted at Loughborough University by Pitcher et al. (2003) [1] on an optically accessed single cylinder engine. Designed to be
representative of a four-cylinder Lotus engine with 1.8-litre displacement volume, the single cylinder has the same characteristics as the production engine. The inlet valves are angled at 68 ° with a base diameter of 31 mm. The single cylinder engine is equipped with an active valve timing system. The engine specifications can be summarised in the table below:

<table>
<thead>
<tr>
<th>Specifications</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore (mm)</td>
<td>80.5</td>
</tr>
<tr>
<td>Stroke (mm)</td>
<td>88.2</td>
</tr>
<tr>
<td>Connecting rod length (mm)</td>
<td>131</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>10.5:1</td>
</tr>
<tr>
<td>Number of valves</td>
<td>4</td>
</tr>
<tr>
<td>Inlet port angle (°)</td>
<td>30</td>
</tr>
<tr>
<td>Pent roof angle (°)</td>
<td>22.3</td>
</tr>
<tr>
<td>Displacement volume (litre)</td>
<td>0.45</td>
</tr>
</tbody>
</table>

The experimental data was conducted and provided by Pitcher et al. (2003) [1]. For these tests, only air is inserted through the ports into the optically accessible cylinder. The axial and radial mean velocities of points defined within the cylinder are recorded on three different planes, namely plane 1, 2 and 3. Plane 1 is the cross-plane, cutting inlet and outlet ports at y = 0 mm; plane 2 is the centre-plane of the cylinder at x = 0 mm and plane 3 is the cross-plane, cutting inlet and outlet ports at 18 mm from the centre-line at y = - 18 mm. Figure 4.1 illustrates those three planes from different views for a better understanding. Plane 1 and plane 3 are separated by 18 mm on the y-axis. Plane 3 is used to measure an offset cross-section of one inlet valve and one exhaust valve. The points on planes 1, 2 and 3, set to measure mean velocities, are defined by six lines on the z-axis from - 10 mm to - 60 mm every 10 mm (- 10, - 20, - 30, - 40, - 50, - 60), 0 mm being top dead centre (TDC). Points are defined on those lines every 5 mm, from - 35 to 35 mm on planes 1 and 2, and from - 30 to 30 mm on plane 3, due to a smaller cross-section. It should be noted that the centre-line values were not recorded during the experiments.
Figure 4.1 Experimental planes 1, 2 and 3 on three views: (a) top view, (b) side view, (c) isometric projection

The measurement points are illustrated in Figure 4.2. For planes 1 and 2, measurements are made on 6 lines, recording 14 points for each line, which gives a total of 84 points per plane. As plane 3 is 18 mm from the centre-line, the cross-section is smaller and only 12 points are recorded which gives a total of 72 points for plane 3.

4.1.1 Spark-ignition valve timing experimental data

The work conducted on the optical single cylinder can be categorised in two main parts. First, using typical spark-ignition valve lift and timing at an engine speed of 1500 revolutions per minute (rpm). For each of these points, the mean velocities respective to
their planes are recorded separately every 4 crank angle degrees (CAD). A maximum inlet valve lift of 8.5 mm is seen at 460 CAD and the inlet valve duration is 278 CAD. The maximum exhaust valve lift of 8 mm occurs at 256 CAD with a lift duration of 272 CAD. An illustration of the valve timings is presented in Figure 4.3. A small valve overlap can be seen at TDC gas exchange. The data is comprised of one axial and one radial measurement of mean velocity for each of the 240 points, over the three planes reported in time, for every 4 CAD over the cycle. This gives a total of 86 400 values for the spark-ignition valve timing LDA measurements. For the study, the full LDA measurements of 86 400 values obtained and provided by Pitcher et al. (2003) [1] are reprocessed onto graphs, to time-dependent axial and radial mean velocity, for each 240 points of the three planes. Hence, a full velocity map of the cylinder is produced. However, due to the amount of data, only two lines of six points from plane 1 will be presented in the following figures. On each side of the cylinder, the points are separated 30 mm from the centre-line, which should depict the high velocities and rotational vortices. The rest of the results are regrouped, summarised and will be presented later for comparison with the computational fluid dynamics (CFD) calculations.

Figure 4.3 Spark-ignition valve timings used during the laser Doppler anemometry experiments
An illustration of the selected points on plane 1 is shown in Figure 4.4.

Figure 4.5 depicts the axial mean velocities, of those points reported in time, for the intake and compression stroke. Despite the inlet valves opening shortly before TDC gas exchange, it can be seen from the figure that the mean axial velocity is nil at the beginning of the intake stroke; explained by the fact that the piston has not reached the specific depth inside the cylinder for each figure. This event occurs at 394 CAD, 410 CAD, 424 CAD, 436 CAD, 448 CAD and 461 CAD for 10 mm, 20 mm, 30 mm, 40 mm, 50 mm and 60 mm, respectively. Shortly after the piston moves downwards, a high peak of velocity can be seen for each line, due to the valves being opened already by 5.42 mm at 400 CAD reaching the maximum lift at 460 CAD. The behaviour is similar for both sides of the piston with the -35 mm vertical line of points showing higher velocity peaks. Those peaks are seen at later crank angles as the piston reaches lower lines from 436 CAD at 10 mm gradually to 500 CAD at 60 mm. The peak values reduce as the piston reaches lower cylinder levels from 34.3 m/s at 20 mm gradually to 16.3 m/s at 60 mm. The velocities decrease thereafter, as the cylinder vacuum is almost reduced to the atmospheric pressure. The piston is going up from 540 CAD and the velocities are seen as negative for the -35 mm vertical line of points, meaning the air direction is upward. The velocities on the right side of the cylinder are also decreasing, but remain positive almost until the end of the compression stroke, signifying that the air direction is still downward even if the piston is going up.
Figure 4.5 Axial mean velocity at the -30 mm (left) and +30 mm radial line (right) for 10 mm, 20 mm, 30 mm, 40 mm, 50 mm and 60 mm axial lines for the spark-ignition valve timing at 1500 rpm
4.1.2 Controlled auto-ignition valve timing experimental data

The second category of LDA measurements is conducted using a shorter valve lift and timing, which is representative of controlled auto-ignition (CAI). These experiments were conducted and provided by Pitcher et al. (2003) [1] for engine speeds of 1500 rpm and 2000 rpm. The inlet valves lift has a maximum of 3.6 mm at 505 CAD and the exhaust valves lift has a maximum of 3.6 mm at 215 CAD. The lift duration is 188 CAD for both the inlet and exhaust valves. The exhaust valves open, exhaust valves close, inlet valves open and inlet valves close occur at 131 CAD, 319 CAD, 421 CAD and 609 CAD, respectively. The inlet and exhaust valves profiles are represented in Figure 4.6.

![CAI valve lift and timing used during the laser Doppler anemometry experiments](image)

Once again, the full LDA measurement values obtained and provided by Pitcher et al. (2003) [1] are reprocessed onto graphs, to time-dependent axial and radial mean velocities, for each of the 240 points on the three cutting-planes. A full velocity map of the cylinder is produced for CAI valve timing at engine speeds of 1500 rpm and 2000 rpm. As for the SI valve timing, the same two lines of six points from plane 1 will be presented in figures, due to the amount of data. Figure 4.7 depicts the cylinder axial mean velocities for the points located on the symmetrical cutting-plane at a distance of - 30 mm and + 30 mm from the centre-line.
Figure 4.7 Axial mean velocity at the - 30 mm (left) and + 30 mm radial line (right) for 10 mm, 20 mm, 30 mm, 40 mm, 50 mm and 60 mm axial lines for the controlled auto-ignition valve timing and 3.6 mm valve lift at 1500 rpm
For those measurements, the cylinder is running at 1500 rpm with a CAI valve timing and a valve lift of 3.6 mm. The left side of the cylinder, which represents the entrance of air flow through the inlet valves, depicts higher levels of velocity compared to the exhaust side. The cylinder axial velocities reach higher values at the top of the cylinder; a maximum of 50.7 m/s for the 10 mm line gradually decreasing to a maximum of 23.5 m/s at the 60 mm line.

The cylinder axial mean velocities are depicted in Figure 4.8 for an engine speed of 2000 rpm. As for 1500 rpm, the entrance of air flow through the inlet valves depicts higher levels of velocity compared to the exhaust side of the cylinder. The peaks of velocity seen are higher compared to an engine speed of 1500 rpm. The maximum velocity reaches 71.4 m/s for the 10 mm line linearly decreasing to 27.5 m/s for the 60 mm line.
Figure 4.8 Axial mean velocity at the -30 mm (left) and +30 mm radial line (right) for 10 mm, 20 mm, 30 mm, 40 mm, 50 mm and 60 mm axial lines for controlled auto-ignition valve timing and 3.6 mm valve lift at 2000 rpm for a full cycle.
4.1.3 LDA error analysis

The first LDA experiment was successfully conducted in 1964 [9]. The method has been under continuous development to improve measurement accuracy ever since, mainly focusing on the optical, electronic and flow measurement aspects of LDA systems [10, 11]. Frequency shifting is a method where one of the laser beams is passed through an acousto-optic modulator, known as a Bragg cell. The transparent medium of the Bragg cell is excited by ultrasonic sound waves, to produce a frequency shift on the second beam. The shift in the frequency of the fringes now enables the measurement of both stationary and particles travelling in opposing directions [12]. One form of optical error, chromatic aberration, or fringe distortion, can occur with non-symmetrical laser beam refractions on the medium interface [13, 14]. It generally results in an over-estimation of the measured turbulence quantities. The range constraints and calibration of the sensors are also sources of error. The distance at which they take measurements has to be precisely defined [15, 16, 17]. Another source of error in LDA systems is the flow velocity bias caused by the difference of sample rates. As LDA systems measure the frequency of particles through the fringes created by the laser beams, the high flow velocity is sampled more often than low flow velocity. Particle averaging bias is used to normalise the measurement sample size, leading to an additional source of error [18, 19, 20, 21]. Larger errors have been reported for air flow measurements. A correction factor is usually applied to minimise the error due to averaging bias effect [22, 23]. The data size is also an important factor to consider in reducing measurement error [24]. Velocity gradient broadening causes reading fluctuations even in steady flow due to the difference in particle velocities for a specific location within the boundary layer [25, 26, 27]. Also, finite transit time broadening is a measurement error linked to signal processing time and the number of fringes. As signal processing time is shortened, fewer fringes are included in the frequency calculation, which leads to measurement velocity fluctuations and increases the measured variance of the velocity signal [28]. Finally, in non-stationary flow measurements, where velocity variations are observed due to flow periodicity, appropriate data processing is necessary to resolve fluctuations [29, 30, 31]. Additionally, sources of noise, such as electronic noise, photodetector noise, preamplifier circuit thermal noise and light/reflections from ambient or external sources, are all commonly found to affect LDA signals.
4.2 Single cylinder thermodynamics engine data

Experiments on a single cylinder thermodynamics engine running at 2000 rpm were also conducted and provided by Pitcher et al. (2003) [1]. The cylinder geometry is identical to the optically accessible cylinder used for the LDA experimental work. The single cylinder thermodynamics engine specifications can be summarised in the table below:

<table>
<thead>
<tr>
<th>Table 4.2 Single cylinder thermodynamics engine specifications</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore (mm)</td>
</tr>
<tr>
<td>Stroke (mm)</td>
</tr>
<tr>
<td>Connecting Rod Length (mm)</td>
</tr>
<tr>
<td>Test Speed (rpm)</td>
</tr>
<tr>
<td>Compression ratio</td>
</tr>
<tr>
<td>Number of Valves</td>
</tr>
<tr>
<td>Fuel Injection</td>
</tr>
<tr>
<td>Fuel Type</td>
</tr>
<tr>
<td>Mode</td>
</tr>
<tr>
<td>Burnt mixture residual concentration</td>
</tr>
</tbody>
</table>

The single cylinder thermodynamics engine experiments are conducted using a shorter valve lift and timing compared to the standard spark-ignition set-up. Using a valve lift of 6 mm, the inlet and exhaust valve timings are varied, to retain the residual burnt mixture within the cylinder at the event exhaust valves close (EVC) for the next cycle. Six valve timings are used to retain residual values of 36 %, 41 %, 46 %, 51 %, 55 % and 59 %. The corresponding events and durations for inlet valves open (IVO), inlet valves close (IVC), exhaust valve open (EVO) and EVC are listed in Table 4.3. The lift durations for both inlet and exhaust valves decrease as the percentages of residual increase.
Table 4.3 Inlet and exhaust valves timing details

<table>
<thead>
<tr>
<th>Residuals</th>
<th>IVO CAD</th>
<th>IVC CAD</th>
<th>EVO CAD</th>
<th>EVC CAD</th>
<th>Inlet CAD</th>
<th>Exhaust CAD</th>
</tr>
</thead>
<tbody>
<tr>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>36</td>
<td>427</td>
<td>576</td>
<td>142</td>
<td>291</td>
<td>149</td>
<td>149</td>
</tr>
<tr>
<td>41</td>
<td>433</td>
<td>576</td>
<td>142</td>
<td>285</td>
<td>143</td>
<td>143</td>
</tr>
<tr>
<td>46</td>
<td>438</td>
<td>576</td>
<td>142</td>
<td>280</td>
<td>138</td>
<td>138</td>
</tr>
<tr>
<td>50</td>
<td>443</td>
<td>576</td>
<td>142</td>
<td>275</td>
<td>133</td>
<td>133</td>
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<tr>
<td>55</td>
<td>448</td>
<td>576</td>
<td>142</td>
<td>270</td>
<td>128</td>
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</tr>
<tr>
<td>59</td>
<td>453</td>
<td>576</td>
<td>142</td>
<td>265</td>
<td>123</td>
<td>123</td>
</tr>
</tbody>
</table>

The valves profiles are illustrated in Figure 4.9 for the inlet and 4.10 for the exhaust. It can be noted that IVC and EVO occur at the same crank angle position for all valve timings. The amount of residual retained in the cylinder is affected only by the timing at which the inlet valves open and the exhaust valves close. Opening the inlet valves early will increase the amount of fresh charge into the cylinder, therefore, reducing the total quantity of residual. The corresponding exhaust timing strategy is to close the valves late to exhaust the burnt gases and clear the cylinder volume ready for the next fresh charge.

Figure 4.9 Controlled auto-ignition inlet valve timings
A fast data acquisition system is used to acquire the engine parameters for each valve setting. 300 cycles are recorded with a resolution of 0.5 CAD. However, due to cyclic variations of the cylinder pressure, an average pressure trace is calculated from the 300 cycles of data for each valve timing. An illustration of the average cylinder pressures is represented in Figure 4.11. The cylinder pressures are plotted for each valve timing corresponding to residual concentrations ranging from 36% to 59%.

Figure 4.10 Controlled auto-ignition exhaust valve timings
Figure 4.11 300 cycles averaged cylinder pressure inside the thermodynamic engine for (a) 36 %, (b) 41 %, (c) 46 %, (d) 51 %, (e) 55 % and (d) 59 % residual gases
A close-up of the pressure peaks after top dead centre firing (TDCF) for all valve timings is shown in Figure 4.12. Depending on the residual level, the maximum combustion pressure after auto-ignition varies from 32.4 to 37.5 bar. At the exception of 36 % residual where the maximum pressure increases as the residual concentration increases. Also, the peak timing occurs earlier as the residual concentration increases.

![Graph showing cylinder pressure peaks during the expansion stroke for all valve timings](image)

**Figure 4.12 Close-up of the cylinder pressure peaks during the expansion stroke for all valve timings**

A close-up of the pressure peaks for all the valve timings at TDC gas exchange is shown in Figure 4.13. At the end of the exhaust stroke, the pressure increases as the piston is moving up and the valves are all closed. The pressure rises until reaching a maximum at TDC gas exchange. The maximum pressure is seen higher as the residual concentration increases, gradually increasing from 11.2 bar for 36 % residual to 15.4 bar for 59 % residual. As no chemical reaction occurs at that time, the variation of pressure is directly due to the remaining amount of mixture left in the cylinder when the exhaust valves close, before being compressed.
Figure 4.1 Close-up of the cylinder pressure peaks during the exhaust stroke for all valve timings

The heat release rate can be calculated using the cylinder pressure. A simplified equation to calculate the heat release rate is presented below [8]:

$$\frac{dQ_n}{d\theta} = \frac{\gamma}{\gamma - 1} P \frac{dV}{d\theta} + \frac{1}{\gamma - 1} V \frac{dp}{d\theta}$$

(4-1)

where $\frac{dQ_n}{d\theta}$ is the apparent net heat release rate in J/deg, V is the gas volume in m³, $\theta$ is the crankshaft angle (deg), P is the cylinder pressure in Pa and $\gamma$ is the ratio of specific heats, the heat capacity at constant pressure $C_p$ over the heat capacity at constant volume $C_v$. The equation assumes a uniform pressure and temperature in time within the cylinder, a cylinder content modelled as an ideal gas, a negligible enthalpy and the ideal gas law universal gas constant $R$ applicable. More complex methods of heat release analysis have been studied for gas properties, heat transfer and crevice effects.

As the cylinder geometry in this study does not contain a piston crevice, it is assumed
that a simple heat release rate calculation can be applied. As one of the variables in equation 4-1 is the ratio of specific heats, its variation during the cycle needs to be studied to know if a constant value can be used in the equation. A cylinder pressure analysis shows that the ratio of specific heats varies during the cycle as shown in Figure 4.14.

A close-up of the specific heats ratio around TDCF is depicted in Figure 4.15. The heat release rate (HRR) calculation will be conducted from the moment of auto-ignition until all the fuel has been oxidised. The ratio of specific heats varies from 1.275 to 1.305 around TDCF as depicted in the figure. A small variation of the specific heat ratio has a low impact on the HRR calculation, only altering its magnitude by +/- 1.2%. It means that an average value of 1.29 can be used for the calculation and should give a good approximation of HHR.
The apparent net heat release rate can be calculated using equation 4-1 as presented in Figure 4.16. As the apparent net heat release rate is calculated from the cylinder pressure, any irregularities of the pressure will lead to fluctuations of HRR. It demonstrates that the average cylinder pressure representative of the 300 measured cycles still shows pressure fluctuations. An error analysis of the cylinder pressure has shown high cyclic variations between the 300 pressure cycles, in particular at TDCF (0 CAD), EVC (265 - 291 CAD) and IVC (576 CAD).
The maximum pressure fluctuation between the cycles is presented in Figure 4.17. It can be seen from the figure that the fluctuation of cylinder pressure reaches a maximum around TDCF, which will affect the apparent net heat release rate calculation even on average values. Observing the apparent net heat release rate calculation variation, it can be seen that the values fluctuate from negative to positive at every crankshaft angle degree. An average of two values every CAD would cancel the fluctuations of HHR.
Figure 4.17 Cyclic pressure variations of 300 cycles

After filtering the measured average pressure cycle against irregularities, the apparent net heat release rate shows more consistent trends as depicted in Figure 4.18.

Figure 4.18 Apparent net heat release rate after pressure filtering
References


Chapter 5: Numerical modelling methodology and boundary conditions

Before defining the transient motions occurring in the cylinder during the cycle, it is necessary to briefly describe the engine geometry and its moving components. Hence, the piston motion and valve lift are defined. Finally, the mesh, the port deactivation and the boundary condition are described.

5.1 Numerical modelling

5.1.1 Description of piston motion

The engine mechanism consists of the crankshaft, connecting rod, piston and valves. Details of the calculations of piston position and velocity, in function of the crankshaft angle and connecting rod length, can be found in the appendices. The instantaneous piston velocity $U_p$ can be expressed as:

$$\dot{U}_p = U_p \frac{\pi}{2} \left( \sin \theta + \frac{A \sin \theta \cos \theta}{\sqrt{L^2 - A^2 \sin^2 \theta}} \right)$$  \hspace{1cm} (5-1)

where $\overline{U}_p$ is the average piston speed, $\theta$ is the crankshaft angle, $L$ is connecting rod length and $A$ is crankshaft radius.

5.1.2 Description of valve motion

The other moving parts, which must be considered in dynamic mesh modelling, are the inlet and exhaust valves. To match the experimental work conducted by Pitcher et al. (2003) [1], the same valve lift and timings are applied to each study. The spark-ignition (SI) and controlled auto-ignition (CAI) valve timings, with a 3.6 mm valve lift, are implemented for the calculations which correspond to the laser Doppler anemometry (LDA) experimental work conducted by Pitcher et al. (2003) [1]. The various CAI valve timings with a 6 mm valve lift, used to retain different quantities of residual gases, are set for the calculations which correspond to the thermodynamic single cylinder experiments. A coordinate system is defined independently for each valve. The valve profiles for inlet and exhaust are inserted into Fluent using text files, which enumerate a list of valve
positions corresponding to the crankshaft angle relative to their own coordinate systems. Figure 5.1 compares the SI and the CAI valve lift and timing with the corresponding piston displacement, plotted against the crankshaft angle in degrees (CAD). With a maximum lift of 8.5 mm and 8 mm for the inlet and exhaust valves with SI timing; the CAI valves show a maximum lift of 3.6 mm for both inlet and exhaust valves. In this figure, the shorter timing seen for the CAI valves is used to trap residual gases into the cylinder.

![Figure 5.1 Spark-ignition and controlled auto-ignition valve lift with the corresponding piston position](image)

5.1.3 Obtaining the engine geometry

To gain access, the cylinder head must be dismounted, in order to make manual measurements of engine combustion chamber dimensions. Also, an accurate measurement of the pent roof angle, the inlet, and exhaust ports dimensions can be increasingly challenging due to inaccessibility. Moreover, the assumption of geometry for these parts could affect the inlet flow and the resulting vortices in the cylinder. The solution adopted is to obtain a negative cast of the inlet port and the cylinder head geometry. The exhaust port can be measured and its geometry estimated, as its effect on
flow occurs later during the cycle at the exhaust stroke. The cylinder head is removed and faced downward in order to be able to pour the melted rubber to make a negative cast; the valves are removed and measured. To avoid a possible leak in the valve guides, due to the absence of valves in the casting process, the valve holes are sealed. Also, a seal is used to stop any leakage from the entrance of the inlet and exhaust ports. The melted rubber is poured into the inlet port through the cylinder head before solidifying at ambient temperature. Once the rubber becomes solid, the steel frames are removed and the cast is cut at the twin-port junction to be removed. It should be noted here that the virtual representation of this volume corresponds to the real inside surface of the inlet port. Hence, the cast is measured and the corresponding cylinder, valves and inlet port are designed into the software ‘Solid Edge’. The geometry can then be imported into the pre-processing software Gambit to create the mesh and set boundary layers ready for the computational fluid dynamics (CFD) calculations.

5.1.4 Dynamic mesh type

Figure 5.2 shows three different types of dynamic mesh used in Fluent: layering, spring smoothing, and local re-meshing. The features of these three mesh types can be briefly described as follows:

- **Layering**

Layering can be used when the motion of the body is purely linear. It creates or suppresses rows of cells depending on a split/collapse factor defined in Fluent. The mesh shapes for layering are confined to quadrilateral cells for the two-dimensional (2D) mesh, or hexahedron and prism cells for the three-dimensional (3D) mesh. Its application is limited by collapsing cells if \( h < \alpha c h_{\text{ideal}} \) and by splitting if \( h < (1 + \alpha s) h_{\text{ideal}} \). Here, \( h \) is the current height of the cell, \( \alpha c \) is the collapse factor and \( \alpha s \) is the split factor. \( h_{\text{ideal}} \) has to be defined in the dynamic zone section and should be about the same height of a normal cell in the model. Figure 5.2(a) shows the layering mesh type for 410 CAD and 490 CAD available for the lower part of the cylinder below top dead centre (TDC). As the piston is moving down from TDC to bottom dead centre (BDC), cells will be created on the lower part of the cylinder. The cells will collapse when the piston is moving up from BDC to TDC. Layering is ideal to model the valves or the piston movements in a cylinder, but the mesh imposed on the cylinder has to be composed of hexahedrons and prisms for 3D
geometries. The layering mesh option is also illustrated in Figure 5.2(c) for the upper part of the valve and the valve stem.

- **Spring smoothing**
  Spring smoothing is used when the motion is small and the existing cells are compressed or expanded. If the spring constant factor $k$ is set to be equal to 1, the effect of the piston motion will be mainly around the interface between the piston and cylinder wall. When $k$ is set to 0, the piston movement will affect the whole mesh. When the boundary node relaxation $\beta$ is set to 0, it was found that the quality of cells generated near the piston and wall is poor, while $\beta = 1$ will give good quality cells. Figure 5.2(b) shows the spring smoothing mesh type at 360 CAD and 490 CAD for the upper part of the cylinder above TDC. As the piston moves down from TDC to BDC, cells in the upper part of the cylinder expand; From BDC to TDC, cells in the upper part of the cylinder are compressed. This mesh option is used in this study to allow the valves to move within the same meshed volume; the upper part of the mesh. If the valves were to cross the lower part of the mesh with layering option, the simulation would crash.

- **Local re-meshing**
  Local re-meshing can be used when the motion involves both translation and rotation, usually in conjunction with the adoption of 2D triangular mesh or 3D pyramids and tetrahedrons. It re-meshes the cells adjacent to the moving body when the specified settings have been exceeded. The controlling parameters in local re-meshing are minimum length scale, maximum length scale, maximum cell skewness and maximum face skewness. The re-mesh size interval can be set to 1. Figure 5.2(c) illustrates the local re-meshing type mesh underneath the valve. As the valves move down, and if the re-mesh interval is set to 1, those cells close to the valves are re-meshed every time step when the minimum length scale and cell skewness specified are exceeded. It can be used for modelling the valve movement when the valve axis is not parallel to the piston axis. Due to the complexity of the geometry, the inlet port and the upper part of the cylinder are meshed with pyramid and tetrahedron cells together with the valves. This necessitates the use of local re-meshing for the valve movement, in particular for the mesh cells adjacent to the valve lower surface.
Figure 5.2 Dynamic mesh types applied to the model

An additional strategy used in this study to allow the valves motion in the model is to add virtual surfaces, which will form a layer between the static part of the geometry and the moving valves. Therefore, the valves motion can occur without affecting the mesh cells in the static geometry. The layering and re-meshing options occur in the static volume independently from moving volumes (valves). Using this method, there is no stretching of the original mesh cell due to the valves motion. Additionally, the valves and valve stems are set with the layering option, to allow cell layers to be created as the valves motion occur.

5.1.5 Hybrid mesh and port deactivation
The simulations are set to match a step size of 1 CAD when possible and 0.5 CAD when a moving part is included. If the full cycle of 720 CAD is calculated with a step angle size of 0.5 CAD, the simulations take 1440 steps per cycle to complete. However, during dynamic movement of the piston and valves in CFD simulations, the creation of negative cells can occur (depending on the geometry) and can cause computational crashes. One way to avoid negative cells is to reduce the step angle size down to 0.05 CAD when
needed. Hence, the dynamic movement is reduced between two steps which will limit the variation of the temperature, pressure and cell distortion in the model. Figure 5.3 represents the change in step angle size for the first cycle, for an engine speed of 1500 revolutions per minute (rpm) with SI valve timing. It can be noted that the step angle size is reduced to avoid simulation crashes, which can occur when the pressure difference between the cylinder and the ports is high, typically around the events exhaust valves open (EVO) and inlet valves close (IVC).

![Figure 5.3 Variation of crankshaft angle step size](image)

A strategy that can be used to save computational time is to deactivate the inlet and exhaust ports when their respective valves are closed. When the ports are deactivated, the number of cells totalled 79 356 at TDC and 244 222 at BDC. For SI timing, the inlet and exhaust valves have a lift duration of 278 CAD. With a safe port activation margin of 1 CAD before and after the valve movements, this means that each port (inlet and exhaust) can be deactivated for 440 CAD over the cycle of 720 CAD. This method can save approximately 40 % of the computational time for SI timing and 55 % of the computational time for 3.6 mm CAI timing. Higher levels of residuals modelled by shorter lift durations can lead to higher computational time-saving. A representation of
port (de)activations of the inlet and exhaust port during the cycle is shown in Figure 5.4. It can be seen that the activation of the ports is related to the valve movement, and only necessary for those events.

Figure 5.4 Ports deactivation and activation for the spark-ignition model with corresponding valve movement for the (a) inlet port and (b) exhaust port
An illustration of the corresponding activations and deactivations of ports is presented in Figure 5.5 to show their effect on events and geometry changes. From the start of the cycle at top dead centre firing (TDCF) at 0 CAD, the events are defined into the SI timing computational solutions and could be summarised as follows:

- The inlet and exhaust ports are both deactivated.
  From TDCF until 129 CAD Fig. 5.5 (a)

- The inlet port remains deactivated; the exhaust port is activated.
  From 129 CAD until 331 CAD Fig. 5.5 (b)

- For the valves overlap, the exhaust port remains activated; the inlet port is activated.
  From 331 CAD until 403 CAD Fig. 5.5 (c)

- The inlet port remains activated; the exhaust port is deactivated.
  From 403 CAD until 609 CAD Fig. 5.5 (d)

- The exhaust port remains deactivated; the inlet port is deactivated.
  From 609 CAD until 849 CAD (129 CAD on the next cycle) Fig. 5.5 (e)

Figure 5.5 Illustration of the spark-ignition cylinder geometry with and without the ports for (a) from top dead centre firing to 129 CAD, (b) from 129 CAD to 331 CAD, (c) from 331 CAD to 403 CAD, (d) from 403 CAD to 609 CAD and (e) from 609 CAD to 849 CAD
To reduce computational time, the CFD calculations could start from inlet valves open (IVO) at 331 CAD as only air is considered to be compared to the LDA data and no combustion would occur at TDCF. However, it signifies that the exhaust port would be activated and the exhaust valves open. To obtain accurate results, the cylinder turbulences should be considered prior to the intake stroke, i.e. during the exhaust stroke. This implies that the CFD calculations should start at TDCF or between TDCF and EVO when both intake and exhaust valves are closed so no turbulence is generated from the ports.

For the second set of simulations, the 3.6 mm valve lift and timing for CAI operation, the deactivation and activation of the inlet and exhaust ports are depicted in Figure 5.4. A longer duration of deactivation occurs for the CAI valve timings when compared to the SI valve timings. The number of cells in the model is reduced for a longer part of the cycle, meaning the computational time-saving will be higher for the simulation in CAI mode. Also, as none of the valves are open at TDC, the CFD calculations could start at either TDC gas exchange or TDCF. To reduce computational time, the CFD calculations should start at TDC gas exchange. The fresh charge was composed of air during the LDA measurements and, as no combustion would occur at TDCF, the temperature of the cylinder would not be affected by the auto-ignition. Also, no turbulences would be generated from the ports as the valves are all closed.
Figure 5.6 Ports deactivation and activation for the 3.6 mm controlled auto-ignition timing model with corresponding valve movement for the (a) inlet port and (b) exhaust port
Starting from TDC gas exchange, the corresponding model geometry changes are presented in Figure 5.7. The events are defined into the CAI timing computational solutions and could be summarised as follows:

- The inlet and exhaust ports are both deactivated.
  
  From TDC gas exchange (360 CAD) until 421 CAD  
  \( \text{Fig. 5.7 (a)} \)

- The exhaust port remains deactivated; the inlet port is activated.
  
  From 421 CAD until 609 CAD  
  \( \text{Fig. 5.7 (b)} \)

- The exhaust port remains deactivated; the inlet port is deactivated.
  
  From 609 CAD until 720 CAD. In case the CFD calculation continues after 720 CAD onto the next cycle, the event with both ports deactivated is still applicable until 851 CAD (131 CAD on the next cycle)  
  \( \text{Fig. 5.7 (c)} \)

- The inlet port remains deactivated; the exhaust port is activated.
  
  From 851 CAD until 1039 CAD (from 131 CAD until 319 CAD on the next cycle)  
  \( \text{Fig. 5.7 (d)} \)

- The inlet port remains deactivated; the exhaust port is deactivated.
  
  From 1039 CAD until 1440 CAD (from 319 CAD until 720 CAD on next cycle)  
  \( \text{Fig. 5.7 (e)} \)

**Figure 5.7** Illustration of the controlled auto-ignition timing changes of geometry with and without the ports for (a) from 360 CAD to 421 CAD, (b) from 421 CAD to 609 CAD, (c) from 609 CAD to 851 CAD, (d) from 851 CAD to 1039 CAD and (e) from 1039 CAD to 1440 CAD
5.2 Numerical details

The area $A_{in}$ is directly obtained from the software Gambit ($A_{in} = 1.45 \times 10^{-3}$ m$^2$). The perimeter $p$ of the inlet is also obtained ($p = 0.15$ m). The numerical details for the engine geometry and speed can be calculated. The hydraulic diameter $d_e$ of the entrance of the inlet port is defined by:

$$d_e = \frac{4A_{in}}{p} = 38.5 \times 10^{-3} m$$  \hspace{1cm} (5-2)

where $A_{in}$ is the wetted area of the entrance of the inlet port and $p$ denotes the perimeter.

The piston stroke is found to be 88.2 mm and the connecting rod length 131 mm. The average piston velocity for 1500 rpm and 2000 rpm is calculated and found to be 4.41 m/s and 5.88 m/s, respectively. It can be assumed that the flow velocity induced inside the inlet port will be higher than the one in the cylinder, due to the chamber vacuum and inlet surface restriction. Therefore, the minimum Reynolds number is defined inside the cylinder at 1500 rpm. Any other part of the model will give a higher value for the Reynolds number. The Reynolds number can be determined for the combustion chamber at 1500 rpm:

$$Re = \frac{\rho Ud_e}{\mu} = 11624$$  \hspace{1cm} (5-3)

Since the Reynolds number inside the combustion chamber is greater than the critical value of 2300, it can be concluded that the flow through the whole cylinder is turbulent. Thus, employment of turbulence models in the simulation is necessary. Considering the flow inside the cylinder to be characterised by swirl and tumble, three models are selected for comparison. A natural choice for turbulence modelling is the standard k-$\varepsilon$ model [2]. It gives good results for moderately complex behaviour like jet impingement, separating flows, swirling flows and secondary flows. The standard two-equation k-$\varepsilon$ model solves two transport equations of the turbulent kinetic energy $k$ and its dissipation rate $\varepsilon$ for the eddy viscosity. Suited for modelling rotating turbulent flows in engines, the
renormalisation group (RNG) k-ε model [3] derived from the standard k-ε model is also considered. The standard k-ε model has a similar form to the RNG k-ε model except for the coefficients. The realisable k-ε model [4], a variation of the standard k-ε model with a different approach to closure is also considered. Due to the number of equations to solve, the Reynolds stress model appears increasingly challenging for integration with chemical kinetics reactions in later stages of the study to calculate auto-ignition.

5.3 Numerical validation

To validate the numerical modelling, different simulations are set to investigate the possible variations of mean velocity, vorticity, turbulent kinetic energy and cylinder pressure due to the following variables:

- The turbulence model used
- The convergence criteria
- The change of crank angle step size during the cycle
- The effects of deactivation and activation of the exhaust and inlet ports
- The cyclic variation
- The length of the inlet port
- The grid resolution and mesh quality

Most of the validation simulations were conducted at an early stage of the study on the geometry with spark-ignition valve timing. As the same geometry is used for CAI, but with different valve timings, it is assumed that the results obtained with SI settings are valid for both valve timings.
5.3.1 Turbulence models

Three turbulence models are examined in the current study: k-ε standard, k-ε RNG, k-ε realisable. Multiple simulations are run to investigate the variations between the turbulence models on the same geometry using the same settings. Prior simulations indicated that negligible variations of cylinder pressure (less than 0.01 bar) were recorded between the three turbulence models. However, the mean velocity in the cylinder is demonstrating higher variations. Further simulations are run to plot the differences of axial mean velocity, between the LDA experimental values obtained by Pitcher et al. (2003) [1] and CFD calculations, for four points spaced equally on the symmetry cutting-plane of the cylinder as shown in Figure 5.8. These points should reveal variations of the flow behaviour across the cylinder where high levels of turbulence are expected due to the tumble phenomenon.

The axial mean velocity at the four points for each turbulence model is compared to the measured data as depicted in Figure 5.9.
Figure 5.9 Axial mean velocity at the four points for three turbulence models

The velocity difference between the three turbulence models and the LDA measured data obtained by Pitcher et al. (2003) [1] is presented in Figure 5.10. The k-ε standard model seems to perform better than the other two k-ε models. It is assumed that the same flow
behaviour is occurring on other cross section planes of the cylinder. The $k$-$\varepsilon$ standard is therefore selected to conduct all the simulations presented in this study.

Figure 5.10 Axial mean velocity difference compared to the laser Doppler anemometry data for the four selected points
5.3.2 The convergence criteria
Calculations are conducted to quantify the turbulence variations in the cylinder between different convergence criteria accuracies. The purpose is to detect at which level the change of residuals demonstrates no improvement of in-cylinder velocities and turbulences for the solution. For the first simulation case, all the residuals defined as the continuity, the momentum and the k and ε transport equations are set to $10^{-1}$. The residuals are then reduced by a factor of 10 until a compromise between computational time and accuracy can be found. Figure 5.11 illustrates the average vorticity of all the points on the symmetrical cross section plane for residuals criteria values of 0.1, 0.01 and 0.001. It can be seen that the vorticity is consistent for all three values of residuals following the same trends. However, a large difference can be spotted between 0.1 and lower residual values.

![Graph showing average vorticity on the symmetry plane for various convergence residual levels.](image)

**Figure 5.11 Average vorticity on the symmetry plane for various convergence residual levels**

Figure 5.12 depicts the difference of vorticity between each residual level case, which also represents the error. The comparison between residuals at 0.1 and 0.01 demonstrates a large vorticity difference of up to 45 s$^{-1}$. The vorticity difference between residuals at 0.1 and 0.001 is also very large. However, comparing residuals of 0.01 and 0.001 shows little difference. It can therefore be concluded that all residuals can be set at 0.01, which
gives results close to high accuracy settings (lower residuals) while saving computational time, as additional iterations have smaller accuracy benefits.

To confirm findings, the mean velocity is also compared for two of the points selected on the lower part of the cylinder (axial 60 mm) for the symmetrical cross section plane as shown in Figure 5.13. The negative radial part of the cylinder, which corresponds to the area underneath the inlet valves, demonstrates a higher difference of velocities as shown in Figure 5.13(a), up to 0.12 m/s. The positive part of the cylinder shows velocity differences up to 0.65 m/s. It is noticed that the residuals at 0.1 compared to any lower residual levels are depicting the highest difference. Once again, as the residuals at 0.01 and 0.001 show the lowest velocity discrepancies, it confirms that residuals can be set at 0.01 without affecting the mean velocity at lower parts of the cylinder. The same behaviour is expected for the higher part of the cylinder.
Figure 5.13 Root-mean-square mean axial velocity difference between convergence residual levels for points at an axial level of 60 mm for (a) +30 mm radial position and (b) -30 mm radial position.
5.3.3 Crank angle step size

CFD calculations are conducted to determine the error as the crank angle step size changes during the cycle. In order to avoid computational crashes, the crank angle step size has to be reduced for the critical parts of the cycle, when component motion is inducing high variations of velocity in surrounding mesh cells i.e. when the valves open or close. It is found that the crank angle step size needs to be varied for values in the range of 0.05 to 1 CAD for the dynamic motions as shown previously in Figure 5.3. Hence, for this study, one simulation is conducted with a changing crank angle step size while another is conducted with a constant 0.05 CAD per step. The difference between the two calculations demonstrates less than 0.012 bar of cylinder pressure. Therefore, additional simulations are run to investigate the velocity and turbulence differences.

The difference of axial mean velocity between the two calculations is depicted in Figure 5.14 for one point in the cylinder (axial 60 mm; radial - 30 mm). It is noted that all the points studied demonstrated the same level of velocity difference, particularly for the peak seen after 540 CAD. In this figure, the difference reaches a maximum 0.088 m/s on a maximum scale of almost 20 m/s, which is an acceptable level of error for the gain of computational time. However, as no major differences have been seen for the cylinder pressure and velocities, the turbulence parameter needs to be studied.

![Figure 5.14 Effects of crank angle step size changes on velocity inside the cylinder](image-url)
For instance, the difference in terms of average vorticity for the symmetry plane is reported in Figure 5.15. A maximum difference of 4 s\(^{-1}\) is seen in the figure at 600 CAD while the maximum vorticity value is found to be 459 s\(^{-1}\) at around 400 CAD. The highest vorticity difference is seen particularly for the compression stroke after the inlet valves close. It is therefore concluded that the crank angle step size can be varied during the cycle to avoid crashes and highly reduce the computational time whilst maintaining consistent results.

Figure 5.15 Effects of crank angle step size changes on vorticity for the cross section valve symmetry plane
5.3.4 Deactivation and activation of the exhaust and inlet ports

The effects of deactivation or activation of the inlet port are studied. Simulations are run to investigate possible leakage at the inlet port junction and also the turbulence variation that sudden port activation can cause. One of the simulations is conducted using activation as well as deactivation. In another calculation, both ports are set to be activated for the full duration of the simulation. It is assumed that the deactivation of the exhaust port has a minimal effect on exhaust flow and in-cylinder turbulences for the fresh charge of the next cycle. The effect of the exhaust port deactivation during the exhaust stroke is therefore not studied. The preliminary simulations conducted to investigate the cylinder pressures demonstrate a negligible difference. Again, additional simulations are set to study other flow parameters. For instance, Figure 5.16 depicts the difference of mean velocity recorded on two of the points inside the cylinder (axial 60 mm; radial - 30 mm and axial 60 mm; radial + 30 mm). It can be seen from the figure that the mean velocity difference between the two models reaches a maximum of 0.0038 m/s, which is considered negligible on a scale of 17.4 m/s. As no significant differences between the models are found, additional calculations are simulated to study in-cylinder turbulences. The same conclusions are drawn for vorticity, which represents the in-cylinder turbulences where a difference of less than 2.3 s\(^{-1}\) is found over a maximum vorticity value of 459 s\(^{-1}\). Hence, the inlet and exhaust ports can be activated and deactivated during the cycle to reduce computational time, by reducing the number of mesh cells without altering the cylinder pressure, velocities and in-cylinder turbulences.
Figure 5.16 Effects of inlet port deactivation on cylinder velocity for (a) axial 60 mm; radial - 30 mm and (b) axial 60 mm; radial + 30 mm
5.3.5 The cyclic variation

An additional study was conducted to assess the cyclic variation. The turbulences were nil at the start of the simulation at cycle one. The cylinder vacuum, created during the cycle due to the closed valve and moving piston, was affected by the existing pressure inside the cylinder, the ports and the valve timing. Starting from cycle one, four cycles were calculated to demonstrate the difference of average mean velocity on the symmetry cutting plane between the cycles. A low difference between two cycles meant that a stability of pressure and velocity was reached. Using the CAI 3.6 mm valve timing and an engine speed of 1500 rpm, a representation of the mean velocity during the intake stroke for four cycles is shown in Figure 5.17. During the intake stroke, the mean velocity reaches a peak value. The cyclic variation at that peak shows a difference of 2 m/s between the four cycles. It can be seen on the figure that cycle 2, 3 and 4 are almost superimposed. Higher stability is found for the second cycle but still shows a lower mean velocity compared to the third cycle. The fourth cycle demonstrates the same level of mean velocity as the third cycle and almost matching results. It is assumed that the different valve timings will not alter those results, as a higher valve lift can only increase the stability of pressure and velocities inside the cylinder. Hence, all simulations should run three cycles where only the results from the third cycle should be presented for the rest of the study using all valve timings and lifts.

![Figure 5.17 Cyclic variation of mean velocity for the controlled auto-ignition 3.6 mm valve timing at 1500 rpm](image-url)
5.3.6 The length of the inlet port

An extended length version of the inlet port represented in Figure 5.18 is developed to investigate the effect of flow directionality from the inlet wall surface on in-cylinder turbulences and velocities. Again, the simulations do not show a significant cylinder pressure difference between the two inlet port models (maximum 0.041 bar). Additional simulations are therefore calculated on vorticity and velocity inside the cylinder to confirm the results for the inlet and compression stroke. The maximum vorticity difference seen on the cutting plane between the models reaches 23.2 s\(^{-1}\) over a maximum vorticity value of 459 s\(^{-1}\) and the highest velocity difference seen on the maximum of the four points selected reaches 0.24 m/s over a maximum vorticity value of 34 m/s for the point at an axial location 10 mm and radial - 30 mm. It can be considered negligible when compared to the full scale of the parameters measured. Hence, the model with a shorter inlet port can be selected for the study to reduce the number of mesh cells used, as the flow direction does not seem affected.

![Figure 5.18 Illustration of the shorter (a) and the longer inlet port models (b)]
5.3.7 Grid resolution and mesh quality

Finally, a grid dependency study is conducted to determine the mesh size for the best compromise between the quality of the results and the computational time. In order to improve the mesh quality of the full model, a hybrid mesh is used. The combustion chamber is meshed separately in hexahedrons and prism cells while the exhaust and inlet ports are meshed in tetrahedrons and pyramids cells due to the complex geometry. Mesh sizes of 3 mm, 2 mm and 1.5 mm are compared to assess the numerical diffusion of the model. It is assumed that the exhaust port mesh size is not affecting the flow inside the cylinder at a critical time of the cycle. Therefore, the exhaust port mesh size is kept at 3 mm, for the three cases. Due to the details needed for the definition of the clearance volume and movement of the valves, some parts were meshed under 1 mm cell size. The mesh quality of the model at TDC is depicted in Figure 5.19. The cells are coloured by equisize skew quality with the highest mesh quality represented by a ratio close to 0 while a poor quality mesh is seen with a ratio close to 1.

![Mesh quality of the model coloured by equisize skew](image)

Figure 5.19 Mesh quality of the model coloured by equisize skew
Table 5.1 defines the detailed mesh cell count of each part of the geometry.

<table>
<thead>
<tr>
<th>Grid Resolution</th>
<th>Intake Port Cell Count</th>
<th>Exhaust Port Cell Count</th>
<th>Volume Clearance Cell Count</th>
<th>Displacement Volume Cell Count</th>
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</thead>
<tbody>
<tr>
<td>Coarse</td>
<td>36 972</td>
<td>19 009</td>
<td>60 510</td>
<td>76 544</td>
</tr>
<tr>
<td>Grid 1 (3 mm)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Medium</td>
<td>56 181</td>
<td>19 009</td>
<td>79 356</td>
<td>164 866</td>
</tr>
<tr>
<td>Grid 2 (2 mm)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fine</td>
<td>129 064</td>
<td>19 009</td>
<td>106 169</td>
<td>285 597</td>
</tr>
<tr>
<td>Grid 3 (1.5 mm)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 5.2 defines the total mesh count at TDC and BDC.

<table>
<thead>
<tr>
<th>Grid Resolution</th>
<th>Total Number of Cells at TDC (including inlet and exhaust ports)</th>
<th>Total Number of Cells at BDC (including inlet and exhaust ports)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coarse</td>
<td>116 491</td>
<td>193 035</td>
</tr>
<tr>
<td>Grid 1 (3 mm)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Medium</td>
<td>154 546</td>
<td>319 412</td>
</tr>
<tr>
<td>Grid 2 (2 mm)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fine</td>
<td>254 242</td>
<td>539 839</td>
</tr>
<tr>
<td>Grid 3 (1.5 mm)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The total number of cells at BDC is plotted against the grid resolution in Figure 5.20. It can be seen that the total cells of the model are increasing exponentially as the mesh size is refined.
The volume average vorticity is compared for the three different grids for a full cycle as shown in Figure 5.21.

Also, the cylinder average turbulent kinetic energy is compared for the three different grids in Figure 5.22. A large difference is recorded between the coarse and medium grids. The comparison between the medium and fine grids shows a smaller difference in terms
of vorticity and turbulent kinetic energy. As a result, the medium grid is selected to conduct the study and reduce the computational time, without compromising the accuracy through numerical diffusion.

![Figure 5.2 Turbulent kinetic energy compared for three different grids](image)

For the selected grid resolution, the mesh quality can be studied. The total number of cells reach 154 546 at TDC. When the mesh quality is characterised by the equisize skew, the statistics showed that 92 890 cells have a factor of 0 - 0.4. A high mesh quality is seen with a ratio close to 0 and a poor mesh quality has a ratio close to 1. When the mesh quality is characterised by the equiangle skew, the statistics show that 85 448 cells have a factor of 0 - 0.4. This indicated that 60.1% of the mesh cells are high quality when defined by the equisize skew and 55.3% of the cells are high quality by equiangle skew.

A detailed repartition is given in Table 5.3. The cell number increases gradually until the piston reaches BDC. It is indicated from the simulation that the total number of cells reaches 319 412 at BDC. 80.7% of the mesh cells if considered by equisize skew are high quality while 78.4% of the dynamic mesh cells if judged by equiangle skew are high quality. A comparison of the mesh quality for both the start and end of the simulation indicates that a significant increase in the number of cells occurs with a mesh quality
factor of 0 - 0.1. The rest of the cylinder cells are included into the 0.1 - 0.3 range category, which is still high-quality mesh.

Table 5.3 Equiangle & equisize repartition at top dead centre

<table>
<thead>
<tr>
<th>Quality range</th>
<th>Number of cells</th>
<th>%</th>
<th>Quality range</th>
<th>Number of cells</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0 - 0.1</td>
<td>12 457</td>
<td>8.06 %</td>
<td>0.0 - 0.1</td>
<td>5 860</td>
<td>3.79 %</td>
</tr>
<tr>
<td>0.1 - 0.2</td>
<td>18 483</td>
<td>11.96 %</td>
<td>0.1 - 0.2</td>
<td>10 951</td>
<td>7.09 %</td>
</tr>
<tr>
<td>0.2 - 0.3</td>
<td>27 442</td>
<td>17.76 %</td>
<td>0.2 - 0.3</td>
<td>21 640</td>
<td>14.00 %</td>
</tr>
<tr>
<td>0.3 - 0.4</td>
<td>34 509</td>
<td>22.33 %</td>
<td>0.3 - 0.4</td>
<td>46 997</td>
<td>30.41 %</td>
</tr>
<tr>
<td>0.4 - 0.5</td>
<td>24 986</td>
<td>16.17 %</td>
<td>0.4 - 0.5</td>
<td>34 872</td>
<td>22.56 %</td>
</tr>
<tr>
<td>0.5 - 0.6</td>
<td>18 579</td>
<td>12.02 %</td>
<td>0.5 - 0.6</td>
<td>21 487</td>
<td>13.90 %</td>
</tr>
<tr>
<td>0.6 - 0.7</td>
<td>12 108</td>
<td>7.83 %</td>
<td>0.6 - 0.7</td>
<td>9 753</td>
<td>6.31 %</td>
</tr>
<tr>
<td>0.7 - 0.8</td>
<td>3 814</td>
<td>2.47 %</td>
<td>0.7 - 0.8</td>
<td>2 567</td>
<td>1.66 %</td>
</tr>
<tr>
<td>0.8 - 0.9</td>
<td>1 537</td>
<td>0.99 %</td>
<td>0.8 - 0.9</td>
<td>317</td>
<td>0.21 %</td>
</tr>
<tr>
<td>0.9 - 1.0</td>
<td>633</td>
<td>0.41 %</td>
<td>0.9 - 1.0</td>
<td>102</td>
<td>0.07 %</td>
</tr>
<tr>
<td>0.0 - 1.0</td>
<td>154 546</td>
<td>100.00 %</td>
<td>0.0 - 1.0</td>
<td>154 546</td>
<td>100.00 %</td>
</tr>
</tbody>
</table>

A detailed repartition is given in Table 5.4. Thus, the quality of the dynamic mesh modelling for the simulation of the flow inside the combustion chamber is improved from TDC to BDC by generating new cells of high-quality mesh.

Table 5.4 Equiangle & equisize repartition at bottom dead centre

<table>
<thead>
<tr>
<th>Quality range</th>
<th>Number of cells</th>
<th>%</th>
<th>Quality range</th>
<th>Number of cells</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0 - 0.1</td>
<td>135 501</td>
<td>42.42 %</td>
<td>0.0 - 0.1</td>
<td>128 903</td>
<td>40.36 %</td>
</tr>
<tr>
<td>0.1 - 0.2</td>
<td>52 606</td>
<td>16.47 %</td>
<td>0.1 - 0.2</td>
<td>45 075</td>
<td>14.11 %</td>
</tr>
<tr>
<td>0.2 - 0.3</td>
<td>35 141</td>
<td>11.00 %</td>
<td>0.2 - 0.3</td>
<td>29 339</td>
<td>9.19 %</td>
</tr>
<tr>
<td>0.3 - 0.4</td>
<td>34 509</td>
<td>10.80 %</td>
<td>0.3 - 0.4</td>
<td>46 997</td>
<td>14.71 %</td>
</tr>
<tr>
<td>0.4 - 0.5</td>
<td>24 986</td>
<td>7.82 %</td>
<td>0.4 - 0.5</td>
<td>34 872</td>
<td>10.92 %</td>
</tr>
<tr>
<td>0.5 - 0.6</td>
<td>18 579</td>
<td>5.82 %</td>
<td>0.5 - 0.6</td>
<td>21 487</td>
<td>6.73 %</td>
</tr>
<tr>
<td>0.6 - 0.7</td>
<td>12 108</td>
<td>3.79 %</td>
<td>0.6 - 0.7</td>
<td>9 753</td>
<td>3.05 %</td>
</tr>
<tr>
<td>0.7 - 0.8</td>
<td>3 814</td>
<td>1.19 %</td>
<td>0.7 - 0.8</td>
<td>2 567</td>
<td>0.80 %</td>
</tr>
<tr>
<td>0.8 - 0.9</td>
<td>1 537</td>
<td>0.48 %</td>
<td>0.8 - 0.9</td>
<td>317</td>
<td>0.10 %</td>
</tr>
<tr>
<td>0.9 - 1.0</td>
<td>633</td>
<td>0.20 %</td>
<td>0.9 - 1.0</td>
<td>102</td>
<td>0.03 %</td>
</tr>
<tr>
<td>0.0 - 1.0</td>
<td>257 756</td>
<td>80.70 %</td>
<td>0.0 - 1.0</td>
<td>250 314</td>
<td>78.37 %</td>
</tr>
<tr>
<td>0.0 - 1.0</td>
<td>319 412</td>
<td>100.00 %</td>
<td>0.0 - 1.0</td>
<td>319 412</td>
<td>100.00 %</td>
</tr>
</tbody>
</table>
Figures 5.23 and 5.24 depict the cell quality repartition difference between TDC and BDC in total cell number and percentage, respectively. It can be seen that the mesh cell creation from TDC to BDC is improving the mesh quality cells for both equisize and equiang skew by a significant amount. Hence, the overall mesh quality from TDC to BDC is improved by over 20 %.

Figure 5.23 Repartition of Equisize at top dead centre and bottom dead centre in total cells number and percentage
Figure 5.24 Repartition of Equiangle at top dead centre and bottom dead centre in total cells number and percentage
5.4 Boundary conditions and initial values

As the simulations have to be validated using current experimental data, the simulations are conducted to match the experimental conditions as closely as possible. As the LDA experimental work was conducted at atmospheric conditions by Pitcher et al. (2003) [1], no fuel was injected and the cylinder mixture can therefore be considered as non-reactive. The operating pressure inside the cylinder and the inlet port is assumed to be at 101 325 Pa with an air inlet temperature of 15 °C. The gas properties set into the software are defined as a simplified air composition following the ideal gas law. Since no fuel was injected during the experimental work, the consideration of a simple version of air composition containing 78 % of nitrogen (N₂), 21 % of oxygen (O₂) and 1 % of argon (Ar) by volume is a good approximation of the exact composition of dry atmospheric air composed of 78.084 % of N₂, 20.947 % of O₂, 0.934 % of argon (Ar), 0.033 % of carbon dioxide (CO₂), the other species representing 0.002 % of the total volume. The consideration of air relative humidity can be discarded. The change in air mass due to the addition of relative humidity to dry atmospheric air can be considered negligible. For instance, the addition of water vapour to dry air only reduces the density of the air by a small amount as the molecular mass of water (18 g/mol) is lighter than molecular mass of dry air (28 g/mol). Therefore, the density selected is the one of atmospheric dry air at 15 °C, 1.225 kg/m³. The dynamic viscosity is set to \( \mu = 1.79 \times 10^{-5} \) kg/m.s.

The boundary conditions are:

- The inlet port surface is set as inlet pressure. It allows the air to enter the inlet port, depending on the in-cylinder vacuum when the inlet valves open. The pressure set on the inlet port surface is equal to the atmospheric conditions i.e. 101 325 Pa, 18 °C, 78 % of N₂, 21 % of O₂ and 1 % of Ar. The engine is naturally aspirated, which means only a small restriction can be caused by the intake filter. Therefore, the inlet port pressure could be considered equal to atmospheric, and no gauge pressure is set in addition to the operating pressure on the inlet surface.

- The exhaust port surface is set as outlet pressure, which allows the cylinder gas mixture to exit the cylinder freely through the exhaust port, depending on the cylinder pressure when the exhaust valves open. It is assumed that no restriction of flow due to after
treatment occurred during the experimental LDA measurements conducted by Pitcher et al. (2003) [1]. Hence, no gauge pressure is set in addition to the exit operating pressure; the atmospheric pressure.

- The initial pressure inside the cylinder can be assumed to be almost equal to the atmospheric pressure at specific timings during the cycle. During the exhaust stroke, the piston is moving upward increasing the cylinder pressure. When the exhaust valves open, the air contained in the cylinder exits through the exhaust port due to the difference of pressure within the cylinder. The in-cylinder pressure reduces until equilibrium with the exhaust port pressure is reached. It can be assumed that the pressure inside the cylinder is close to atmospheric conditions when the exhaust valves are closing. The simulations should all start at the event exhaust valves close (EVC), as the cylinder pressure is known. Moreover, as three cycles are necessary to reduce the cyclic variations of pressure and turbulence, an approximation of the cylinder pressure is only used to initialise the first cycle of the simulation. As the cylinder pressure of the following cycles will reach equilibrium, the results presented for the third cycle should be stable.

- The valves are set to be moving walls in the simulation. The valve lifts are defined using the user defined functions (UDF) to implement a position profile which is updated for each step of the simulations.

- The convergence criteria adopted in the simulation are as follows:

  (1) The continuity is set to $10^{-2}$;
  (2) The momentum is set to $10^{-2}$;
  (3) The k and $\varepsilon$ transport equations are set to $10^{-2}$;
  (4) No energy equation is considered for this part of the study.

- The near-wall treatment employs a standard wall function. As the mesh size selected is 2 mm, the centre-point of the first layer of cells in the cylinder is spaced 1 mm apart from the wall surface avoiding the flow to be in the viscous zone. It is noticed from the simulation that Y+ values fell between 30 and 500, thus ensuring the validity of the application of the standard k-$\varepsilon$ model, to model the flow inside the cylinder.
5.5 Concluding remarks

This chapter presents the modelling considerations and numerical validation steps. A validation of the model was intended between the CFD prediction and LDA experimental results. Conclusions drawn from this part of the study were summarised as follows:

(1) The standard k-ε turbulence model seemed to perform better than the two other k-ε models and was therefore selected to conduct all simulations presented in this study.

(2) The convergence criteria study showed that the residuals could be set to $10^{-2}$ without compromising the results.

(3) The cyclic variation study showed that the fourth cycle demonstrated the same level of mean velocity as the third cycle. It was concluded that the results had converged at the third cycle which would be presented for the rest of the study using all valve timings and valve lifts.

(4) The study conducted on the length of the inlet port has shown that the model with a shorter inlet port could be selected for the study to reduce the number of mesh cells as the flow direction was not affected.

In this study, the dynamic mesh option was used for the CFD simulation of transient flow inside the cylinder, taking into consideration the movement of the piston and valves. The three types of dynamic mesh were implemented in the model; layering, spring smoothing and local remeshing. The layering mesh option was used to create the part representing the displacement volume in the cylinder. Due to the complexity of the geometry, the clearance volume and ports were meshed using tetrahedron, pyramid and prism cells. For the grid resolution and mesh quality study, it was found that:

(1) A mesh study was conducted and revealed that the overall mesh quality was improved by over 20% as the piston was moving down from TDC to BDC.
(2) A grid meshing size of 2 mm showed the best compromise between the computational time required to complete the simulation and the corresponding results of volume average vorticity, average plane vorticity and turbulent kinetic energy.

Finally, a methodology for reducing computational time was presented. The conclusions drawn from the computational time reduction method were summarised as follows:

(1) During the CFD calculations, the ports were deactivated while their respective valves were closed to reduce the number of mesh cells. It has shown to save up to 40% of the total computational time for spark-ignition valve timing and up to 55% for the CAI 3.6 mm valve timing, when compared to simulations without ports deactivations. The port deactivations have demonstrated no alteration of the results for the cylinder pressure, velocities and in-cylinder turbulences.

(2) The crank angle step size was varied during the cycle to adapt to the dynamic motion of the valves and save computational time, while maintaining a consistency of the results (average plane vorticity and mean velocity).
References


Chapter 6: In-cylinder flow of spark-ignition valve timing

Although the experimental studies on flow inside internal combustion (IC) engines using the laser Doppler anemometry (LDA) and particle tracking velocimetry (PTV) can provide a physical insight into the real flows inside the cylinder [1, 2], the use of such experimental technology is usually expensive and it is still impossible to obtain the entire flow details for IC engines in practice. As an alternative, the use of computer-aided design and computational fluid dynamics (CFD) has become popular for IC engine optimisation and design. However, the results of CFD modelling have to be validated against relevant experiments. One of the advantages of CFD modelling is that the settings for simulations can be recorded and these will provide a basis for further studies. CFD modelling of turbulent flows inside a combustion chamber of vehicle engines have been used for many years [3, 4, 5, 6, 7, 8, 9 and 10].

This chapter presents the computational fluid dynamics modelling results of the transient flow structure inside the cylinder of a four valve Lotus engine single cylinder at a speed of 1500 revolutions per minute (rpm) during the intake and compression stroke. A dynamic mesh is created to simulate the movement of the piston and standard spark-ignition valve timing. The CFD simulations replicate the experimental work, where only air was inserted into a driven optically accessible single cylinder. The first part of this chapter compares the calculated mean velocities against the reprocessed time-dependent axial and radial mean velocities, obtained from LDA measurements provided by Pitcher et al. (2003) [11], aiming for a validation of the numerical model. Calculated from 400 crank angle degree (CAD) to 640 CAD, the CFD results show an overall agreement with the LDA measurements of 78.3 %. The second part of the chapter presents the development of the flow pattern inside the cylinder at the symmetrical cross section where the tumble motions and their centre are described for 450 CAD and 540 CAD. Results are presented for the variation of turbulence parameters such as turbulence intensity (TI), turbulence kinetic energy (TKE) and turbulence dissipation rate (TDR) during the intake and compression stroke.
6.1 Model validation

The experimental measurement conducted and provided by Pitcher et al. (2003) [11] are described in details in Chapter 4 on three different cutting-planes, namely 1, 2 and 3. Plane 1 is the symmetry plane, cutting inlet and outlet ports at Y = 0 mm; Plane 2 is the centre-plane of the cylinder at X = 0 mm and Plane 3 is the offset plane, cutting inlet and outlet ports at 18 mm from the centre-line at Y = -18 mm. The measurement points are spaced horizontally every 10 mm from -10 mm to -60 mm and vertically every 5 mm from -35 to 35 mm on planes 1 and 2, from -30 to 30 mm on plane 3 due to a smaller cross-section. An illustration of these points is recapitulated in Figure 6.1.

![Figure 6.1](image)

**Figure 6.1 Calculated points corresponding to the laser Doppler anemometry measurements on (a) plane 1, (b) plane 2 and (c) plane 3**

Two components of mean velocity relative to their planes are recorded in time for each point during the experimental work. As the numerical simulations are set to match the experimental settings and conditions, the same velocity components of each corresponding LDA measurement point on planes 1, 2 and 3 are calculated and recorded separately for every crank angle step of the simulations. The same valve profiles are used with a maximum inlet valve lift of 8.5 mm and maximum exhaust valve lift of 8 mm. As for the LDA measurements, the events inlet valves open (IVO), inlet valves close (IVC), exhaust valves open (EVO) and exhaust valves close (EVC) occur at 331 CAD, 609 CAD, 130 CAD and 402 CAD, respectively.
A comparison between experimental and numerical results can be drawn for model validation. 84 measurement points on planes 1 and 2, and 72 points on plane 3 are measured. The CFD calculations give a total of 2137 values in time during the intake stroke and compression stroke for each of the 240 measurement points on the 3 planes. These values are reported on graphs for an easier comparison between CFD and LDA. 240 points with two velocity components each, for 2137 time steps gives around one million values to be processed. 480 figures are created to visualise a time-dependent map of mean velocity inside the cylinder. However, due to the amount of data, the results of two vertical lines of axial velocity on plane 1 are presented in the following figures for a comparison between the LDA data and numerical calculations. On each side of the cylinder, the points are separated 30 mm from the centre-line as shown in Figure 6.2. The selection of the points should illustrate the tumble phenomenon.

![Figure 6.2 Selected points on plane 1](image)

The rest of the results are averaged to describe the overall accuracy of the CFD model for all points of planes 1, 2 and 3.
The axial mean velocities of those points are represented in Figure 6.3 for both the experimental and calculated values. Observing the results for both CFD and LDA, it can be concluded that:

- The CFD calculations are in good agreement with the LDA in particular for the positive radial line of points.

- The top half of the cylinder is demonstrating nearly matching results.

- The positive radial part of the cylinder is showing more accurate results than the negative part.

- The CFD results show an over-prediction of the negative radial line of points. This is particularly true for the bottom half of the cylinder.

The 480 figures obtained from all 240 measured and calculated points cannot be presented fully in this chapter. Therefore, an average result is necessary so that the overall performance of the model can be presented. In order to define how the numerical model predicts the flow patterns inside the whole cylinder, each point of the specific plane can be averaged for its own value in time. It should be noted that the top dead centre firing (TDCF) position occurs at 720 CAD.
Figure 6.3 Axial mean velocity on the -30 mm (left) and +30 mm radial line (right) for 10 mm, 20 mm, 30 mm, 40 mm, 50 mm and 60 mm axial lines
Figure 6.4 represents the average mean velocity on plane 1 of the LDA data and the CFD results. It is calculated by using all the points located on plane 1 for an average value in time. For each point, the root-mean-square (RMS) of the two-dimensional (2D) mean velocity is calculated as a combination of the axial and radial velocities projected on the plane. To be noted that each line of points is reached by the piston at different crankshaft angles. When the piston passes through the cylinder lines, the velocity recorded is equal to the piston speed for a short period of time. This produces irregularities on the figure between 394 CAD and 460 CAD, between 620 CAD and 684 CAD. It can be seen that the CFD calculation is under-predicting the mean velocity during the second half of the intake stroke, but also over predicting the velocity for the first half of the compression stroke.

![Figure 6.4 Plane 1 average root-mean-square two-dimensional mean velocity](image)

Figure 6.4 Plane 1 average root-mean-square two-dimensional mean velocity

Figure 6.5 depicts the average mean velocity difference between the LDA data and the CFD results for the points located on plane 1. The maximum difference shown is 2.33 m/s.
Figure 6.5 Average root-mean-square velocity difference between the laser Doppler anemometry data and the computational fluid dynamic results for the points located on plane 1

The velocity difference can be converted into a percentage as depicted in Figure 6.6. A high-velocity difference is found between 650 CAD and 685 CAD and can be explained by a large velocity difference compared to a low mean velocity at the end of the compression stroke.

Figure 6.6 Plane 1 root-mean-square velocity difference between laser Doppler anemometry data and the computational fluid dynamic results reported as a percentage
The process has to be repeated for each of the three planes to give the accuracy per plane. The values can be compared to give the performance per plane. The three plane accuracy can be averaged to give an estimated overall accuracy of the model. The LDA data is available from 400 CAD to 680 CAD, but it would possible to increase the number of points and planes in the CFD calculations, to obtain further details of the cylinder mean velocities. However, the additional calculated values would not be compared to any experimental work for the model validation.

Table 6.1 is showing the resulting average value of mean velocity for each plane. Overall, the CFD model shows an accuracy of 72.45%. It is noted that the percentage accuracy of the model is impaired at the end of the compression stroke. Considering a part of the cycle, with a minimum mean velocity of 2 m/s, would allow obtaining a more representative value of CFD accuracy.

<table>
<thead>
<tr>
<th>Plane</th>
<th>Average model accuracy (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Plane 1</td>
<td>71.02 %</td>
</tr>
<tr>
<td>Plane 2</td>
<td>75.85 %</td>
</tr>
<tr>
<td>Plane 3</td>
<td>70.49 %</td>
</tr>
<tr>
<td>3 planes average</td>
<td>72.45 %</td>
</tr>
</tbody>
</table>

From 400 CAD to 640 CAD, the overall prediction of the model is increased to 78.32% as seen in Table 6.2.

<table>
<thead>
<tr>
<th>Plane</th>
<th>Average model accuracy (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Plane 1</td>
<td>80.75 %</td>
</tr>
<tr>
<td>Plane 2</td>
<td>78.71 %</td>
</tr>
<tr>
<td>Plane 3</td>
<td>75.51 %</td>
</tr>
<tr>
<td>3 planes average</td>
<td>78.32 %</td>
</tr>
</tbody>
</table>
6.2 Results for the in-cylinder turbulence

The CFD results obtained can be used to describe the development of the intake flow pattern inside the cylinder using velocity vectors. Two typical piston positions of 450 CAD and 540 CAD are selected to characterise the flow field development inside the cylinder, which corresponds to the second half of the intake stroke. At these angles, the corresponding displacement of the inlet valves is 8.41 mm and 3.12 mm for 450 CAD and 540 CAD, respectively. It should be noted here that the maximum inlet valve lift of 8.5 mm occurs at an angle of 460 CAD, corresponding to a piston displacement of 59.2 mm.

Figure 6.7 shows the velocity field development in the symmetry cutting-plane for two crankshaft angles. At an angle of 450 CAD, the tumble motion is just formed, as seen in Figure 6.7a. The highest velocity of the flow occurs at the region marked as 1, at approximately 40 m/s. It can be seen that the main part of the high-velocity flow is at the top of the cylinder and around the valves. The flow diverges around the valve to generate two counter-rotating tumble vortices 2 and 3. Such counter-rotating flow is deflected by the cylinder wall and piston, resulting in the loss in intensity of the vortices. It can be seen that the clockwise tumble vortex 2 is stronger than 3 at this stage. The vortices rotational centre is marked as 4. At this angle, the piston velocity is 6.95 m/s and the openness of the valve is 98.94 % of the maximum valve lift. The maximum velocity found from the simulation in the symmetry plane is 7.31 m/s at 434 CAD. Since the valves are nearly fully opened at this angle, the incoming flow can easily enter the cylinder with less valve obstruction. This velocity difference can be expressed as a factor between the piston area and the inlet wetted area. The bore is equal to 0.0805 m, which gives a piston area of 5.09 \times 10^{-3} m^2. The inlet hydraulic diameter of 0.0385 m gives a wetted area of 1.16 \times 10^{-3} m^2. With an instantaneous piston velocity of 6.95 m/s, the corresponding multiplying coefficient between the wetted area of the inlet and the piston surface of 4.38 would give a velocity of 30.44 m/s at the inlet surface. This can be explained by the additional flow restriction around the valves. It can also be due to a time delay of air flow between the piston and inlet surface.
Figure 6.7b depicts the flow pattern at an angle of 540 CAD. At this angle, the piston velocity is nil and the valve lift of 3.12 mm represents an openness of 36.7 %. Although the flow velocities have reduced as a result of a reduction of the piston speed, when the angle is greater than 434 CAD, the overall flow inside the cylinder is strongly affected by the inertia of the tumble motion. The flow at 1 still diverges around the valve to generate two counter-rotating tumble vortices 2 and 3 as in Figure 6.7a. The conical jet marked 3 evolves into a larger rotating vortex inside the cylinder. The strength of the vortices has now developed, compared to the previous flow behaviour at 450 CAD. The anti-clockwise rotating tumble 3 is reaching a maximum of 15 m/s while 2 is attaining 8 m/s. However, the turbulence seen as 4 in Figure 6.7b is moving up in the cylinder. It is noticed that a secondary vortex marked 5 is formed at the bottom left-hand side of the cylinder as a result of the interaction of flow deflection by the piston, the inertia of the impinging jet and their differences in strength. This clockwise vortex confirms that the rotating tumble vortex 2 is faster than vortex 3. The sizes of the two major tumble vortices increase due to the increase in cylinder volume.
As differences of velocity on the symmetry plane have been observed during the intake stroke, this could also lead to variations of the turbulence parameters during the compression stroke, which in turn could affect the mixing of the charge prior to combustion. Monitoring the turbulence parameters at specific points, located at the top of the cylinder, should reveal their variations as the clearance volume is accessible during the full cycle. Figure 6.8 shows the location of the points selected to conduct a comparison.
of the TI, the TKE and the TDR. All the points are located 3 mm higher than the piston maximum upper position, top dead centre (TDC). Six points are dispatched around the valves on the radial cutting-plane located at 0 mm on the axial cylinder axis z.

Figure 6.8 Selected points for comparison of the turbulence parameters for (a) side view and (b) top view
Figure 6.9 depicts the variations of turbulence parameters during the intake and compression stroke at points located on the radial cutting plane at a \( z = 0 \) mm axial cylinder position (3 mm above TDC). The inlet valves open at 331 CAD and by 360 CAD (TDC gas exchange) the valve lift is 0.7 mm. As the inlet valve lift increases further, all the turbulence parameters rise progressively until reaching a maximum value, different for each point. The peak value occurs at different crankshaft angles for the different locations in the clearance volume. The peak of turbulence seen at the point \( x = -30 \) mm; \( y = 0 \) mm; \( z = 0 \) mm can be explained by its proximity to the inlet valves. As the points distance with the inlet valves rises, increasing their position on the x-axis, the maximum value gradually decrease and occurs at a later crankshaft angle. The flow being directed by the valves to form the tumble and swirl phenomena is stronger around the valves. The maximum valve lift occurs at 460 CAD and the turbulence parameters are already seen to decrease. At the end of the intake stroke, the piston speed reduces and the turbulences decrease for all the points within the clearance volume. As the piston is moving up and increasing speed during the compression stroke, the points see their turbulence parameters rising again. As the inlet valves are now closed since 609 CAD, only the piston movement is affecting the turbulences, which explains lower levels compared to the intake stroke. However, differences in terms of TI and TKE are still present for the points in the clearance volume at TDCF (720 CAD) which could affect the mixing of air and fuel. It is expected that the high levels of turbulence parameters, seen at the end of the compression stroke, will directly affect the flame propagation.
Figure 6.9 TI (a), TKE (b) and TDR (c) on the selected points within the clearance volume.
6.3 Concluding remarks

This chapter presents the results of numerical calculations on the transient flow structure inside an engine cylinder at 1500 rpm during the intake and compression stroke. A dynamic mesh is created to simulate the movement of the piston and the valves. A standard spark-ignition valve timing is applied to replicate the experimental work. The first part aims to validate the model by comparing experimental and simulated data. It is found that the calculations are in good agreement with the LDA measurements provided by Pitcher et al. (2003) [11], in particular for the positive radial line of points and the top half of the cylinder. An over-prediction is noticed for the negative radial lines of points at the bottom half of the cylinder. Overall, the CFD calculations seemed to match the LDA data reasonably well with an overall averaged agreement of 78.3 % for the spark-ignition valve timing from 400 CAD to 640 CAD.

The second part of the chapter depicts the development of the flow pattern inside the cylinder at the symmetrical cross section and also the variation of turbulence levels for different points selected in the clearance volume. The conclusions drawn from this part can be summarised as follows:

(1) The simulation of the transient flow inside the cylinder has clearly revealed the existence of tumble phenomenon for the inlet stroke. This has been reported previously by experimental studies in this area of research. Tumble motion was developed significantly during the intake stroke.

(2) As the movements of the valves and piston are modelled, vortex centres change inside the cylinder. The tumble centre is moving upwards between 450 CAD and 540 CAD. The predicted flow behaviour shows the creation of a secondary vortex at the bottom of the cylinder in opposing rotation to the primary vortex.

(3) The variation of turbulence levels such as TI, TKE and TDR have been drawn for the intake and compression stroke. For all turbulence parameters, a peak value, relative to the distance with the inlet valves, occurs as the inlet valves open at different crankshaft angles for the various locations in the clearance volume. The turbulence parameters start to
decrease before the maximum valve lift is reached. As the piston is moving up and increasing speed during the compression stroke, the turbulence parameters rise again. However, differences in terms of TI and TKE are still present for the points in the clearance volume at TDCF which could affect the mixture quality and the flame propagation.
**References**


Chapter 7: Results and discussions for controlled auto-ignition valve timings

The first part of this chapter presents the results of the computational fluid dynamics (CFD) calculations of transient air flow characteristics inside a single cylinder at speeds of 1500 and 2000 revolutions per minute (rpm) in controlled auto-ignition (CAI) mode with 3.6 mm valve lift timing. The calculated three-dimensional mean velocities are validated against the time-dependent axial and radial mean velocity laser Doppler anemometry (LDA) data provided by Pitcher et al. (2003) [1]. The simulations replicate the experimental work, where only air was inserted into a motored optical engine. The numerical results show workable agreements with the LDA measurements of 75.1 % at 1500 rpm and 73.4 % at 2000 rpm. The second part of this chapter describes the development of the flow pattern inside the cylinder at the symmetrical cross section, where the tumble phenomenon and its vortex change are described for the intake and compression stroke. Also, the turbulence intensity (TI), the turbulence kinetic energy (TKE) and turbulence dissipation rate (TDR) are presented for a better understanding of the effect of engine speed on the generated turbulences. The effects of engine speed on charge amount and charge delay are also presented and discussed.
7.1 Model validation

The numerical calculations aim to replicate the LDA experimental work conducted and provided by Pitcher et al. (2003) [1] on a single cylinder in CAI mode as presented in Chapter 4. Two mean velocity components relative to their planes are compared against each corresponding LDA measurement point. Points are selected on three different cutting-planes, namely 1, 2 and 3. Plane 1 is the symmetry plane cutting inlet and outlet ports at \( y = 0 \) mm; Plane 2 is the centre-plane of the cylinder at \( x = 0 \) mm and Plane 3 is the offset plane cutting inlet and outlet ports at 18 mm from the centre-line at \( y = -18 \) mm. On planes 1 and 2, the measurement points are spaced horizontally every 10 mm from -10 mm to -60 mm and vertically every 5 mm from -35 to 35 mm, respectively and from -30 to 30 mm on plane 3, due to a smaller cross-section. A recapitulation of the planes and the measurement points is illustrated in Figure 7.1.

![Figure 7.1](image)

**Figure 7.1 Calculated points corresponding to the laser Doppler anemometry measurements on (a) plane 1, (b) plane 2 and (c) plane 3**

Using a lift of 3.6 mm for the inlet and exhaust valves in the simulations, the two velocity components per point are recorded separately for each of the time steps during the cycle (2249 time steps for 1500 rpm and 1835 time steps for 2000 rpm). 84 measurement points for planes 1 and 2, and 72 points for plane 3 are recorded at 1500 rpm and 2000 rpm during the engine cycle. Hence, two million values are processed into time-dependent graphs for the two engine speeds. 960 figures are created to visualise a time-dependent map of mean velocity inside the cylinder. However, due to the amount of data, the results of two vertical lines of axial velocity on plane 1 are
presented into the following figures, for a comparison between the LDA data and numerical calculations. On each side of the cylinder, the points are separated 30 mm from the centre-line as shown in Figure 7.2. The selection of the points should illustrate the difference of tumble motion between the two engine speeds.

![Figure 7.2 Selected points on plane 1](image)

Figure 7.2 Selected points on plane 1

The rest of the results can be averaged to describe the overall accuracy of the CFD model for all points of planes 1, 2 and 3. Combining those results should give a global performance value of the model for the three planes.
The axial mean velocities of those points are represented on the following figures for both the experimental and numerical values at 1500 rpm in Figure 7.3 and 2000 rpm in Figure 7.4. It should be noted that the top dead centre firing (TDCF) position can be found at 0 crank angle degree (CAD) and 720 CAD. Observing the axial mean velocity from both numerical (CFD) and measured (LDA) results at 1500 rpm and 2000 rpm engine speeds, it can be concluded that:

- The calculations are reasonably comparative to the LDA measurements.

- The results show better agreement at 1500 rpm than 2000 rpm.

- The calculated results show nearly matching velocities, when compared to LDA measurements, for the positive radial line of points (+ 30 mm). This corresponds to the side of the cylinder where the exhaust valves operate. An under-prediction of the velocity is seen around 540 CAD from 5 m/s on the axial position 40 mm increasing to 12.4 m/s on the axial position 60 mm for an engine speed of 2000 rpm.

- An over-prediction of the calculated results for the negative radial line of points (- 30 mm) is seen around 515 CAD. This corresponds to the half of the cylinder where the inlet valves operate. For 1500 rpm, the mean velocity difference is seen increasing from 5.8 m/s on the axial position 10 mm to 17.1 m/s at 60 mm. A different pattern is seen for 2000 rpm with an under-prediction of the calculated values of 10.9 m/s at an axial position of 10 mm changing into an over-prediction of 12.1 m/s at 30 mm increasing to 21.6 m/s at 60 mm.
Figure 7.3 Axial mean velocity at the -30 mm (left) and +30 mm radial line (right) for 10 mm, 20 mm, 30 mm, 40 mm, 50 mm and 60 mm axial lines for 1500 rpm
Figure 7.4 Axial mean velocity at -30 mm (left) and +30 mm radial line (right) for 10 mm, 20 mm, 30 mm, 40 mm, 50 mm and 60 mm axial lines for 2000 rpm
All the 240 measurement points are distributed on the three planes. Each point, on each plane, has around 2100 time dependent values (depending on model version and speed) for axial and radial mean velocity, obtained with a numerical calculation for the two engine speeds of 1500 rpm and 2000 rpm. Each velocity point obtained by LDA measurement has 180 values in time for 720 CAD, one every 4 CAD. This gives an excessive amount of data. Therefore, an averaging method is necessary to describe the overall performance of the model.

In order to define how the numerical model predicts the flow patterns inside the whole cylinder, each point of the specific plane has been averaged over time, as shown in Figure 7.5. It should be noted that each line of points is reached by the piston at different crankshaft angles. This produces irregularities on the results seen between 42 CAD and 119 CAD, between 258 CAD and 326 CAD for the power and exhaust stroke, between 405 CAD and 461 CAD, and between 616 CAD and 686 CAD for the intake and compression stroke, respectively.
Comparison between experimental and numerical results of the root-mean-square (RMS) values of the axial and radial velocity components are shown in Figures 7.6 and 7.7. Figure 7.6 shows plane 1 average RMS velocity difference between LDA and CFD results. The maximum difference is found to occur during the intake stroke, 9.43 m/s at 496 CAD for 1500 rpm and 7.6 m/s at 480 CAD for 2000 rpm. For the rest of the cycle, the calculation predicted the mean velocity with less than 1.8 m/s difference at 1500 rpm during the compression, power and exhaust stroke. The difference in results between the calculations and measurements is higher at 2000 rpm, as compared to those obtained at 1500 rpm.
Figure 7.6 Average root-mean-square differences between calculated and measured velocities at (a) 1500 rpm and (b) 2000 rpm for the points located on plane 1.

When converted into percentage in Figure 7.7, the calculation is showing reasonable agreement against the measured data. The high peaks of velocity difference seen around 52, 304, 412 and 664 CAD can be explained by a large difference value compared to a low mean velocity.
The process has to be repeated for each of the three planes 1, 2 and 3 to give the accuracy per plane. The three plane accuracies can then be averaged to represent the overall accuracy of the model. The first line of points in the cylinder ( - 10 mm ) is defined from 40 CAD to 320 CAD and 400 CAD to 680 CAD from the experimental part. The numerical calculation can give further details of the cylinder mean velocities, but these values cannot be compared to the experiments, due to lack of measurements at those points. Table 7.1 provides average values of mean velocity for each of the three
planes selected. Overall, the calculated results show an accuracy of 75.1\% and 73.4\% for 1500 rpm and 2000 rpm, respectively.

Table 7.1 Average model accuracy from 0 CAD to 720 CAD for each plane at engine speeds of 1500 rpm and 2000 rpm

<table>
<thead>
<tr>
<th></th>
<th>RMS difference (m/s)</th>
<th>Model accuracy (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1500 rpm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Plane 1</td>
<td>0.792</td>
<td>73.35%</td>
</tr>
<tr>
<td>Plane 2</td>
<td>0.789</td>
<td>78.05%</td>
</tr>
<tr>
<td>Plane 3</td>
<td>0.950</td>
<td>73.78%</td>
</tr>
<tr>
<td>3 planes average</td>
<td>0.844</td>
<td>75.06%</td>
</tr>
<tr>
<td>2000 rpm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Plane 1</td>
<td>1.158</td>
<td>68.23%</td>
</tr>
<tr>
<td>Plane 2</td>
<td>0.746</td>
<td>78.87%</td>
</tr>
<tr>
<td>Plane 3</td>
<td>0.903</td>
<td>73.16%</td>
</tr>
<tr>
<td>3 planes average</td>
<td>0.936</td>
<td>73.42%</td>
</tr>
</tbody>
</table>

7.2 Results for the in-cylinder turbulence
The calculated results are used to describe the development of the intake flow pattern inside the cylinder using velocity vectors. Five typical crankshaft angles are selected to characterise the flow field development inside the cylinder before the power stroke: top dead centre (TDC) gas exchange at 360 CAD, 450 CAD, 540 CAD, 630 CAD and TDCF at 720 CAD.

Figure 7.8 shows the velocity field development at the inlet port symmetry plane for five crankshaft angles. The crankshaft angle value of 360 CAD in Figure 7.8 represents TDC gas exchange of the 3rd cycle when the cycle to cycle variation is negligible. At this crank angle, no difference in velocity is observed. The inlet valves are not yet opened, as they start to open at 421 CAD. At 434 CAD, the piston position is 39 mm where the piston speed reaches a maximum of 7.31 m/s and 9.75 m/s for 1500 rpm and 2000 rpm, respectively. At 450 CAD, the corresponding inlet valve lift is 1 mm, the piston position is 51.75 mm and the piston speed decreases to 6.95 m/s and 9.26 m/s for 1500 rpm and 2000 rpm, respectively. The velocity fields are proportionally distributed at 450 CAD, gradually higher, close to the piston surface and smaller close to TDC, as
presented in Figure 7.8. The level of velocity difference seen between 1500 rpm and 2000 rpm varies from 0 at the top of the cylinder to 2 m/s close to the piston. It should be noted here that the maximum inlet valve lift of 3.6 mm occurs at a crankshaft angle of 505 CAD, corresponding to a piston displacement of 82.7 mm and the piston speed reduced to 2.9 m/s. At a crank angle value of 540 CAD, the corresponding inlet valve lift is reduced to 2.5 mm. The piston position reaches bottom dead centre (BDC) at 88.2 mm and the piston speed is decreased to 0 before starting a negative speed for the compression stroke. The location of the inlet valves in-flow is marked as 1 in the figure, which depicts stronger velocity vectors for 2000 rpm than for 1500 rpm. The area marked as 2 is seen to be at 25 m/s for both 1500 rpm and 2000 rpm, but the maximum velocity at that point is reported at a lower position for 1500 rpm when compared to 2000 rpm. It can be seen that the tumble motion is clearly forming, stronger at 2000 rpm than at 1500 rpm. At the area marked 3, the velocity is seen at 13.6 m/s for 1500 rpm and 25 m/s for 2000 rpm. The area marked 4 depicts velocities of 18 m/s for 1500 rpm and 35 m/s for 2000 rpm. It shows a consequent difference for both engine speeds, as only an increase of 500 rpm can double the velocity levels on this plane under the inlet valves. It can be noted that two vortices are seen forming at 540 CAD; the lower vortex centre, marked 6, is the same for both speeds but the velocity levels are nearly doubled, 12 m/s for 1500 rpm and 25 m/s for 2000 rpm. The middle vortex’s centre 5 is reported at different locations, 2000 rpm being higher in the cylinder than 1500 rpm. However, a maximum velocity of 14 m/s is found for both engine speeds. The inlet valves are closing at 605 CAD. The velocity field reduces consequently, as seen in the figure for 630 CAD. The turbulence levels reported here show a difference between 1500 rpm and 2000 rpm of nearly twice the maximum velocities for the tumble motion at 630 CAD. At 720 CAD, higher velocity fields are observed at 2000 rpm compared to 1500 rpm.
As the two engine speeds have shown differences of velocity fields, additional parameters can be studied to investigate the effect of engine speed on the turbulences, which could affect the mixing of the charge prior to combustion. Various points at the
top of the cylinder within the clearance volume are selected, to allow monitoring the turbulence parameters fully during the intake and compression stroke. Figure 7.9 shows the location of the points selected to conduct a comparison of the turbulence intensity, the turbulence kinetic energy and the turbulence dissipation rate. All the points are located 3 mm higher than the piston maximum upper position, TDC. Six points are dispatched around the valves on the radial cutting-plane located at 0 mm on the axial cylinder axis z.

**Figure 7.9** Selected points for comparison of the turbulence parameters for (a) side view and (b) top view
Figure 7.10 illustrates the turbulence intensity, the turbulence kinetic energy and the turbulence dissipation rate for the points located on the radial cutting plane at a $z = 0$ mm axial cylinder position (3 mm above TDC) at 1500 rpm during the intake and compression stroke. Two important areas in the figure should be noted, the intake stroke from 360 CAD to 540 CAD and compression stroke from 540 CAD and 720 CAD. The inlet valves open at 421 CAD, and by 451 CAD the valve lift is already reaching 1 mm. The three quantities have similar profiles. As the inlet valve lift increases, all the turbulence parameters rise progressively until reaching a maximum value different for each point. The highest values are seen at the points $x = 0$ mm ; $y = 0$ mm ; $z = 0$ mm and $x = -30$ mm ; $y = 0$ mm ; $z = 0$ mm. These results are expected due to the proximity of the points to the inlet valves, opening during the intake stroke, resulting in a strong merging flow at the symmetry cutting plane. The peak values for the turbulence parameters are occurring around 490 CAD. The maximum valve lift occurs at 405 CAD and the turbulence parameters are already seen to decrease. At the end of the intake stroke, the piston speed reduces and the turbulences decrease for all the points within the clearance volume. At the start of the compression stroke, the values are still decreasing until 585 CAD. As the piston is moving up and increasing speed during the compression stroke, the points see their turbulence parameters rising again. The inlet valves close at 609 CAD, which explains lower values compared to the intake stroke. However, different values for the turbulence intensity, turbulence kinetic energy and turbulence dissipation rate are recorded for the points in the clearance volume at TDCF (720 CAD). For instance, at TDCF, the turbulence intensity varies between 1.83 % and 2.46 % for all the points. Also, the turbulence kinetic energy depicts values between 3.8 m$^2$/s$^2$ and 9.5 m$^2$/s$^2$ at TDCF and between 946 m$^2$/s$^3$ and 2283 m$^2$/s$^3$ for the turbulence dissipation rate.
Figure 7.10 Turbulence intensity (a), turbulence kinetic energy (b) and turbulence dissipation rate (c) on the selected points at 1500 rpm
Figure 7.11 depicts the turbulence intensity, the turbulence kinetic energy and the turbulence dissipation rate for the same points during the intake and compression stroke at an engine speed of 2000 rpm. The trends for the three parameters are very similar when compared to 1500 rpm. The differences between the engine speeds can be described in two parts: the turbulence maximum values and the duration of the turbulences. The engine speed is increased by a third from 1500 rpm and 2000 rpm. One of the main differences noted between engine speeds of 1500 rpm and 2000 rpm is that the peak values seen during the intake stroke are mostly consistent with a 33 % increase. Also, the duration of the peak value during the intake stroke is increased by up to 11.5 CAD when compared to 1500 rpm. The variation of the values is similar at TDCF compared to 1500 rpm. At the top of the cylinder, the TI, TKE and TDR vary between 2.1 % and 3.4 %, between 6.5 m²/s² and 17 m²/s² and between 1 870 m²/s³ and 5 505 m²/s³ at TDCF, respectively.

In conclusion, the two engine speeds display similar trends for all three quantities TI, TKE and TDR during the intake stroke and compression stroke. As the engine speed is increased by a third, the peak values depict approximately a 33 % rise. When increasing the engine speed by 33 %, the duration of the peaks during the intake stroke is extended by up to 11.5 CAD. The most significant conclusion is found to be the differences of turbulence seen at different locations in the clearance volume prior to auto-ignition. It is clear that engine speed is an important factor contributing to cylinder turbulences. It is concluded that engine speed could affect mixture quality by mixing the air, the fuel and the residual gases, through turbulence levels in particular, at the end of the compression stroke where all turbulence levels are seen higher for 2000 rpm when compared to 1500 rpm.
Figure 7.11 Turbulence intensity (a), turbulence kinetic energy (b) and turbulence dissipation rate (c) on the selected points at 2000 rpm
7.3 Engine speed effect on charge delay

Prior to inlet valves open (IVO), the cylinder pressure is related only to the mixture density and the piston position, which governs the cylinder volume. The combustion chamber is a closed volume and the in-cylinder flow velocity is proportional to the piston velocity, and the distance from the piston, due the expansion of the air and cylinder vacuum. This was demonstrated by the velocity magnitude at the symmetry cutting plane in Figure 7.8.

A comparison is presented for a speed of 1500 rpm in Figure 7.12(a) and 2000 rpm in Figure 7.12(b). The average cylinder axial velocities during the intake stroke are illustrated for the radial cutting plane located 10 mm below TDC. The corresponding inlet valve timing and piston velocity are also presented. Similar plane velocity behaviour is observed for both engine speeds. When the inlet valves open, the difference of pressure between the inlet port and the cylinder vacuum forces the air inside the combustion chamber. Despite the piston speed reducing from IVO, the plane average velocity increases and reaches a peak value higher than the current piston speed. This can be explained by the vacuum still being present in the cylinder and the inertia of air. The main difference between the two engine speeds can be seen in terms of velocity magnitude. For 1500 rpm, the magnitude is nearly matching the piston speed, while being almost 2 m/s under the piston speed at 2000 rpm.
Figure 7.12 Average axial velocity for the cutting plane located 10 mm below top dead centre during the intake stroke for (a) 1500 rpm and (b) 2000 rpm

When the two engine speeds are plotted onto the same graph, the charge velocity is very similar as shown in Figure 7.13. For the two engine speeds, the charge enters the cylinder at the same velocity rate. However, the engine speed of 2000 rpm shows higher velocity levels and a longer duration of charge intake. It suggests that both engine
speeds do not have the same amount of charge intake. Observing the density results confirmed this finding as the volume at TDCF is similar for both engine speeds, $5.57 \times 10^{-5}$ m$^3$. The mixture density at TDCF was found to be 9.71 kg/m$^3$ for 1500 rpm and 9.8 kg/m$^3$ for 2000 rpm. This gives a trapped mass contained in the cylinder of 541 mg and 546 mg for 1500 rpm and 2000 rpm, respectively. The trapped mass at TDCF represents the fresh charge intake and the residual air trapped from the previous cycle. It corresponds to an increase of the amount of fresh charge by 0.9 % when compared to 1500 rpm. It can therefore be concluded that an increase of engine speed results in a higher amount of charge intake, therefore changing the concentration value for the residual gases and altering the air-fuel ratio (AFR).

![Graph](image)

**Figure 7.13** Plane average axial velocity during the intake stroke for engine speeds of 1500 rpm and 2000 rpm

The charge delay can be expressed in terms of crankshaft angle degree difference, between piston velocity and charge velocity, at same velocity levels. A comparison of the charge delay for both engine speeds is presented in Figure 7.14. The valve timing is identical for both engine speeds and the charge delay starts at the same location on the graph. It demonstrates that the engine speed has no effect on the cylinder vacuum prior to IVO as it is a closed volume. At 438 CAD, the valve lift is less than 0.1 mm and the charge velocity is already delayed by 63 CAD compared to the piston speed.
As the valves open further, the charge delay increases for both engine speeds. It can be noted that the air delay increases to a higher level for 2000 rpm when compared to 1500 rpm. The charge delays reach maximum values of 75.5 CAD and 80.5 CAD for 1500 rpm and 2000 rpm, respectively. As the valves timing, valves restriction and cylinder vacuum are the same for both speeds, the difference of charge delay can only be explained by the change of piston velocities. It indicates that the velocity rate of the charge entering the cylinder is already at maximum due to the valves restriction. For the case of 1500 rpm, the rate at which the charge enters the cylinder is greater than the piston velocity, which leads to a decrease of charge delay. The valves open further and the charge delay is found to reduce at a faster rate for 1500 rpm than 2000 rpm, reaching 43.3 CAD and 75 CAD at 474 CAD for 1500 rpm and 2000 rpm, respectively. A higher engine speed increases the charge delay during the intake stroke.

Figure 7.14 Charge delay on the radial cutting plane located 10 mm below top dead centre for the two engine speeds of 1500 rpm and 2000 rpm during the intake stroke

Important variations of velocity are observed between the two engine speeds. It is expected that engine speed could affect the mixing of fuel for port injected fuel engines and the amount of charge entering the cylinder.
7.4 Concluding remarks

In this chapter, a dynamic mesh CFD simulation of transient flow inside an internal combustion engine cylinder is conducted, taking into consideration the movement of the piston and valves. The first part intends to validate the model through comparison between experimental and calculated data. It is found that the calculations are in reasonable agreement with the LDA measurements conducted and provided by Pitcher et al. 2003 [1], in particular at the positive radial direction. An over-prediction is noticed for the negative radial direction between 450 CAD and 630 CAD. Overall, the CFD calculations seemed to match the LDA data reasonably well with an overall averaged agreement of 75.1 % at 1500 rpm and 73.4 % at 2000 rpm for the 3.6 mm CAI valve timing, against the corresponding experimental measurements.

The second part of this chapter describes the development of the flow pattern inside the cylinder at the symmetrical cross section, where the tumble phenomenon and its vortex change are found to be different between the two engine speeds studied. The main vortex centre is found to be higher for 2000 rpm as compared to 1500 rpm engine speed. At the cylinder wall just below the inlet valves, the velocity is nearly doubled in value when comparing the two engine speeds. Therefore, increasing the engine speed is found to create a stronger tumble motion.

Also, the two engine speeds display similar trends for all three quantities TI, TKE and TDR during the intake stroke and compression stroke. The two engine speeds displayed similar trends for all three turbulence quantities TI, TKE and TDR during the intake stroke and compression stroke. As the engine speed was increased by a third, the peak values rose accordingly. However, the duration of the turbulence peaks during the intake stroke was extended by up to 11.5 CAD. The turbulence quantities have been found to vary at the different locations in the clearance volume and between engine speeds prior to auto-ignition.

For the two engine speeds, the charge enters the cylinder at the same velocity rate. However, the engine speed of 2000 rpm shows higher velocity levels and a longer duration of charge intake. An increase of engine speed results in a higher amount of
charge intake. The valve timing is identical for both engine speeds and the charge delay starts at the same timing already delayed by 63 CAD compared to the piston speed. As the valves open, the charge delay increases for both engine speeds. The air delay increases to a higher level for 2000 rpm when compared to 1500 rpm. Also, a higher engine speed increases the charge delay during the intake stroke.

It is clear that engine speed is an important factor contributing to cylinder turbulences. It is concluded that engine speed could affect mixture quality by mixing the air, the fuel and the residual gases, through turbulence levels in particular, at the end of the compression stroke where all turbulence levels are seen higher for 2000 rpm when compared to 1500 rpm. Engine speed could also affect the amount of charge entering the cylinder which will alter the AFR.
Reference

Chapter 8: Effects of valve timings on the fresh charge, residual gas mixing and auto-ignition

This chapter presents the results of the computational fluid dynamics (CFD) calculations combined with chemical kinetics inside an engine cylinder running at a speed of 2000 revolutions per minute (rpm). The simulations replicate the experimental work conducted and provided by Pitcher et al. 2003 [1] on a single cylinder engine where gasoline was injected into the inlet port in controlled auto-ignition (CAI) mode. Six different valve timings are applied to the model, with a valve lift of 6 mm, to retain various burnt mixture residual concentrations within the cylinder. The calculated results are validated against experimental measurements of the cylinder pressure. The first part of this chapter describes the engine parameters and settings used in both the experiments and the simulations respectively. Calculations of the air composition and fuel quantity injected during the tests are also presented and discussed. Finally, the effects of the valve timings on the fresh charge velocity along with the mixing and temperature of the charge are revealed.

8.1 Engine initial parameters and simulation settings

8.1.1 The chemical kinetics model

A typical gasoline mixture is mainly composed of alkanes, cycloalkanes and alkenes. Alkanes, also called saturated hydrocarbons, are a chemical compound of carbon and hydrogen linked exclusively by single bonds. The generic chemical formula is $\text{C}_n\text{H}_{2n+2}$ where $n$ is the number of carbon atoms. They are saturated compounds with no cyclic structure like butane ($\text{C}_4\text{H}_{10}$), which is formed of four carbon atoms connected in a line with ten hydrogen atoms around. Each carbon atom has four connections. The two central carbon atoms have two single bonds with other carbon atoms and two with hydrogen atoms. The two carbon atoms at the extremities of the molecular structure have three single bonds to hydrogen atoms and one bond to the central carbon atoms. Cycloalkanes are a type of alkane which contain one or more rings of carbon atoms in their molecule structure. Their general formula is $\text{C}_n\text{H}_{2(n+1-g)}$, where $g$ is the number of carbon rings within the structure. An example would be cyclopropane ($\text{C}_3\text{H}_6$) where three carbon atoms are connected by the same length bond to form a perfect triangular
shape surrounded by hydrogen atoms (two hydrogen atoms per carbon atom). Alkenes (or olefins) are unsaturated chemical compounds containing at least one carbon to carbon double bond. The generic chemical formula is $C_nH_{2n}$ [2]. The simplest of the alkenes is ethylene ($C_2H_4$), each having a double bond between the two carbon atoms, each having two single bonds with hydrogen atoms.

Gasoline is distilled directly from crude oil. The composition of gasoline varies by the distillation process used by a refinery, the grade of crude oil used and the octane rating required. Once distilled, additives like toluene ($C_7H_8$) and benzene ($C_6H_6$) are used to raise the octane number, improving auto-ignition limits and avoiding knock. Some mixtures also contain significant quantities of ethanol ($C_2H_5OH$) as a partial fuel alternative. The typical hydrocarbon components of gasoline are butane, iso-butane, heptane, hexane, cyclohexane, pentane, iso-pentane, benzene, toluene, cyclohexane, octane and iso-octane. A gasoline mixture contains more than 150 separate compounds, although as many as 1000 have been identified in some blends. In chemistry, isomers are compounds which share the same molecular formula but have different structural geometries. With the same number of carbon and hydrogen atoms, the bonds which join them are connected differently. Octane ($C_8H_{18}$) is an alkane which has 18 structural isomers like methylheptane, dimethylhexane, iso-octane and trimethylpentane. Octane and its isomers, which are highly flammable, are the main components of gasoline. The simulations aim to match the experimental work conducted on the thermodynamics single cylinder engine where gasoline was used as fuel. Researchers have shown the combustion process of gasoline can be modelled using 1036 species and 4238 reactions [3]. Mechanisms for gasoline surrogates include n-heptane, iso-octane, toluene and $C_5$-$C_6$ olefins [4] which reach as many as 1389 species and 5935 reactions. As the number of species and reactions increases the computational time of CFD calculations exponentially, it is clear that the use of such a model is currently limited by available computer capabilities. Each reaction adds an equation to be solved, for each crank angle step of the cycle. Hence, a reduced chemical kinetics model has to be used in this study. As the exact composition of the fuel used during the experimental work is unknown, an assumption has to be made to set the reactant in the software. A simpler approach is to consider that gasoline is modelled using a mixture of n-heptane and iso-octane as an
approximation [5]. The research octane number (RON) of octane is defined as 100 while heptane is defined as 0. The correct octane number of the entire fuel mixture can be obtained by using the appropriate amount of octane and heptane. A mixture of 87 % octane and 13 % heptane (by volume) was selected for this study, to represent a fuel mixture of 87 RON [6]. Using the densities of 703 kg/m³ for octane and 679.5 kg/m³ for heptane, the fuel concentration by volume can be converted into a mass fraction. The fuel mixture content is 87.4 % of C₈H₁₈ and 12.6 % of C₇H₁₆ by mass.

Also, a reduced chemical kinetics model with 32 species and 55 reactions [7] is selected to conduct the study. The reaction mechanism produces adequate results to calculate the ignition delay and burn rates of an iso-octane and n-heptane mixture in CAI engines. An interaction between iso-octane and n-heptane is included in the chemical kinetics model. The two-stage ignition profile, typical of controlled auto-ignition of heptane, is modelled with low and high-temperature chain reactions. A fully detailed list of species and reactions is available in the appendices section.

### 8.1.2 Air composition, stoichiometry and air-fuel ratio

During the combustion process, the oxygen reacts with the fuel. The ratio of fuel to oxygen defines the mixture properties, rich if there is more fuel and lean if there is more oxygen. Stoichiometry is defined as the equilibrium where all molecules of oxygen react with all molecules of the fuel, both reactant and oxidant being consumed. Hydrocarbon fuels have different atomic compositions with various contents of carbon and hydrogen changing the stoichiometry value. For the calculation of stoichiometry and the air-fuel ratio (AFR), the air composition needs to be taken into account. A detailed list of species contained in atmospheric dry air is presented in Table 8.1. The concentration is shown in parts per million by volume (ppmv).
Table 8.1 Composition of dry atmospheric air per volume

<table>
<thead>
<tr>
<th>Species</th>
<th>Molecular formula</th>
<th>Concentration (ppmv)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen</td>
<td>N₂</td>
<td>780 840.00</td>
</tr>
<tr>
<td>Oxygen</td>
<td>O₂</td>
<td>209 460.00</td>
</tr>
<tr>
<td>Argon</td>
<td>Ar</td>
<td>9 340.00</td>
</tr>
<tr>
<td>Carbon dioxide</td>
<td>CO₂</td>
<td>390.00</td>
</tr>
<tr>
<td>Neon</td>
<td>Ne</td>
<td>18.18</td>
</tr>
<tr>
<td>Helium</td>
<td>He</td>
<td>5.24</td>
</tr>
<tr>
<td>Methane</td>
<td>CH₄</td>
<td>1.79</td>
</tr>
<tr>
<td>Krypton</td>
<td>Kr</td>
<td>1.14</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>H₂</td>
<td>0.55</td>
</tr>
<tr>
<td>Nitrous oxide</td>
<td>N₂O</td>
<td>0.30</td>
</tr>
<tr>
<td>Carbon monoxide</td>
<td>CO</td>
<td>0.10</td>
</tr>
<tr>
<td>Xenon</td>
<td>Xe</td>
<td>0.09</td>
</tr>
<tr>
<td>Ozone</td>
<td>O₃</td>
<td>0.07</td>
</tr>
<tr>
<td>Nitrogen dioxide</td>
<td>NO₂</td>
<td>0.02</td>
</tr>
<tr>
<td>Iodine</td>
<td>I₂</td>
<td>0.01</td>
</tr>
</tbody>
</table>

The corresponding atomic weights in unified atomic mass units (u) are presented in Table 8.2.

Table 8.2 Atomic weight (u)

<table>
<thead>
<tr>
<th>Element</th>
<th>Atomic weight (u)</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>14.006700</td>
</tr>
<tr>
<td>O</td>
<td>15.999400</td>
</tr>
<tr>
<td>Ar</td>
<td>39.948000</td>
</tr>
<tr>
<td>C</td>
<td>12.010700</td>
</tr>
<tr>
<td>Ne</td>
<td>20.179700</td>
</tr>
<tr>
<td>He</td>
<td>4.002602</td>
</tr>
<tr>
<td>H</td>
<td>1.007940</td>
</tr>
<tr>
<td>H₂</td>
<td>1.007830</td>
</tr>
<tr>
<td>Kr</td>
<td>83.798000</td>
</tr>
<tr>
<td>Xe</td>
<td>131.293000</td>
</tr>
<tr>
<td>I</td>
<td>126.904470</td>
</tr>
<tr>
<td>S</td>
<td>32.065000</td>
</tr>
</tbody>
</table>

Using the concentration values from Table 8.1 and the atomic weight values from Table 8.2, the air composition by mass can be expressed in percentage, as shown in Table 8.3.
Table 8.3 Calculated dry air composition by mass in percentage

<table>
<thead>
<tr>
<th>Species</th>
<th>Composition (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen (N₂)</td>
<td>75.5127%</td>
</tr>
<tr>
<td>Oxygen (O₂)</td>
<td>23.1381%</td>
</tr>
<tr>
<td>Argon (Ar)</td>
<td>1.2881%</td>
</tr>
<tr>
<td>Carbon dioxide (CO₂)</td>
<td>0.0593%</td>
</tr>
<tr>
<td>Other species</td>
<td>0.0019%</td>
</tr>
</tbody>
</table>

Only the species considered in the chemical kinetics model can be included in the air composition. It can be seen that four species are representing the majority of the mass and all other remaining species represent only a very small fraction of the air composition. The engine reference conditions, selected for this part of the study, are based on international standards organisation (ISO) documents. ISO 8528/1 and ISO 3046/1 define the engine testing reference conditions to be 25 °C for the air inlet temperature, 100 kPa for the operating pressure and a relative humidity of 30 % in air. The dry air can be assumed to be an ideal gas with a constant specific heat capacity of $C_p = 1005 \text{ J/kg.K}$. The ideal gas law can be expressed in its common form:

$$PV = nRT$$  \hspace{1cm} (8-1)

where $P$ is the absolute pressure of the gas, $V$ is the volume of the gas, $n$ is the amount of gas substance, $R$ is the ideal gas constant (equal to the product of Boltzmann’s constant and Avogadro’s constant which gives $8.314 \text{ J.K}^{-1}\text{.mol}^{-1}$) and $T$ is the absolute temperature in K. The amount of gas substance is equal to the mass divided by the molar mass:

$$n = \frac{m}{M}$$  \hspace{1cm} (8-2)

The density of the gas is equal to the mass divided by the volume:

$$\rho = \frac{m}{V}$$  \hspace{1cm} (8-3)

where $\rho$ is the air density. Replacing terms 8-2 and 8-3 in equation 8-1 gives:

$$P = \rho \frac{R}{M} T$$  \hspace{1cm} (8-4)
where \( \frac{R}{M} \), which represents the specific gas constant, is equal to 287 J/kg.K for dry air.

This form of the equation relates density to pressure and temperature. Re-arranged from equation 8-4, the density can be expressed as:

\[
\rho = \frac{P}{R} \frac{M}{T}
\]  

(8-5)

The density of dry air, for the given temperature of 25 °C and a pressure of 100 kPa, is 1.184 kg/m³. The relative humidity of 30 % can now be introduced into the equation. As for air, water vapour can also be treated as an ideal gas. When mixed together, the total pressure \( P \) can be defined as:

\[
P = P_{\text{water}} + P_{\text{air}}
\]  

(8-6)

where \( P_{\text{water}} \) is the partial pressure of water vapour and \( P_{\text{air}} \) is the partial pressure of dry air. At a temperature of 25 °C and a pressure of 100 kPa, the partial pressure for saturated water vapour is equal to 3.17 kPa. For this value of pressure, the air is saturated in water vapour, which means the relative humidity in the air is equal to 100 %. A relative humidity of 30 % represents a partial pressure of 0.95 kPa. Therefore, the partial pressure of dry air is equal to 99.05 kPa, which is the difference between the total pressure and the partial pressure of water vapour. As stated previously, \( R \) is equal to 8.314 J.K⁻¹.mol⁻¹. The molar mass of water \( M_{\text{water}} \) is 0.018 kg/mol while the molar mass of dry air \( M_{\text{air}} \) is 0.029 kg/mol.

The specific gas constant of water vapour \( \frac{R}{M_{\text{water}}} \) can be calculated and is found to be equal to 461.5 J/kg.K. The specific gas constant of dry air \( \frac{R}{M_{\text{air}}} \) obtained previously is 287 J/kg.K. For one cubic metre of dry air with 30 % relative humidity, the mass of each component can be calculated as follows:

\[
m_{\text{air}} = \frac{P_{\text{air}}V}{R_{\text{air}}T}
\]  

(8-7)
which gives 1.16 kg.

\[ m_{\text{water}} = \frac{P_{\text{water}}V}{R_{\text{water}}T} \]  

(8-8)

which gives 6.9 g.

As the mass of each gas species has been obtained, the composition can be deduced. 99.4 % of the gas composition is dry air and 0.6 % is water vapour. The new composition of air (by mass), including 30 % relative humidity at standard conditions, is shown in Table 8.4.

<table>
<thead>
<tr>
<th>Nitrogen (N\textsubscript{2})</th>
<th>75.0620 %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oxygen (O\textsubscript{2})</td>
<td>23.0000 %</td>
</tr>
<tr>
<td>Argon (Ar)</td>
<td>1.2804 %</td>
</tr>
<tr>
<td>Water vapour (H\textsubscript{2}O)</td>
<td>0.5969 %</td>
</tr>
<tr>
<td>Carbon dioxide (CO\textsubscript{2})</td>
<td>0.0589 %</td>
</tr>
<tr>
<td>Other species</td>
<td>0.0019 %</td>
</tr>
</tbody>
</table>

Table 8.4 Air composition with 30 % relative humidity at 25 °C (% by mass)

For stoichiometric combustion of a typical gasoline, the AFR is found to be between 14.6:1 and 15.3:1 but depends on the gasoline blend. Two atoms of oxygen are needed to oxidise one atom of carbon and one atom of oxygen is necessary for the oxidation of two hydrogen atoms. Using the atomic weight presented in Table 8.2, the weight ratio of oxygen can be calculated and found to be 2.664:1 for carbon and 7.937:1 for hydrogen. In other words, 2.66 kg of oxygen is needed for the oxidation of 1 kg of carbon and 7.94 kg of oxygen is needed for the oxidation of 1 kg of hydrogen. By mass, octane is composed of 84.1 % carbon for 15.9 % hydrogen (C\textsubscript{8}H\textsubscript{18}) and heptane is 83.9 % carbon for 16.1 % hydrogen (C\textsubscript{7}H\textsubscript{16}). The stoichiometric AFR is found to be 15.22:1 and 15.27:1 for octane and heptane respectively. For a mixture of 87.4 % of octane and 12.6 % of heptane by mass, the stoichiometric AFR becomes 15.23:1. As CAI operation is running with a lean mixture of fuel to reduce the peak of pressure at top dead centre firing (TDCF), the actual AFR will be much higher than the stoichiometric AFR.
8.1.3 Calculation of fuel amount injected from apparent net heat release rate

Calculated from the filtered experimental cylinder pressure, using Equation 4-1 from Chapter 4, the apparent net heat release rate (HRR) is presented in Figure 8.1 for each valve timing.

(a)

(b)
The total fuel injected, during the experiments on the single cylinder, can be calculated. The apparent net HRR, in Joules per degree, can be integrated over its duration in crankshaft angle degrees. A visual reading of each HRR curve gives the start and the
end of the heat release for the integration duration in crank angle degree (CAD). The results of the integrals give the total energy released by the fuel over time during the cycle. A fuel mixture with an octane number of 87 is composed of 87.4 % octane and 12.6 % heptane (by mass). The low heating value (LHV) of the fuels is known, 44.57 MJ/kg for octane and 44.43 MJ/kg for heptane. The overall mixture LHV is found to be 44.55 MJ/kg. The total fuel energy released into the cylinder can now be calculated, as presented in Table 8.5.

### Table 8.5 Start and end timing for HRR

<table>
<thead>
<tr>
<th>Residual gases</th>
<th>36 %</th>
<th>41 %</th>
<th>46 %</th>
<th>51 %</th>
<th>55 %</th>
<th>59 %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Start of HRR</td>
<td>-18.5</td>
<td>-9.5</td>
<td>-9.5</td>
<td>-7.5</td>
<td>-9.5</td>
<td>-11.5</td>
</tr>
<tr>
<td>(CAD)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>End of HRR</td>
<td>15.5</td>
<td>25.5</td>
<td>18.5</td>
<td>19.5</td>
<td>21.5</td>
<td>15.5</td>
</tr>
<tr>
<td>(CAD)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Calculated total fuel energy (J)</td>
<td>363.8</td>
<td>381.3</td>
<td>391.4</td>
<td>377.4</td>
<td>351.1</td>
<td>333.2</td>
</tr>
<tr>
<td>Calculated fuel amount (mg)</td>
<td>8.17</td>
<td>8.56</td>
<td>8.79</td>
<td>8.47</td>
<td>7.88</td>
<td>7.48</td>
</tr>
</tbody>
</table>

The total fuel energy can be plotted on a graph for each residual gases level to check consistency between valve timings as presented in Figure 8.2.

![Figure 8.2 Fuel energy calculated for each valve timing](image-url)
The corresponding fuel quantity is presented in Figure 8.3 for each case. The results suggest that the amount of fuel varied during the test with a lower amount of fuel required for high residual gases levels. This can be explained by the lower amount of oxygen available for combustion at high residual gases levels. Hence, the fuel injected is reduced to maintain the AFR higher than stoichiometric. The average fuel amount is found to be 8.22 mg for all cases.

![Figure 8.3 Fuel amount calculated for each valve timing](image)

8.1.4 Engine initial parameters

The measured cylinder pressures for each valve timing are stored in files using the ACAP software. The pressures corresponding to events inlet valves open (IVO), inlet valves close (IVC), exhaust valves open (EVO) and exhaust valves close (EVC) can be obtained from the measurements. Although the simulations can start at any point and run several cycles until convergence of temperature and pressure, a convenient point to start the simulation is at the IVO event. All the chemical reactions occurring during the expansion stroke have been completed and the cylinder contains only residual gases following the exhaust stroke. Also, the CFD calculations start prior to IVO where the cylinder turbulences would be affected by the intake flow. From the measured data the cylinder temperatures, for all the valve timings, are given at EVC. All the valves are closed between the two events EVC and IVO, therefore, the same mixture remains in the cylinder. For the same substance at different sets of conditions, the combined gas
law can be applied to deduce the temperature at IVO using the values at EVC. Avogadro’s law states that for a given mass of an ideal gas at a constant pressure and temperature, the volume and the amount of gas are directly proportional.

\[
\frac{V}{n} = k \tag{8-9}
\]

where \(k\) is a constant, \(V\) and \(n\) are the cylinder volume and the amount of substance of the gas, respectively. A direct consequence of Avogadro’s law is that the ideal gas constant \(R\) is the same for all gases. Using the ideal gas law (8-1) for two conditions of pressure, temperature and volume can be expressed as:

\[
P_1V_1 = n_1RT_1 \tag{8-10}
\]

and

\[
P_2V_2 = n_2RT_2 \tag{8-11}
\]

The combined gas law equation can now be expressed as:

\[
\frac{P_1V_1}{n_1T_1} = \frac{P_2V_2}{n_2T_2} \tag{8-12}
\]

The cylinder temperatures are calculated from measured pressure data, calculated cylinder volume and initial measured EVC temperatures. The CFD simulation initial CAD, cylinder temperature and cylinder pressure are presented in Table 8.6.
Table 8.6 CFD simulation initial parameters

<table>
<thead>
<tr>
<th>Valve timing</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Measured residual</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>gases</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>36</td>
<td>41</td>
<td>46</td>
<td>51</td>
<td>55</td>
<td>59</td>
</tr>
<tr>
<td>Simulation starting</td>
<td>CAD</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>angle (IVO)</td>
<td>427</td>
<td>433</td>
<td>438</td>
<td>443</td>
<td>448</td>
<td>453</td>
</tr>
<tr>
<td>Cylinder temperature</td>
<td>K</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>753.6</td>
<td>766.8</td>
<td>779.4</td>
<td>766.2</td>
<td>756.6</td>
<td>740.5</td>
</tr>
<tr>
<td>Cylinder pressure</td>
<td>kPa-abs</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>143.3</td>
<td>139.5</td>
<td>144.2</td>
<td>135.1</td>
<td>127.0</td>
<td>119.7</td>
</tr>
</tbody>
</table>

It should be noted that any cylinder pressure and temperature can be set as initial values. The purpose of using realistic initial values is to save computational time by reaching a faster convergence by reducing cyclic variations.

8.2 Model validation and calibration

A comparison of calculated and experimental cylinder pressure for each valve timing at an engine speed of 2000 rpm is shown in Figure 8.4. The CFD simulation showed that using valve timing 1 auto-ignition is not possible. The results were confirmed by Osei-Owusu et al. (2007) [8]. The maximum mixture temperature reached during compression is too low. This is mainly due to a low burnt mixture concentration retained in the cylinder, due to a long exhaust valve duration or a low amount of fuel injected. CFD simulations have shown that for this valve timing, a minimum of 11.63 mg of fuel must be injected in order for the auto-ignition to occur. It suggests spark assistance was needed during the experimental work. The consequences of the mixture misfire in the CFD simulation, using valve timing 1, are an under-prediction of the cylinder pressure at TDCF and an over-prediction of the cylinder pressure at TDC gas exchange. The peak of pressure at TDC gas exchange is found to be under-predicted by the rest of the CFD simulations compared to the measured data, except for valve timing 6. As the fuel type is known and the fuel quantity injected has been calculated, the valve parameters are the only variables which can alter the pressure at TDC gas exchange. This could indicate that a combination of the valve lift profile, timing, geometry (or the discharge coefficient (Cd)) used in the CFD simulations is not identical to the ones used during the experimental tests.
Cylinder average pressure (bar-abs)

(a)

Valve timing 1: Measured pressure
Valve timing 1: Simulated pressure

TDC gas exchange
TDCF

Cylinder average pressure (bar-abs)

(b)

Valve timing 2: Measured pressure
Valve timing 2: Simulated pressure

TDC gas exchange
TDCF
Figure 8.4 Comparison of CFD calculated and measured experimental cylinder pressures for valve timing (a) 1, (b) 2, (c) 3, (d) 4, (e) 5 and (f) 6.
The simulation results are presented in Table 8.7. The quantity of residual gas contained in the cylinder can be defined as the trapped mass at EVC over the trapped mass at IVC. The calculated residual gases are under-predicted compared to the measured ones, along with the pressures, at TDC gas exchange.

Table 8.7 Measured and calculated residual gases for all valve timings

<table>
<thead>
<tr>
<th>Valve timing</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Measured residual gases</td>
<td>%</td>
<td>36</td>
<td>41</td>
<td>46</td>
<td>51</td>
<td>55</td>
</tr>
<tr>
<td>Measured pressure at TDC gas exchange</td>
<td>bar</td>
<td>11.25</td>
<td>12.35</td>
<td>14.14</td>
<td>14.61</td>
<td>15.16</td>
</tr>
<tr>
<td>Calculated pressure at TDC gas exchange</td>
<td>bar</td>
<td>12.06</td>
<td>10.29</td>
<td>11.34</td>
<td>12.64</td>
<td>14.06</td>
</tr>
<tr>
<td>Calculated cylinder trapped mass at IVC</td>
<td>g</td>
<td>N/A</td>
<td>0.345</td>
<td>0.338</td>
<td>0.335</td>
<td>0.334</td>
</tr>
<tr>
<td>Calculated cylinder trapped mass at EVO</td>
<td>g</td>
<td>N/A</td>
<td>0.136</td>
<td>0.145</td>
<td>0.16</td>
<td>0.176</td>
</tr>
<tr>
<td>Calculated residual gases</td>
<td>%</td>
<td>N/A</td>
<td>39.40</td>
<td>43.00</td>
<td>47.60</td>
<td>52.60</td>
</tr>
</tbody>
</table>

For the purpose of the model validation, the valve timings are adjusted by matching the calculated pressure to the measured pressure at TDC gas exchange. The corrected pressures at TDC gas exchange should retain the same amount of residual gases as retained in the experimental work. The corresponding simulated pressures are presented in Figure 8.5 and are compared to the measured pressures. It can be seen that auto-ignition occurs late for valve timing 1. The rest of the CFD simulated pressures concur with the measured data.
Valve timing 3: Measured pressure
Valve timing 3: Simulated pressure
Valve timing 4: Measured pressure
Valve timing 4: Simulated pressure
Cylinder average pressure (bar-abs)
CAD
TDC gas exchange
TDCF
Figure 8.5 Calculated and experimental cylinder pressures for the new valve timings matching the pressure at TDC gas exchange (a) 11.25 bar, (b) 12.35 bar, (c) 14.14 bar, (d) 14.61 bar, (e) 15.16 bar and (f) 15.44 bar
A close-up of the cylinder pressures around TDCF is presented in Figure 8.6. The comparison shows reasonable agreement between the calculated and experimental pressures.
(c) Cylinder average pressure (bar-abs) vs. CAD

Valve timing 3: Measured pressure
Valve timing 3: Simulated pressure

(d) Cylinder average pressure (bar-abs) vs. CAD

Valve timing 4: Measured pressure
Valve timing 4: Simulated pressure
Figure 8.6 Cylinder pressures around TDCF for valve timings (a) 1, (b) 2, (c) 3, (d) 4, (e) 5 and (f) 6.
The adjusted values for the events IVO, IVC, EVO and EVC, to obtain the measured pressures at TDC gas exchange, are presented in Table 8.8.

### Table 8.8 Adjusted values for the inlet and exhaust valve timings

<table>
<thead>
<tr>
<th>Valve timing</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure at TDC gas exchange</td>
<td>bar</td>
<td>11.33</td>
<td>12.35</td>
<td>14.13</td>
<td>14.65</td>
<td>15.16</td>
</tr>
<tr>
<td>IVO CAD</td>
<td>438.7</td>
<td>442.9</td>
<td>450.1</td>
<td>451.8</td>
<td>453.3</td>
<td>454.1</td>
</tr>
<tr>
<td>IVC CAD</td>
<td>577</td>
<td>577</td>
<td>577</td>
<td>577</td>
<td>577</td>
<td>577</td>
</tr>
<tr>
<td>EVO CAD</td>
<td>143</td>
<td>143</td>
<td>143</td>
<td>143</td>
<td>143</td>
<td>143</td>
</tr>
<tr>
<td>EVC CAD</td>
<td>281.3</td>
<td>277.1</td>
<td>269.9</td>
<td>268.2</td>
<td>266.7</td>
<td>265.9</td>
</tr>
<tr>
<td>Inlet valves lift duration CAD</td>
<td>138.3</td>
<td>134.1</td>
<td>126.9</td>
<td>125.2</td>
<td>123.7</td>
<td>122.9</td>
</tr>
<tr>
<td>Exhaust valves lift duration CAD</td>
<td>138.3</td>
<td>134.1</td>
<td>126.9</td>
<td>125.2</td>
<td>123.7</td>
<td>122.9</td>
</tr>
</tbody>
</table>

The simulated values from the adjusted valve timings are presented in Table 8.9. For the valve timings used, the simulations are over-predicting the trapped mass by up to 7 % for low residual gases levels and under predicting the trapped mass by 1.6 % for 59 % residual gases. However, the calculated residual gases levels are more realistic than the measured data, as they are consistent with the pressure at TDC gas exchange.

### Table 8.9 Measured and calculated residual gases for all valve timings

<table>
<thead>
<tr>
<th>Valve timing</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Measured residual gases %</td>
<td>%</td>
<td>36</td>
<td>41</td>
<td>46</td>
<td>51</td>
<td>55</td>
</tr>
<tr>
<td>Measured pressure at TDC gas exchange bar</td>
<td>11.25</td>
<td>12.35</td>
<td>14.14</td>
<td>14.61</td>
<td>15.16</td>
<td>15.44</td>
</tr>
<tr>
<td>Calculated pressure at TDC gas exchange bar</td>
<td>11.19</td>
<td>12.34</td>
<td>14.14</td>
<td>14.65</td>
<td>15.16</td>
<td>15.42</td>
</tr>
<tr>
<td>Calculated cylinder trapped mass at IVC g</td>
<td>0.326</td>
<td>0.336</td>
<td>0.328</td>
<td>0.328</td>
<td>0.33</td>
<td>0.331</td>
</tr>
<tr>
<td>Calculated cylinder trapped mass at EVO g</td>
<td>0.14</td>
<td>0.156</td>
<td>0.172</td>
<td>0.178</td>
<td>0.185</td>
<td>0.19</td>
</tr>
<tr>
<td>Calculated residual gases %</td>
<td>%</td>
<td>42.9</td>
<td>46.6</td>
<td>52.3</td>
<td>54.1</td>
<td>56.2</td>
</tr>
</tbody>
</table>
The calculated results show that the residual gases concentration is almost proportional to the pressure peak at TDC gas exchange even with the change in fuel quantity between each case. A comparison of these values is presented in Figure 8.7.

Figure 8.7 Comparison of measured and calculated residual gases level against pressure at TDC gas exchange

8.3 Results and discussion
For the purpose of the current study, the amount of fuel injected in the following CFD simulations remains constant at the measured average value of 8.22 mg. It highlights the sole effect of the residual gases on the engine variables. Further, the compression ratio remains at 10.5:1 with the valve lift remaining at 6 mm. The CFD simulation valve timings could be further adjusted, to retain the same quantity of trapped residual gases as the test data (36 %, 41 %, 46 %, 51 %, 55 % and 59 %). However, the CFD simulation settings do not include spark assistance. This suggests the 36 % residual gases case will fail to auto-ignite. The 41 % residual gases case could also fail to auto-ignite due to a lower quantity of fuel injected (8.22 mg instead of 8.56 mg). Instead of adjusting the valve timings to the exact residual gases levels as the test data, the valve
events, which matched the pressure at TDC gas exchange, are used for the CFD simulations with constant fuel injection. The quantity of residual gas can be calculated again, from the CFD simulation results, for each valve timing. These values are found to be 43.2 %, 47 %, 53.1 %, 54.5 %, 55.7 % and 56.2 % for valve timings 1 to 6 respectively. The corresponding mixture composition, prior to and after auto-ignition, can also be calculated. An ideal full clean stoichiometric combustion will follow the equations $2 \text{C}_8\text{H}_{18} + 25 \text{O}_2 \rightarrow 16 \text{CO}_2 + 18 \text{H}_2\text{O}$ for octane and $\text{C}_7\text{H}_{16} + 11 \text{O}_2 \rightarrow 7 \text{CO}_2 + 8 \text{H}_2\text{O}$ for heptane, which produces only carbon dioxide and water. A comparison of the mixture concentrations between IVC and EVO is presented in Table 8.10, at an engine speed of 2000 rpm, for all valve timings. At IVC, the mixture contains the fresh charge of air, the fuel and the quantity of residual gases trapped from the previous cycle. It should be noted that the residual gases molecular weight is higher than the molecular weight of air. Therefore, the mass fraction of fuel is increasing with higher residual gases concentrations, despite the total amount of fuel injected into the inlet port remaining constant at 8.22 mg for all valve timings. The AFR is defined as the mass of the fresh charge of air over the mass of fuel. By definition, the calculation of the AFR does not take into account the residual oxygen in the residual gases, caused by the lean mixture. The formula, therefore, under-predicts the AFR for this particular application. The air-fuel equivalence ratio, lambda ($\lambda$), is defined by the actual AFR over the stoichiometric AFR, which also under-predicts the total quantity of oxygen available for combustion. When a lean mixture and trapped residual gases are used as a method to control auto-ignition, the correct method is to calculate the oxygen ratio between the total amount of oxygen prior to auto-ignition and the oxygen needed for the oxidation of the fuel. Hence, the total oxygen available is the oxygen contained in the fresh charge added to the residual oxygen in the burnt mixture. As the oxygen concentration in the residual gases is lower than in the fresh charge, higher residual fractions lead to a lower amount of oxygen in the overall mixture.
Table 8.10 Mixture composition by mass at IVC and EVO

<table>
<thead>
<tr>
<th>Mixture concentration at IVC (% of mass)</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Valve timing</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Calculated residual gases</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Octane (C₈H₁₈)</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Heptane (C₇H₁₆)</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nitrogen (N₂)</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Oxygen (O₂)</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Argon (Ar)</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Carbon dioxide (CO₂)</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water vapour (H₂O)</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lambda including O₂ in residual gases</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Mixture concentration at EVO (% of mass)</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen (N₂) after combustion</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Oxygen (O₂) after combustion</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Argon (Ar) after combustion</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Carbon dioxide (CO₂) after combustion</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water (H₂O) after combustion</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
The cylinder pressures for the adjusted CFD simulations with a fixed quantity of injected fuel for all valve timings are presented in Figure 8.8. The peak of pressure occurs as late as 15.7 CAD after TDCF for the lowest amount of residual gases. As the amount of residual gases increases, the peak of pressure gradually occurs earlier, occurring at 8.9 CAD after TDCF for the highest amount of residual gases.

![Figure 8.8 Cylinder pressure at TDCF for all valve timings](image)

The corresponding cylinder average temperatures are presented in Figure 8.9. It can be seen that the temperature gradually increases as the residual gases increases. This is particularly evident from EVC until TDCF. The expansion stroke has a very low-temperature variation between the cases. The variation of temperature is mainly governed by the amount of residual gases exiting the cylinder. The inlet valve timing has been found to have a much lesser effect on cylinder temperature than the exhaust valve timing.
8.3.1 Effects of valve timing on mixture velocity

The comparison between calculated and measured pressures showed reasonable agreement for all six valve timings. Following the validation of the model, the CFD simulations can be used to highlight the phenomena occurring within the cylinder inaccessible for measurements. The difference in velocities within the cylinder, for each valve timing, can be presented for the adjusted set of CFD simulations with a fixed injected fuel quantity for all valve timings. A radial-plane can be selected to present the average velocity from IVO for all cases. The selection of the plane location is limited, as a position too high in the cylinder would interfere with the valves crossing the plane, whereas a position too low in the cylinder would only be available for a fraction of the cycle. For these reasons, the plane selected is 10 mm below TDC on the cylinder axis. Figure 8.10 depicts the average mean velocity on the plane for the valve timings. The peak mean velocity is seen reducing from 12.68 m/s to 9.22 m/s for residual concentrations increasing from 43 % to 56 %. Also, due to the inlet valve opening later, the peaks are seen at a later crank angle from 43 % to 56 % residual gases, occurring from 484.8 CAD to 499 CAD. When compared with the piston speed, the velocities demonstrate different charge delivery due to the valve timing.
8.3.2 Effects of valve timing on mixture inhomogeneities

The effect of valve timing on the fresh charge delivery has been investigated. Various fresh charge velocities occurring at different valve timings could affect the mixture concentration and temperature at different locations within the cylinder. Monitoring the gasoline mass fraction at different locations within the cylinder should reveal differences in mixture concentration during the intake and compression stroke. Further, monitoring the mixture temperature at various locations within the cylinder should uncover the quantity and variation of residual gases, within the mixture for each valve timing, during the cycle. Figure 8.11 shows the location of the points selected to conduct a comparison of the gasoline and residual gases concentrations within the cylinder. As the piston reaches TDC (which is a value of - 3 mm on the axial axis), all the points have to be located within the clearance volume to allow monitoring of the quantities during the full cycle. Seven points are selected, which are spread out on the 0 mm radial-plane, with the centre point being located at \( x = 0 \) mm, \( y = 0 \) mm and \( z = 0 \) mm. To be noted that the point at \( x = -30 \) mm; \( y = -17 \) mm; \( z = 0 \) mm has been removed as it is located in the path of one of the inlet valves.
During the experimental work, conducted by Pitcher et al., the fuel was injected into the inlet ports. To replicate the test engine configuration and simplify the modelling of fuel injection, the air-fuel mixture was assumed to be premixed within the inlet ports of the model. As a result, the air-fuel ratio for each mixture remained constant. The fresh charge quantity and the mixture concentration were known. Monitoring the quantity of fuel during the cycle allows the study of the ratio between the air-fuel mixture and the residual gases within the cylinder. The fuel mass fraction can be defined as the ratio of
fuel mass to the overall mixture mass. It is expressed as the mass of fuel contained in the mixture over the total mass of the mixture, including the mass of the fresh charge and the mass of the residual gases in the cylinder. For instance, a fuel-free fresh charge would give a value of zero for the fuel mass fraction. On the contrary, a pure fuel intake without retained gases would give a fuel mass fraction value of one. As the fuel is oxidising during the combustion process, the fuel mass fraction decreases. Also, the HRR analysis from Chapter 4 revealed that the fuel energy release occurs prior to TDCF. Figure 8.12 depicts the variation of fuel mass fraction within the clearance volume during the intake and compression stroke, at different locations on the 0 mm axial axis. Monitoring the fuel mass fraction until TDCF means that some of the fuel would have already been oxidised. To prevent this discrepancy, the fuel mass fraction is recorded only until 30 CAD before TDCF. As the calculated residual gases only show a small variation between valve timings 3, 4, 5 and 6, the fuel values for the valve timings 1, 2, 3 and 6 only, will be depicted to simplify the presentation of the results. Prior to IVO, the cylinder content is only composed of residual gases, so the fuel mass fraction is nil. The fuel mass fraction increases shortly after IVO. All valve timings show a large variation of fuel mass fraction at different locations within the cylinder between IVO and IVC (470 CAD and 550 CAD respectively). It demonstrates that the fresh charge does not reach all of the points within the cylinder equally. This is mainly due to the turbulence phenomena of tumble and swirl, demonstrated in Chapter 6 and Chapter 7. The highest fuel concentration is found to occur at the cylinder centre-point (where \( x = 0 \) mm, \( y = 0 \) mm and \( z = 0 \) mm) for all cases. The peak value corresponds to the fresh charge entering the cylinder as it is passing through the centre-point with a full concentration, comprising mainly of nitrogen, oxygen and gasoline. For the centre-point, at the corresponding crank angles, the fresh charge is not diluted with the residual gases. The fresh charge entering the cylinder creates a tumble motion which progressively mixes the residual gases with air and fuel, reducing the fuel mass fraction seen at specific points. After the fuel mass fraction peak, it reduces, which demonstrates a dilution of the fresh charge with the residual gases, for all locations. Fuel mass fraction in the cylinder progressively reduces, until reaching 690 CAD or - 30 CAD TDCF. However, even at this crank angle, all the points do not have the same fuel concentration.
(a) and (b) show the fuel mass fraction as a function of CAD for different positions within the cylinder. The graphs represent the fuel mass fraction at specific locations as indicated by the coordinates $(x, y, z)$.

- **(a)**: Fuel mass fraction for positions $(x = 0 \text{ mm}; y = 0 \text{ mm}; z = 0 \text{ mm})$, $(x = 30 \text{ mm}; y = 0 \text{ mm}; z = 0 \text{ mm})$, $(x = 0 \text{ mm}; y = 30 \text{ mm}; z = 0 \text{ mm})$, $(x = 0 \text{ mm}; y = -30 \text{ mm}; z = 0 \text{ mm})$, $(x = -30 \text{ mm}; y = 0 \text{ mm}; z = 0 \text{ mm})$, $(x = 0 \text{ mm}; y = -17 \text{ mm}; z = 0 \text{ mm})$, and $(x = 30 \text{ mm}; y = -17 \text{ mm}; z = 0 \text{ mm})$.

- **(b)**: Cylinder average fuel mass fraction.
Figure 8.12 Comparison of fuel concentration at different locations within the cylinder for valve timing (a) 1, (b) 2, (c) 3 and (d) 6
As the differences of the fuel mass fraction have been monitored during the cycle (prior to auto-ignition) at different locations within the cylinder, the fuel stratification at specific crankshaft angles can be depicted. Figure 8.13 shows the fuel distribution on the axial planes 1, 2 and 3 for valve timing 1 at -30 CAD TDCF.

![Fuel concentration for valve timing 1 at 690 CAD on axial planes (a) 1, (b) 2 and (c) 3](image)

Figure 8.13 Fuel concentration for valve timing 1 at 690 CAD on axial planes (a) 1, (b) 2 and (c) 3

The fuel distribution (on the same planes) for valve timing 6 are shown in Figure 8.14. The results show that the mixture in the cylinder contains inhomogeneities prior to auto-ignition.
Calculated results are used to obtain the maximum and minimum fuel concentration values, within the entire cylinder volume at 690 CAD. The range around the cylinder average value is obtained by comparing the maximum and minimum to the cylinder average value. The detailed values are presented in Table 8.11 for all valve timings. The results show variations of fuel concentration around the cylinder average value, by up to 90%. Further, it shows that shorter valve lift durations, which lead to higher residual gases concentrations, have a higher fuel fraction distribution prior to auto-ignition. Using shorter valve timing to control auto-ignition, by trapping residual gases, produces a natural charge stratification, which is accentuated with higher residual gases levels.
Table 8.11 Variation of fuel concentration at TDCF - 30 CAD for all valve timings

<table>
<thead>
<tr>
<th>Valve timing</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calculated residual gases</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cylinder average fuel mass fraction</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cylinder minimum fuel mass fraction</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cylinder maximum fuel mass fraction</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Minimum difference with average value</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Maximum difference with average value</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Range around average value</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure 8.15 shows the total temperature at the 7 points located on the 0 mm cylinder axis cross section, after IVO. In the same way that the fuel quantity can represent the concentration of the fresh charge in the cylinder, the temperature can be used to deduce the residual gases concentration at these locations. Once again, only the temperature values for the valve timings 1, 2, 3 and 6 will be depicted, to simplify the presentation of the results. Prior to the inlet valves opening, the cylinder content is only composed of residual gases, for which the temperature is around 600 K to 700 K for the various valve timings. As the fresh charge is introduced through the inlet port, a drop of temperature at these locations is observed, which signifies that the points are in the path of the fresh charge (300 K). Similar to the fuel mass fraction results, all valve timings show variations of temperature at different locations of the cylinder between IVO and IVC (470 CAD to 550 CAD). It demonstrates that the fresh charge does not reach all the points within the cylinder equally. Instead, it progressively mixes with the residual gases leading to an increase of temperature for all locations. At 690 CAD, all points have different temperatures, with ranges of 41 K, 45 K, 67 K and 67 K for valve timings.
1, 2, 3, and 6, respectively. This shows that the temperature range is increasing with residual gases quantity.
Figure 8.15 Comparison of temperature distribution at different locations within the cylinder for valve timing (a) 1, (b) 2, (c) 3 and (d) 6
Temperature distribution at 690 CAD (-30 CAD TDCF) on the planes 1, 2 and 3 for valve timing 1 is shown in Figure 8.16.

![Temperature distribution at 690 CAD for valve timing 1 on axial planes (a) 1, (b) 2 and (c) 3](image)

**Figure 8.16** Temperature distribution for valve timing 1 at 690 CAD on axial planes (a) 1, (b) 2 and (c) 3

Temperature distribution on the same planes for valve timing 6 is shown in Figure 8.17. The results demonstrate that a temperature stratification of the mixture exists within the cylinder prior to auto-ignition.
A cylinder volume-temperature distribution analysis is conducted to check the quantity of mesh cells affected by the temperature stratification within the entire volume, prior to auto-ignition. As most of the cells have the same mesh size, the cell count is representative of the cylinder volume. The temperature distribution of the mesh cells, with a 20 K range, is presented in Figure 8.18 for valve timing 6. For instance, 7360 cells from all elements contained within the cylinder, have temperatures between 810 K and 830 K.
Using the total count of elements in the combustion chamber, the results can be converted into a percentage of the total number of elements for each temperature range as shown in Figure 8.19.
Using a one-degree range to increase accuracy, the results are compared for all valve timings as shown in Figure 8.20. The whole cylinder temperature range was found to gradually increase with residual gases concentration, from 104 K for valve timing 1 to 205 K for valve timing 6. The total count of elements in the cylinder is the same for all cases. As a consequence, the count of elements for each 1 K range decreases gradually from 2.52 % for valve timing 1 to 1.19 % for valve timing 6.

![Figure 8.20 Cylinder temperature distribution at 690 CAD for all valve timings](image)

The temperature distribution ranges are presented in Table 8.12. The results show that the minimum temperature, maximum temperature and temperature range are all increasing with residual gases fractions. Using a shorter valve lift duration to control auto-ignition, by trapping residual gases, produces a natural thermal stratification within the cylinder, which is accentuated with higher residual gases levels.
Table 8.12 Cylinder temperature range at -30 CAD TDCF for all valve timings

<table>
<thead>
<tr>
<th>Valve timing</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calculated residual gases</td>
<td>%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Minimum temperature</td>
<td>K</td>
<td>771</td>
<td>774</td>
<td>794</td>
<td>810</td>
<td>812</td>
</tr>
<tr>
<td>Maximum temperature</td>
<td>K</td>
<td>875</td>
<td>922</td>
<td>963</td>
<td>984</td>
<td>1011</td>
</tr>
<tr>
<td>Cylinder temperature range</td>
<td>K</td>
<td>104</td>
<td>148</td>
<td>169</td>
<td>174</td>
<td>199</td>
</tr>
</tbody>
</table>

A fuel distribution analysis is conducted using an equivalent fuel range, to the
one-degree range temperature study, over a period of 250 K. The results show that the
fuel has an opposite trend to the temperature, for all valve timings. The results are
consistent with each other, as the mixture temperature is the direct consequence of the
mixing of residuals with the fresh charge (which also contains the fuel). The example of
valve timing 6 is presented in Figure 8.21. The x-axis scale has been plotted in
decreasing order to easily compare the temperature distribution and fuel concentration
trends, as well as the percentage of elements.
Figure 8.21 Cylinder temperature distribution (a) compared to the fuel distribution (b) at 690 CAD for valve timing 6
It is found that the valve timing greatly affects the velocity and behaviour of the fresh charge entering the cylinder. The variation of the valve timing affects the dilution of fresh charge during the intake and compression stroke, due to the associated tumble it generates. Each valve timing produces a specific temperature stratification and fresh charge stratification, which are directly opposite.

8.3.3 Comparison with homogeneous charge and temperature

The charge and temperature stratifications have been highlighted. A combustion study can reveal the differences with a fully homogeneous mixture and temperature. The cylinder average temperature, as well as the mixture average concentration, is used to simulate a model with the same quantity of residual gases. The fully homogeneous and the charge and temperature stratification calculations are set with same coefficients for the Chen-Flynn friction model [9] and the Woschni heat transfer model [10], which are widely used to model the friction and heat transfer of engines. Details of the Chen-Flynn friction model and the Woschni heat transfer model can be found in the appendices. The results are presented in Figures 8.22 to 8.25 for valve timing 6. Figure 8.22 depicts the cylinder pressure for both the charge and temperature stratification model and the fully homogeneous model. The pressure peak is higher for the fully homogeneous model as the whole mixture ignites simultaneously.

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*Figure 8.22 Cylinder pressure comparison between a charge stratification and a fully homogeneous model for valve timing 6*
The same trend is observed for the cylinder temperature as shown in Figure 8.23.

Figure 8.23 Cylinder temperature comparison between the charge and temperature stratification model and a fully homogeneous model for valve timing 6

However, the indicated work is improved by the end of the expansion stroke (3.4 J) for this case, with charge and temperature stratifications, as shown in Figure 8.24. This represents an improvement of 2.26 %.

Figure 8.24 Indicated work comparison between the charge and temperature stratification model and the fully homogeneous model for valve timing 6
The results can be explained by the difference of the two HRRs as shown in Figure 8.25. The fully homogeneous mixture and temperature case recorded an HRR peak of 1171 J/deg. The charge and temperature stratifications case shows an extended HRR which improves the indicated work by 3.4 J or 2.26 %.

Figure 8.25 Corresponding HRR for valve timing 6 for (a) Fully homogeneous and (b) Charge and temperature stratification
These findings are consistent with previous investigations aimed at extending the HRR, by increasing turbulences. Longer combustion duration and an extended HRR were obtained by Christensen and Johansson (2002) [11] when using a square bowl piston instead of a flat piston. The design of combustion chamber geometry was also found to affect CAI operation by Christensen et al. (2002) [12] and could be used as a tool for increasing the load range of CAI. Swirl enhancement alone was shown to have little effect on combustion duration by Kong et al. (2003) [13]. However, in the current study, using valve duration to retain residual gases has proven to generate both swirl and tumble as well as cylinder turbulences until auto-ignition. Simulations for different initial temperature distributions in a CAI engine, for the auto-ignition of a turbulent homogeneous mixture of lean hydrogen, were studied by Sankaran et al. (2005) [14]. Turbulence has demonstrated to be a significant influence on the initial location and development of ignition. The findings are also consistent with this study, which showed that using valve duration to retain residual gases, creates natural fuel and temperature stratifications, which are specific to each valve timing.

8.3.4 Valve timing effects on volumetric efficiency, pumping work and heat transfer

Calculated results show that valve timings also affect the pumping work, the volumetric efficiency and the heat transfer. A summary of these values is presented in Table 8.13. A decrease in volumetric efficiency is noted, as the valve lift duration is shortened. This is consistent with retaining mass within the cylinder for increasing residual gases. The friction power variation is found to almost be unaffected between valve timings. The pumping work is increased as the valve lift duration is shortened. This leads to a decrease in the net indicated mean effective pressure when increasing the residual gases levels. The most significant difference between cases, is the average heat transfer, with an increase of 0.44 kW as the valve duration is reduced. The combined effects result in a decrease of indicated power and therefore, a decrease of indicated efficiency by 2%.

Despite the HRR improvement generated by the charge and temperature stratification, the indicated efficiency decreases as the valve duration reduces, due to the cumulative effects of the increase of heat transfer, pumping work and friction power. The use of
valve timing to control auto-ignition is beneficial for combustion and can be used to extend the HRR. This, in turn, can help increase the load limit for CAI engines. However, this improvement results in a penalty, of the cylinder indicated efficiency. Valve timing as a means to control auto-ignition should only be used when the load range is to be improved.

Table 8.13 Engine parameters summary for all valve timings

<table>
<thead>
<tr>
<th>Valve timing</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calculated residual gases</td>
<td>%</td>
<td>42.9</td>
<td>46.6</td>
<td>52.3</td>
<td>54.5</td>
<td>55.7</td>
</tr>
<tr>
<td>Volumetric efficiency</td>
<td>fraction</td>
<td>0.36</td>
<td>0.33</td>
<td>0.28</td>
<td>0.27</td>
<td>0.27</td>
</tr>
<tr>
<td>Friction mean effective pressure (FMEP)</td>
<td>bar</td>
<td>1.022</td>
<td>1.042</td>
<td>1.056</td>
<td>1.057</td>
<td>1.055</td>
</tr>
<tr>
<td>Gross indicated mean effective pressure (IMEP360)</td>
<td>bar</td>
<td>3.41</td>
<td>3.40</td>
<td>3.34</td>
<td>3.33</td>
<td>3.31</td>
</tr>
<tr>
<td>Pumping mean effective pressure (PMEP)</td>
<td>bar</td>
<td>0.21</td>
<td>0.23</td>
<td>0.26</td>
<td>0.27</td>
<td>0.27</td>
</tr>
<tr>
<td>Net indicated mean effective pressure (IMEP720)</td>
<td>bar</td>
<td>3.19</td>
<td>3.17</td>
<td>3.08</td>
<td>3.06</td>
<td>3.04</td>
</tr>
<tr>
<td>Average heat transfer</td>
<td>kW</td>
<td>1.90</td>
<td>2.05</td>
<td>2.25</td>
<td>2.29</td>
<td>2.32</td>
</tr>
<tr>
<td>Indicated power</td>
<td>kW</td>
<td>2.39</td>
<td>2.37</td>
<td>2.30</td>
<td>2.29</td>
<td>2.27</td>
</tr>
<tr>
<td>Gross indicated efficiency</td>
<td>%</td>
<td>41.66</td>
<td>41.53</td>
<td>40.83</td>
<td>40.64</td>
<td>40.48</td>
</tr>
<tr>
<td>Indicated efficiency</td>
<td>%</td>
<td>39.05</td>
<td>38.71</td>
<td>37.65</td>
<td>37.37</td>
<td>37.13</td>
</tr>
</tbody>
</table>
8.4 Concluding remarks on the effects of valve timing on engine parameters

The measured cylinder pressure was used to calculate the HRR, the fuel injected during the experimental work and the cylinder temperature at IVO. A model validation was conducted using the experimental cylinder pressure and the given valve timings. As differences of pressure at TDC gas exchange and residual gases quantity were found between the measured and calculated results, the valve timings were adjusted to match the pressures at TDC gas exchange. Once the calculated pressure was in reasonable agreement with the measured pressure, the CFD simulations were launched with the same quantity of fuel injected for all cases, to investigate the sole effects of valve timing on the engine variables.

8.4.1 Valve timing effects on fresh charge intake

Six valve timings were applied to the model with a valve lift of 6 mm to retain various burnt mixture residual concentrations within the cylinder. Differences of charge intake between all cases were observed during the intake stroke. The charge intake depicts lower peaks of velocity as the residual fraction increases. Also, the velocity peaks are seen at later crank angles as the residual gases increase, due to the difference of the valve timing.

8.4.2 Valve timing effects on the mixing of the charge

As each valve timing has a specific intake pattern, differences of the fresh charge dilution were observed during the intake and compression stroke. The calculated results demonstrated a stratification of the fuel concentration and the mixture temperature within the cylinder, which were still present prior to auto-ignition. The fuel and temperature stratification was specific for each valve timing.

8.4.3 Mixture concentration and temperature effects on heat release rate and indicated work

The CFD simulations show that the HRR was extended when the mixture had a temperature stratification and a different fuel concentration, compared to a fully homogeneous charge. The charge and temperature stratifications case shows an improvement of indicated work by 2.26 %. Therefore, the use of valve timing to control
auto-ignition, is beneficial for combustion, as it extends the HRR. This can help to improve the load limit for CAI engines.

8.4.4 Valve timing effects on engine variables

As the valve timing is shortened and the residual gases level increases, the air flow restriction and the cylinder pressure at TDC gas exchange increases. Results have shown an increase of heat transfer, pumping work and friction power, with increasing residual gases levels. Despite the HRR improvement generated by the charge and temperature stratifications, the indicated efficiency decreases as residual gases levels increase. The extension of the HRR results in a penalty of the cylinder indicated efficiency. Valve timing as a means to control auto-ignition should only be used when the load limit of CAI engines is to be improved.
References


Chapter 9: Conclusions derived from the study and recommendation for further work

9.1 Study summary

Limited fossil fuel resources and the impact of pollutant emissions on the environment and health have become urgent problems to solve. An internal combustion engine usually produces nitrogen oxides (NOx), particulate matter (PM), hydrocarbons (HC) and carbon monoxide (CO) emissions. As a result, the emissions levels of new vehicle engines are constantly being reduced to match the revised European emission standards. However, the current progress of research for spark-ignition (SI) and compression-ignition (CI) engines cannot match the emissions targets. An alternative to these two combustion methods, i.e. SI and CI, is called controlled auto-ignition (CAI) and has received significant attention from researchers. The principle is to mix fuel and air homogeneously before compressing the mixture to the point of auto-ignition. Ignition occurs at several places at a time inside the combustion chamber, which makes the fuel/air mixture burn almost simultaneously. Auto-ignition can be controlled to achieve a cleaner combustion and reduced PM emissions along with high engine efficiency. CAI engines achieve extremely low levels of NOx emissions without the use of catalytic aftertreatment, due to a lower combustion temperature. The HC emissions are higher than in SI engines due to the incomplete oxidation during the simultaneous combustion. The CO emissions are also higher than in SI engines due to the gases trapped in the piston crevice, but both HC and CO emissions can be treated by catalytic aftertreatment to meet automotive emission standards. In order to govern the operating conditions in a CAI engine, the control of the fuel/air mixture temperature is key to generating combustion. It can be obtained by varying the compression ratio, by retaining residual gases, recirculating the exhaust gases, pre-heating the intake charge or by increasing the intake charge pressure with a turbocharger or a supercharger. In SI and CI engines, the work output range is complete from low to high load. Adding more fuel/air mixture to the combustion chamber increases the engine output. As the heat release rate is slow, the engine can withstand the extra power provided by the additional fuel during high load operations. In CAI engines, the entire mixture ignites almost simultaneously which creates high peaks of cylinder pressure. The engine design must be robust to withstand
higher pressures and is, therefore, heavier compared to SI and CI engines. Due to the nature of the simultaneous combustion and lean mixture, CAI engines are restricted from low to mid load operations. Various strategies have been studied to improve the load limit of CAI engines, extending the heat release duration and lowering the cylinder pressure peak using dual-fuel injection, water injection or multiple injections. From the various conclusions of researchers, it is clear that CAI engines have the potential to replace conventional combustion methods, such as SI and CI, due to the revised European emission standards. Low NOx and PM emissions along with CI-like efficiencies are the main features of CAI engines. However, the main drawbacks of CAI engines are auto-ignition control and the high energy release rate which restricts CAI load range and speed.

This study presented the computational fluid dynamics (CFD) modelling results of the transient flow inside a Lotus single cylinder engine of 0.45-litre displacement volume. The geometry was obtained by manually measuring a negative casting of the inlet ports and engine cylinder. The CFD calculations took into account the movement of the inlet valves, exhaust valves and the piston. The first part of the study compared the calculated in-cylinder velocities to laser Doppler anemometry (LDA) experimental data available at Loughborough University conducted and provided by Pitcher et al. (2003) [1], where only air was delivered through the ports into a motored, optically accessible, engine cylinder. The available experimental data was reprocessed to illustrate the time-history of mean velocities for all LDA measured points. The first set of CFD simulations was used to validate the model using spark-ignition valve timing with an engine speed of 1500 revolutions per minute (rpm). A map of the time-dependent velocities for 240 points on three cutting planes within the cylinder was populated using figures. A comparison of the results for different turbulence models was conducted as well as a mesh sensitivity study. A turbulence model was selected and using the results, the CFD calculations matched reasonably well the LDA data for the spark-ignition valve timing. An overall average value for the performance of the model was obtained. A method to reduce the computational time of the calculations was presented. The development of the flow field on the cylinder symmetry cutting plane was illustrated. The tumble motions and their centres were described for 450 and 540 crank angle degree (CAD).
The variation of turbulence parameters, such as turbulence intensity (TI), turbulent kinetic energy (TKE) and the turbulent dissipation rate (TDR), during the intake and compression stroke at different locations within the clearance volume, were also discussed.

The second set of CFD simulations was used to validate the model using CAI valve timing with 3.6 mm valve lift for engine speeds of 1500 rpm and 2000 rpm. Again, a map which illustrates the time-history of the velocities at different points in the cylinder was presented for both engine speeds to obtain the overall average performance of the model. The CFD calculations were found to match the LDA measurements reasonably well.

A comparison of the flow field was conducted at specific crankshaft angle positions to examine the engine speed effect on the tumble flow motion. The turbulence parameters were monitored during the cycle to quantify the variations at different locations inside the clearance volume prior to top dead centre firing (TDCF). A conclusion on the effect of engine speed on charge delay and charge amount was presented. Engine speed affected the strength of the tumble motion, the turbulence maximum values and duration during the intake stroke, the charge delay and the amount of fresh charge entering the cylinder. Also, the engine speed has been found to alter the turbulences prior to auto-ignition.

The second part of the study aimed to replicate the thermodynamic single cylinder engine experimental data with gasoline to validate the CFD calculations. With a CAI valve lift of 6 mm at 2000 rpm, six various valve timings were used to retain 36 % to 59 % residual gases in the cylinder. A gasoline surrogate was selected and the air composition calculated to be implemented in the model. The heat release rate (HRR) was calculated from the experimental cylinder pressure trace. To deduce the amount of fuel injected during the experimental work, the integral of the HRR was calculated for each valve timing. Using those values, a set of CFD calculations was performed, combining the CFD code with a chemical kinetics model of 32 species and 55 reactions. Those results were compared to the experimental pressure trace obtained from the
thermodynamics single cylinder engine for model validation. The valve timings were adjusted to match the measurement pressure at top dead centre (TDC) gas exchange for the model to be validated. A new set of CFD calculations was performed with a constant amount of fuel being injected to obtain solely the effect of valve timing on air-fuel ratio (AFR), cylinder pressure, charge velocity, cylinder temperature distribution, fuel concentration and the HRR. Those results were compared to a fully homogeneous mixture model with the same valve timings to obtain conclusions on the HRR and indicated work. Finally, the effects of valve timing on volumetric efficiency, friction power, pumping power, heat transfer, cylinder power and efficiency were studied.

9.2 New contributions to the body of knowledge resulting from this research

The new research contributions found in this study can be listed as follows:

1) The effect of engine speed on the intake charge velocity entering the cylinder of a CAI engine, during the intake stroke.

2) The valve timing effect on the intake charge velocity, entering the cylinder of a CAI engine during the intake stroke.

3) The effect of CAI valve timing on the fuel concentration in the mixture within the cylinder, during the intake and compression stroke.

4) The effect of using CAI valve timing on the temperature distribution within the cylinder, during the intake and compression stroke.

5) The consequence of using CAI valve timing on the combustion duration, compared to a fully homogeneous mixture case.

6) The effect of the fuel and temperature stratification on indicated work in a CAI engine, compared to a fully homogeneous mixture case.

7) The effect of using CAI valve timing on the cylinder indicated efficiency.
9.2.1 Answers to the preliminary scientific/technological questions

The preliminary technological questions can be answered as follows:

- What is the effect of varying the valve timing on the fresh charge amount entering the cylinder, during the intake stroke?

This question was fully answered by calculating the amount of intake charge which entered the cylinder until inlet valve closing (IVC) for all six valve timings used in this study. For instance, gradually shortening the inlet valve opening duration from 138 CAD to 123 CAD decreased the amount of fresh charge in the cylinder at IVC from 57 % to 43 %. Similar results have been found by many researchers when using valve timing to control the auto-ignition of CAI engine mixtures.

- What is the effect of varying the valve timing on the residual gases amount retained within the cylinder, after the exhaust valves close?

This question was answered to a full extent by monitoring the amount of residual gases retained within the cylinder at exhaust valve closing (EVC) for all six valve timing durations of the study. Reducing the exhaust valve opening duration from 138 CAD to 123 CAD increased the amount of residual gas from 43 % to 57 % in this study. These results are consistent with other research studies where the valve timing was varied to control the auto-ignition of CAI engine mixtures.

- What is the effect of valve timing on the mixture ignition timing?

This question was answered fully by numerically simulating the timing of the auto-ignition of the mixture in the cylinder for all six valve timings of the study. As the inlet and exhaust valve opening durations decreased from 138 CAD to 123 CAD, the ignition of the mixture was advanced from 5 CAD after TDCF to 13.5 CAD before TDCF. As many researchers reported, varying the valve timing is a method used to control the in-cylinder mixture temperature, and therefore its point of auto-ignition.
9.2.2 Minor new contributions to the body of knowledge resulting from this research and answers to the corresponding scientific/technological questions

The minor new research contributions and answers to the technological questions can be found below:

- What is the effect of engine speed on the intake charge velocity entering the cylinder of a CAI engine, during the intake stroke?

This question was partly answered as only two engine speeds were monitored in this study, 1500 rpm and 2000 rpm. The cross-section average velocity of the intake charge entering the cylinder during the intake stroke has been found to be higher at 2000 rpm when compared to 1500 rpm. It is concluded that higher engine speeds produce higher intake charge velocities which could affect the mixing of the charge.

- Does the valve timing affect the intake charge velocity, entering the cylinder of a CAI engine during the intake stroke?

This question was fully answered using all six valve timing durations. By comparing the cross-section average intake charge velocity, of the six different valve timings during the intake stroke, it was found that the six valve timing durations, retaining between 43 % and 57 % of residual gases, showed differences of charge intake velocities, during the intake stroke. The intake charge depicted lower velocity peaks as the valve timing duration was shortened. It was also revealed that the velocity peaks occurred at later crankshaft angles during the intake stroke as the valve duration was shortened.

9.2.3 Major new contributions to the body of knowledge resulting from this research and answers to the corresponding scientific/technological questions

The major new research contributions and answers to the technological questions can be found below:

- What is the effect of CAI valve timing on the fuel concentration in the mixture within the cylinder, during the intake and compression stroke?
This question was answered fully for the engine cylinder geometry used in this study, by monitoring the amount of fuel at locations within the clearance volume during the intake and compression stroke and visualising the fuel concentration at cylinder cross-sections 30 CAD before TDCF. As each valve timing has a specific intake pattern, differences in the fresh charge dilution were observed between all the valve timings during both the intake and compression stroke. The calculated results demonstrated a stratification of the fuel concentration within the cylinder, which was still present prior to auto-ignition. The fuel stratification was specific for each valve timing.

What is the effect of using CAI valve timing on the temperature distribution within the cylinder, during the intake and compression stroke?

The effect of valve timing on the temperature distribution of the mixture was fully studied for the engine cylinder geometry used in this study. The temperature was monitored at locations within the clearance volume during the intake and compression stroke. The mixture temperature for three cylinder cross-sections at 30 CAD before TDCF was also recorded. Different intake charge dilutions were observed during the intake and the compression stroke between all valve timings. The calculated results demonstrated a distribution of the mixture temperature within the cylinder until the point of auto-ignition. Like the fuel stratification pattern, the temperature stratification was also found to be specific for each valve timing.

What is the consequence of using CAI valve timing on the combustion duration, compared to a fully homogeneous mixture case?

New findings were revealed for the shortest valve timing duration used in this study, by comparing the valve timing effect on temperature distribution and fuel stratification described previously, to an equivalent fully homogeneous mixture case. The valve timing duration was shortened to retain 57 % of residual gases within the cylinder. The mixture showed a natural temperature distribution and fuel stratification which can only be explained by the shorter valve timing duration. The combustion duration, and therefore the HRR, was extended from 5 CAD to 20 CAD, when compared to its
equivalent fully homogeneous mixture, for the same valve timing. The use of valve timing to control auto-ignition was beneficial for combustion, as it extended the heat release duration.

- What is the effect of the fuel and temperature stratification on indicated work in a CAI engine, compared to a fully homogeneous mixture case?

The effect of the fuel and temperature stratification on the indicated work was studied by comparing the work produced by the mixture with inhomogeneities due to the valve timing duration, against an equivalent fully homogeneous mixture. For the shortest valve timing duration used in this study, which retained 57% of residual gases within the cylinder, the fuel stratification and temperature distribution of the mixture have shown an improvement of the indicated work by 2.26% when compared to a fully homogeneous mixture. The use of valve timing to control auto-ignition was beneficial for combustion as it extended the heat release duration. This ought to improve the load limit for CAI engines. These findings are consistent with previous investigations aimed at extending the HRR, by increasing turbulences. Longer combustion durations were obtained by Christensen and Johansson (2002) [2] when using a square bowl piston instead of a flat piston. The design of combustion chamber geometry was also found to affect CAI operation by Christensen et al. (2002) [3] and could be used as a tool for increasing the load range of CAI engines. Swirl enhancement alone was shown to have little effect on combustion duration by Kong et al. (2003) [4]. However, in the current study, using valve duration to retain residual gases has been proven to generate both swirl and tumble, as well as cylinder turbulences until auto-ignition. Simulations for different initial temperature distributions within a CAI engine, for the auto-ignition of a turbulent homogeneous mixture of lean hydrogen, were studied by Sankaran et al. (2005) [5]. Turbulence has demonstrated to be a significant influence on the initial location and development of ignition. The findings are also consistent with this study, which showed that using valve duration to retain residual gases creates natural fuel and temperature stratifications, which are specific to each valve timing.
What is the effect of using CAI valve timing on the cylinder indicated efficiency?

The effect of using valve timing on the cylinder efficiency was studied for all six valve timings in this study by monitoring the volumetric efficiency, pumping work, heat transfer and indicated efficiency. As the valve lift duration was shortened, the flow restriction caused by the valve increased, which led to a higher amount of residual gases. In turn, it also increased the cylinder pressure at TDC gas exchange. Results have shown an increase in heat transfer, pumping work and friction power with increasing residual gases. Despite the combustion and HRR improvements generated by the charge and temperature stratification, the indicated efficiency has been found to decrease as residual gases increase. The use of valve timing to control auto-ignition could help to improve the load limit for CAI engines but at the expense of indicated efficiency. Additional fuel is necessary to obtain an equivalent cylinder indicated efficiency. It is therefore concluded that valve timing as a method to control auto-ignition should only be used when the load limit of CAI engines is to be improved.

9.3 Recommendations for further work

9.3.1 Further investigation

CFD calculations were conducted using various engine speeds and valve timings. The engine speed has shown to affect the tumble motion, the charge intake amount and the turbulence parameters prior to auto-ignition. Shorter valve timings have shown to stratify the fuel in the charge and temperature within the cylinder prior to auto-ignition, creating inhomogeneities and extending the HRR. This effect could be investigated further using high-speed imaging, laser induced fluorescence or chemiluminescence methods. The results could be compared to other CAI engine studies, which use other methods than shorter valve timings to control auto-ignition, to obtain a relationship between inhomogeneities and load limit improvement. This study focused on the fresh charge being fully homogeneous in the inlet port. Additional considerations to this work could take into account the additional effects of fuel vaporisation both inside the inlet port and directly injected into the cylinder with regards to the fuel and temperature stratification. Also, the effects of different engine speeds combined with a short valve lift duration could highlight an increase in fuel and temperature stratification. In this
study, a gasoline surrogate composed of 87 % octane and 13 % heptane (by volume) was used as the fuel. A different composition of those fuel species could be studied to extend the range of control of auto-ignition. A dual-injection system allowing variable fuel compositions could also be studied to investigate the improvement on HRR by increasing the fuel distribution. Additional control methods, such as cooled EGR and/or turbocharging, could be combined with a shorter valve lift duration, to extend the auto-ignition control range. In the case of direct injection into the cylinder, where the temperature at TDC gas exchange is higher than 1100 K, an additional gasoline injection within the cylinder between EVC and TDC gas exchange could be investigated, to improve the indicated work and therefore, the range limit of CAI engines. Finally, the use of a hot EGR loop instead of a short valve duration could be investigated to reduce the pumping work, improve the volumetric efficiency and the cylinder indicated efficiency. These would make a valuable continuation of this work.

9.3.2 Assumptions on modelling
Extensions to this work could aim to reduce some of the assumptions imposed on CFD modelling, in order to improve the agreement with experimental work. One of the assumptions imposed in this project was that the geometry surfaces were considered as perfectly smooth. Surface imperfections could be considered for parts of the geometry like the clearance volume, ports and piston surfaces. However, this implies that the mesh size needs to be reduced. Due to the mesh size in this study, another assumption introduced was the simulation of the combustion chamber without the spark plug modelled. It could have an effect on the swirl and tumble but was considered to be negligible. With increasing computing capabilities the mesh size can be reduced, which will allow the spark plug to be incorporated into the CFD model.
9.3.3 Improvement of experimental data
Extensions to this work should also include directions for improvement of the experimental data. It was found that the combustion data recorded every 4 CAD showed high variations of in-cylinder pressure, especially seen during valve movement. To increase the accuracy of the data, the frequency of the LDA measurements should be increased. A high variation of the in-cylinder pressure was observed between all 300 cycles for all residual gases concentrations. To reduce those cyclic variations, the ambient temperature, pressure and relative humidity during experimental work should be monitored. The parameters can be expressed relative to the atmospheric conditions. Also, to reduce the cyclic variations, the engine oil temperature should be monitored with the recording of the experimental values starting when temperature values are stable. The average cycle calculation should only start once the temperatures have converged. An ion sensor should be implemented to obtain the exact auto-ignition timing and further validate the CFD calculations combined with the reduced chemical kinetics model. To avoid the pressure transmitters from drifting, a calibration procedure should be implemented at the start of each measurement day. Additional temperature measurements could be added to the set of data (calibrated using a thermal bath). Resistance Temperature Detectors (RTD) could be used for ambient, test cell and intake measurements while thermocouples could be used to record temperatures in the exhaust pipe.

9.3.4 Fuel measurement
The fuel flow rate and the exact composition of the gasoline were not presented in the experimental work. The gasoline was assumed to be composed of 87 % octane and 13 % heptane (by volume) with the fuel amount being calculated from the cylinder pressure and the HRR. The fuel consumption could have been measured with a weighing scale. A longer period of measurement acquisition will increase the accuracy of the results. Also, the gasoline which was used during the experimental work could have been sent for analysis to obtain the components of the blend. A new chemical kinetic model could be developed to include the fuel species obtained from the analysis.
Reference


**Appendix References**

1.1 Engine mechanism

The engine mechanism consists of the crankshaft, connecting rod, and piston. The crankshaft rotates around its axis and its motion is defined by a crank angle $\theta$ relative to this axis. This rotation is converted into the linear motion of the piston through the connecting rod that is attached to the crankshaft. During the inlet stroke, the piston is pulled by the connecting rod and it moves downward linearly from top dead centre (TDC) gas exchange to bottom dead centre (BDC). In the meantime, the two inlet valves are opened whilst the exhaust valves remain closed. This causes a vacuum inside the cylinder, which draws the fuel/air mixture through the inlet port. The displacement of the piston can be determined based on the crankshaft angle, engine stroke and connecting rod length.

It should be noted that the crankshaft radius is half the engine stroke. At TDC the piston reaches its highest position in the cylinder; corresponding to 0 crank angle degree (CAD) for top dead centre firing (TDCF) and 360 CAD for TDC gas exchange. At this position, the corresponding volume (above the piston) is referred to as the clearance volume, $V_{TDC}$. In contrast, BDC is the lowest position of the piston in the cylinder, corresponding to 180 CAD and 540 CAD with a maximum cylinder volume, $V_{BDC}$. The volume difference between 0 CAD and 180 CAD, $V_{BDC} - V_{TDC}$ is called the displacement volume, $V_D$, which can be expressed as:

$$V_D = \frac{\pi}{4} D^2 S$$  \hspace{1cm} (A-1)

where $S$ is the engine stroke and $D$ is the engine bore diameter.
1.2 Description of piston displacement

The cross-section of the reciprocating piston main mechanism inside the cylinder is illustrated in Figure A.1.

![Figure A.1 Main mechanism of a reciprocating piston](image)

To simplify the following schematics, the motion centre lines are represented in blue for the connecting rod and red for the crankshaft. Figure A.2 shows a simplified representation of the linked part of the mechanism.
Three different piston positions are illustrated for their corresponding connecting rod positions and crankshaft angles. TDC and BDC are shown in Figures A.2(a) and A.2(c), respectively. An arbitrary position of the piston is shown in Figure A.2(b). The precise position of the piston can be calculated based on the geometric relationship between the crankshaft, connecting rod and piston. Figure A.3 depicts the geometric relationship between the mechanism components.
For this particular engine cylinder, the connecting rod length $L$ was found to be 0.131 m. The crankshaft radius $A$ is measured at 0.0441 m. All the component dimensions can be expressed using trigonometry relationships. The piston displacement $P_D$ can be expressed as:

$$P_D = A + L - \left(\sqrt{L^2 - A^2 \sin^2 \theta} + A \cos \theta \right)$$ \hspace{1cm} (A-2)

With the piston displacement $P_D$ known, the cylinder volume ($V$) can be calculated. For a given crank angle $\theta$, the actual volume of the cylinder is given by:

$$V = V_{TDC} + \frac{\pi}{4} D^2 P_D$$ \hspace{1cm} (A-3)
The piston position ($P_p$) is shown for a full cycle of 720 CAD in Figure A.4.

Figure A.4 Piston position against crankshaft angle for the engine cylinder

Relative to TDC, the piston position varies from 0 m to -0.0882 m on the y-axis. The engine cylinder strokes, occurring during the cycle, are presented against the corresponding crankshaft angle in the figure. $P_p = 0$ m corresponds to the TDC while $P_p = -0.0882$ m corresponds to the BDC. TDC and BDC occur twice during the cycle. It can be seen from the figure that TDC is reached by the piston at 0 CAD and 360 CAD. It occurs when the connecting rod and crankshaft are in line. The lowest piston position, which is BDC, occurs at a crankshaft angle of 180 CAD and 540 CAD when the connecting rod and the crankshaft are also aligned and orientated in opposing directions. The piston displacement curve shows an asymmetrical trend due to the length of the connecting rod. It can be seen on the graph when the piston reaches the half stroke position of -0.0441 m before 90 CAD and 450 CAD and after 270 CAD and 630 CAD.
The instantaneous piston velocity \( (U_p) \) can be obtained by differentiating equation A-2 with respect to time \( (t) \):

\[
U_p = \frac{dP_D}{dt}
\]

\[
U_p = \frac{\pi}{2} \left( \sin \theta + \frac{A \sin \theta \cos \theta}{\sqrt{L^2 - A^2 \sin^2 \theta}} \right)
\]

\[
\bar{U}_p = 2SN
\]

where \( \bar{U}_p \) denotes the average piston speed, \( S \) is the engine stroke and \( N \) is the crankshaft rotational speed. An engine stroke of 0.0882 m gives an average piston speed of 4.41 m/s for 1500 revolutions per minute (rpm) and 5.88 m/s for 2000 rpm. The instantaneous piston velocity can now be defined by:

\[
U_p = \bar{U}_p \frac{\pi}{2} \left( \sin \theta + \frac{A \sin \theta \cos \theta}{\sqrt{L^2 - A^2 \sin^2 \theta}} \right)
\]

The variation of the instantaneous piston velocity calculated using equation A-5 is shown in Figure A.5.
Again, the velocity curve exhibits an asymmetrical trend for both engine speeds. Shown over 180 CAD, the instantaneous piston velocities and the corresponding average piston velocity are depicted in Figure A.6 for 1500 rpm and Figure A.7 for 2000 rpm.

Figure A.6 Instantaneous piston velocity for 1500 rpm

Figure A.7 Instantaneous piston velocity for 2000 rpm
1.3 Chemical kinetics mechanism

The list of species considered in the study is shown in Table A.1. The molecular mass of the species is defined as dimensionless since it is calculated relative to the atomic mass of an atom of carbon-12, 1/12th to be exact.

Table A.1 List of species for the reduced chemical kinetics model selected

<table>
<thead>
<tr>
<th>Species</th>
<th>Molecular mass (u)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂</td>
<td>2.01594</td>
</tr>
<tr>
<td>O₂</td>
<td>31.99880</td>
</tr>
<tr>
<td>H</td>
<td>1.00797</td>
</tr>
<tr>
<td>O</td>
<td>15.99940</td>
</tr>
<tr>
<td>OH</td>
<td>17.00737</td>
</tr>
<tr>
<td>HO₂</td>
<td>33.00677</td>
</tr>
<tr>
<td>H₂O₂</td>
<td>34.01474</td>
</tr>
<tr>
<td>H₂O</td>
<td>18.01534</td>
</tr>
<tr>
<td>N₂</td>
<td>28.01340</td>
</tr>
<tr>
<td>CO</td>
<td>28.01055</td>
</tr>
<tr>
<td>CO₂</td>
<td>44.00995</td>
</tr>
<tr>
<td>AR</td>
<td>39.94800</td>
</tr>
<tr>
<td>C₇H₁₆</td>
<td>100.20557</td>
</tr>
<tr>
<td>C₇H₁₅</td>
<td>99.19760</td>
</tr>
<tr>
<td>C₇H₁₄</td>
<td>98.18963</td>
</tr>
<tr>
<td>C₇H₁₅OO</td>
<td>131.19640</td>
</tr>
<tr>
<td>C₇H₁₄OOH</td>
<td>131.19640</td>
</tr>
<tr>
<td>OOC₇H₁₄OOH</td>
<td>163.19520</td>
</tr>
<tr>
<td>OC₇H₁₃OOH</td>
<td>146.18783</td>
</tr>
<tr>
<td>OC₇H₁₃O</td>
<td>129.18046</td>
</tr>
<tr>
<td>OC₇H₁₂O</td>
<td>128.17249</td>
</tr>
<tr>
<td>OC₇H₁₀O</td>
<td>126.15655</td>
</tr>
<tr>
<td>C₈H₁₈</td>
<td>114.23266</td>
</tr>
<tr>
<td>C₈H₁₇</td>
<td>113.22469</td>
</tr>
<tr>
<td>C₈H₁₆</td>
<td>112.21672</td>
</tr>
<tr>
<td>C₈H₁₇OO</td>
<td>145.22349</td>
</tr>
<tr>
<td>C₈H₁₆OOH</td>
<td>145.22349</td>
</tr>
<tr>
<td>OOC₈H₁₆OOH</td>
<td>177.22229</td>
</tr>
<tr>
<td>OC₈H₁₅OOH</td>
<td>160.21492</td>
</tr>
<tr>
<td>OC₈H₁₅O</td>
<td>143.20755</td>
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<tr>
<td>OC₈H₁₄O</td>
<td>142.19958</td>
</tr>
<tr>
<td>OC₈H₁₂O</td>
<td>140.18364</td>
</tr>
</tbody>
</table>
The list of reactions considered in the study is shown in Table A.2.

### Table A.2 List of reactions for the reduced chemical kinetics model selected [1]

<table>
<thead>
<tr>
<th>Reactions considered (k = A T^n exp(-E/RT))</th>
<th>A</th>
<th>n</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>C_7H_{15} + O_2 ⇌ C_7H_{15} + HO_2</td>
<td>1.00 × 10^{16}</td>
<td>0.0</td>
<td>46 000</td>
</tr>
<tr>
<td>Reverse Arrhenius coefficients</td>
<td>1.00 × 10^{12}</td>
<td>0.0</td>
<td>0</td>
</tr>
<tr>
<td>C_7H_{15} + O_2 ⇌ C_7H_{15}OO</td>
<td>1.00 × 10^{14}</td>
<td>0.0</td>
<td>0</td>
</tr>
<tr>
<td>Reverse Arrhenius coefficients</td>
<td>2.51 × 10^{13}</td>
<td>0.0</td>
<td>27 400</td>
</tr>
<tr>
<td>C_7H_{13}OO ⇌ C_7H_{14}OOH</td>
<td>1.51 × 10^{11}</td>
<td>0.0</td>
<td>19 000</td>
</tr>
<tr>
<td>Reverse Arrhenius coefficients</td>
<td>1.00 × 10^{11}</td>
<td>0.0</td>
<td>11 000</td>
</tr>
<tr>
<td>C_7H_{14}OO + O_2 ⇌ OOC_7H_{14}OOH</td>
<td>3.16 × 10^{11}</td>
<td>0.0</td>
<td>0</td>
</tr>
<tr>
<td>Reverse Arrhenius coefficients</td>
<td>2.51 × 10^{13}</td>
<td>0.0</td>
<td>27 400</td>
</tr>
<tr>
<td>OOC_7H_{14}OOH ⇌ OC_7H_{13}OOH + OH</td>
<td>8.91 × 10^{10}</td>
<td>0.0</td>
<td>17 000</td>
</tr>
<tr>
<td>C_7H_{16} + OH ⇌ C_7H_{15} + H_2O</td>
<td>1.00 × 10^{13}</td>
<td>0.0</td>
<td>3 000</td>
</tr>
<tr>
<td>OCC_7H_{13}OOH ⇌ OC_7H_{13}O + OH</td>
<td>3.98 × 10^{15}</td>
<td>0.0</td>
<td>43 000</td>
</tr>
<tr>
<td>C_7H_{15} + O_2 ⇌ C_7H_{14} + HO_2</td>
<td>3.16 × 10^{11}</td>
<td>0.0</td>
<td>6 000</td>
</tr>
<tr>
<td>Reverse Arrhenius coefficients</td>
<td>3.16 × 10^{11}</td>
<td>0.0</td>
<td>19 500</td>
</tr>
<tr>
<td>OC_7H_{13}O + O_2 ⇌ OC_7H_{12}O + HO_2</td>
<td>3.16 × 10^{11}</td>
<td>0.0</td>
<td>6 000</td>
</tr>
<tr>
<td>Reverse Arrhenius coefficients</td>
<td>3.16 × 10^{11}</td>
<td>0.0</td>
<td>19 500</td>
</tr>
<tr>
<td>OC_7H_{15}O + HO_2 + O_2 ⇌ OC_7H_{14}O + H_2O + HO_2</td>
<td>3.16 × 10^{13}</td>
<td>0.0</td>
<td>10 000</td>
</tr>
<tr>
<td>OC_7H_{16}O + HO_2 + 5O_2 ⇌ 7CO + 5H_2O + HO_2</td>
<td>3.16 × 10^{13}</td>
<td>0.0</td>
<td>10 000</td>
</tr>
<tr>
<td>C_7H_{14} + HO_2 + 7O_2 ⇌ 7CO + 7H_2O + HO_2</td>
<td>3.16 × 10^{13}</td>
<td>0.0</td>
<td>10 000</td>
</tr>
<tr>
<td>C_8H_{18} + O_2 ⇌ C_8H_{17} + HO_2</td>
<td>1.00 × 10^{16}</td>
<td>0.0</td>
<td>46 000</td>
</tr>
<tr>
<td>Reverse Arrhenius coefficients</td>
<td>1.00 × 10^{12}</td>
<td>0.0</td>
<td>0</td>
</tr>
<tr>
<td>C_8H_{17} + O_2 ⇌ C_8H_{17}OO</td>
<td>1.00 × 10^{14}</td>
<td>0.0</td>
<td>0</td>
</tr>
<tr>
<td>Reverse Arrhenius coefficients</td>
<td>2.51 × 10^{13}</td>
<td>0.0</td>
<td>27 400</td>
</tr>
<tr>
<td>C_8H_{17}OO ⇌ C_8H_{16}OOH</td>
<td>1.14 × 10^{11}</td>
<td>0.0</td>
<td>22 400</td>
</tr>
<tr>
<td>Reverse Arrhenius coefficients</td>
<td>1.00 × 10^{11}</td>
<td>0.0</td>
<td>11 000</td>
</tr>
<tr>
<td>C_8H_{16}OOH + O_2 ⇌ OOC_8H_{16}OOH</td>
<td>3.16 × 10^{11}</td>
<td>0.0</td>
<td>0</td>
</tr>
<tr>
<td>Reverse Arrhenius coefficients</td>
<td>2.51 × 10^{13}</td>
<td>0.0</td>
<td>27 400</td>
</tr>
<tr>
<td>OOC_8H_{16}OOH ⇌ OC_8H_{15}OOH + OH</td>
<td>8.91 × 10^{10}</td>
<td>0.0</td>
<td>17 000</td>
</tr>
<tr>
<td>C_8H_{16} + OH ⇌ C_8H_{17} + H_2O</td>
<td>1.00 × 10^{13}</td>
<td>0.0</td>
<td>3 000</td>
</tr>
<tr>
<td>OC_8H_{15}OOH ⇌ OC_8H_{15}O + OH</td>
<td>3.98 × 10^{15}</td>
<td>0.0</td>
<td>43 000</td>
</tr>
<tr>
<td>C_8H_{17} + O_2 ⇌ C_8H_{16} + HO_2</td>
<td>3.16 × 10^{11}</td>
<td>0.0</td>
<td>6 000</td>
</tr>
<tr>
<td>Reverse Arrhenius coefficients</td>
<td>3.16 × 10^{11}</td>
<td>0.0</td>
<td>19 500</td>
</tr>
<tr>
<td>OC_8H_{15}O + O_2 ⇌ OC_8H_{14}O + HO_2</td>
<td>3.16 × 10^{11}</td>
<td>0.0</td>
<td>6 000</td>
</tr>
<tr>
<td>Reverse Arrhenius coefficients</td>
<td>3.16 × 10^{11}</td>
<td>0.0</td>
<td>19 500</td>
</tr>
<tr>
<td>OC_8H_{14}O + HO_2 + O_2 ⇌ OC_8H_{13}O + H_2O + HO_2</td>
<td>1.58 × 10^{13}</td>
<td>0.0</td>
<td>10 000</td>
</tr>
<tr>
<td>OC_8H_{12}O + HO_2 + 6O_2 ⇌ 8CO + 6H_2O + HO_2</td>
<td>1.58 × 10^{13}</td>
<td>0.0</td>
<td>10 000</td>
</tr>
<tr>
<td>C_8H_{16} + HO_2 + 8O_2 ⇌ 8CO + 8H_2O + HO_2</td>
<td>2.00 × 10^{13}</td>
<td>0.0</td>
<td>10 000</td>
</tr>
<tr>
<td>Interaction reaction</td>
<td>25. ( \text{C}<em>8\text{H}</em>{18} + \text{C}<em>7\text{H}</em>{15} \leftrightarrow \text{C}<em>7\text{H}</em>{16} + \text{C}<em>8\text{H}</em>{17} )</td>
<td>( 5.01 \times 10^{12} )</td>
<td>0.0</td>
</tr>
<tr>
<td>----------------------</td>
<td>--------------------------------</td>
<td>-----------------</td>
<td>-------</td>
</tr>
<tr>
<td>26. ( \text{OH} + \text{H}_2 = \text{H} + \text{H}_2\text{O} )</td>
<td>2.14 \times 10^{08}</td>
<td>1.5</td>
<td>3 449</td>
</tr>
<tr>
<td>27. ( \text{O} + \text{OH} = \text{O}_2 + \text{H} )</td>
<td>2.02 \times 10^{14}</td>
<td>-0.4</td>
<td>0</td>
</tr>
<tr>
<td>28. ( \text{O} + \text{H}_2 = \text{OH} + \text{H} )</td>
<td>5.06 \times 10^{04}</td>
<td>2.7</td>
<td>6 290</td>
</tr>
<tr>
<td>29. ( \text{H} + \text{O}_2 (+\text{M}) = \text{HO}_2 (+\text{M}) )</td>
<td>4.52 \times 10^{13}</td>
<td>0.0</td>
<td>0</td>
</tr>
<tr>
<td>Low-pressure limit</td>
<td>0.00 \times 10^{00}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( 0.105 \times 10^{20} - 0.12570 \times 10^{01} )</td>
<td>H(_2)O enhanced by 0.00 \times 10^{00}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( 0.210 \times 10^{24} - 0.2437 \times 10^{01} )</td>
<td>H(_2) enhanced by 0.00 \times 10^{00}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( 0.152 \times 10^{20} - 0.1133 \times 10^{01} )</td>
<td>H(_2)O enhanced by 0.00 \times 10^{00}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( 0.203 \times 10^{21} - 0.159 \times 10^{01} )</td>
<td>H(_2) enhanced by 0.00 \times 10^{00}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( 0.203 \times 10^{21} - 0.159 \times 10^{01} )</td>
<td>N(_2) enhanced by 0.00 \times 10^{00}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>30. ( \text{H} + \text{O}_2 (+\text{N}_2) = \text{HO}_2 (+\text{N}_2) )</td>
<td>4.52 \times 10^{13}</td>
<td>0.0</td>
<td>0</td>
</tr>
<tr>
<td>Low-pressure limit</td>
<td>0.00 \times 10^{00}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( 0.210 \times 10^{24} - 0.2437 \times 10^{01} )</td>
<td>H(_2)O enhanced by 0.00 \times 10^{00}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>31. ( \text{H} + \text{O}_2 (+\text{H}_2) = \text{HO}_2 (+\text{H}_2) )</td>
<td>4.52 \times 10^{13}</td>
<td>0.0</td>
<td>0</td>
</tr>
<tr>
<td>Low-pressure limit</td>
<td>0.00 \times 10^{00}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( 0.210 \times 10^{24} - 0.2437 \times 10^{01} )</td>
<td>H(_2) enhanced by 0.00 \times 10^{00}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( 0.152 \times 10^{20} - 0.1133 \times 10^{01} )</td>
<td>H(_2)O enhanced by 0.00 \times 10^{00}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>32. ( \text{H} + \text{O}_2 (+\text{H}_2\text{O}) = \text{HO}_2 (+\text{H}_2\text{O}) )</td>
<td>4.52 \times 10^{13}</td>
<td>0.0</td>
<td>0</td>
</tr>
<tr>
<td>Low-pressure limit</td>
<td>0.00 \times 10^{00}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( 0.152 \times 10^{20} - 0.1133 \times 10^{01} )</td>
<td>H(_2) enhanced by 0.00 \times 10^{00}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>33. ( \text{OH} + \text{HO}_2 = \text{H}_2\text{O} + \text{O}_2 )</td>
<td>2.13 \times 10^{28}</td>
<td>-4.8</td>
<td>3 500</td>
</tr>
<tr>
<td>Declared duplicate reaction</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>34. ( \text{OH} + \text{HO}_2 = \text{H}_2\text{O} + \text{O}_2 )</td>
<td>9.10 \times 10^{14}</td>
<td>0.0</td>
<td>10 964</td>
</tr>
<tr>
<td>Declared duplicate reaction</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>35. ( \text{H} + \text{HO}_2 = \text{OH} + \text{OH} )</td>
<td>1.50 \times 10^{14}</td>
<td>0.0</td>
<td>1 000</td>
</tr>
<tr>
<td>36. ( \text{H} + \text{HO}_2 = \text{H}_2 + \text{O}_2 )</td>
<td>8.45 \times 10^{11}</td>
<td>0.7</td>
<td>1 241</td>
</tr>
<tr>
<td>37. ( \text{H} + \text{HO}_2 = \text{O} + \text{H}_2\text{O} )</td>
<td>3.01 \times 10^{13}</td>
<td>0.0</td>
<td>1 721</td>
</tr>
<tr>
<td>38. ( \text{O} + \text{HO}_2 = \text{O}_2 + \text{OH} )</td>
<td>3.25 \times 10^{13}</td>
<td>0.0</td>
<td>0</td>
</tr>
<tr>
<td>39. ( \text{OH} + \text{OH} = \text{O} + \text{H}_2\text{O} )</td>
<td>3.57 \times 10^{04}</td>
<td>2.4</td>
<td>-2 112</td>
</tr>
<tr>
<td>40. ( \text{H} + \text{H} + \text{M} = \text{H}_2 + \text{M} )</td>
<td>1.00 \times 10^{18}</td>
<td>-1.0</td>
<td>0</td>
</tr>
<tr>
<td>H(_2)O enhanced by 0.00 \times 10^{00}</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H(_2) enhanced by 0.00 \times 10^{00}</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>41. ( \text{H} + \text{H} + \text{H}_2 = \text{H}_2 + \text{H}_3 )</td>
<td>9.20 \times 10^{16}</td>
<td>-0.6</td>
<td>0</td>
</tr>
<tr>
<td>42. ( \text{H} + \text{H} + \text{H}_2\text{O} = \text{H}_2 + \text{H}_2\text{O} )</td>
<td>6.00 \times 10^{19}</td>
<td>-1.2</td>
<td>0</td>
</tr>
<tr>
<td>43. ( \text{H} + \text{OH} + \text{M} = \text{H}_2\text{O} + \text{M} )</td>
<td>2.21 \times 10^{22}</td>
<td>-2.0</td>
<td>0</td>
</tr>
<tr>
<td>H(_2)O enhanced by 6.40 \times 10^{00}</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>44. ( \text{H} + \text{O} + \text{M} = \text{OH} + \text{M} )</td>
<td>4.71 \times 10^{18}</td>
<td>-1.0</td>
<td>0</td>
</tr>
<tr>
<td>H(_2)O enhanced by 6.40 \times 10^{00}</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>45. ( \text{O} + \text{O} + \text{M} = \text{O}_2 + \text{M} )</td>
<td>1.89 \times 10^{18}</td>
<td>0.0</td>
<td>-1 788</td>
</tr>
</tbody>
</table>
46. $\text{HO}_2 + \text{HO}_2 \Leftrightarrow \text{H}_2\text{O}_2 + \text{O}_2$  
   $2.00 \times 10^{10}$  
   0.0  
   5 000
47. $\text{H}_2\text{O}_2 + \text{M} \Leftrightarrow \text{OH} + \text{OH} + \text{M}$  
   $1.00 \times 10^{16}$  
   0.0  
   48 000
48. $\text{H}_2\text{O}_2 + \text{H} = \text{HO}_2 + \text{H}_2$  
   $1.98 \times 10^{16}$  
   2.0  
   2 435
49. $\text{H}_2\text{O}_2 + \text{H} = \text{OH} + \text{H}_2\text{O}$  
   $3.07 \times 10^{13}$  
   0.0  
   4 217
50. $\text{H}_2\text{O}_2 + \text{O} = \text{OH} + \text{HO}_2$  
   $9.55 \times 10^{06}$  
   2.0  
   3 970
51. $\text{H}_2\text{O}_2 + \text{OH} = \text{H}_2\text{O} + \text{HO}_2$  
   $2.40 \times 10^{18}$  
   4.0  
   -2 162

<table>
<thead>
<tr>
<th>CO oxidation reactions</th>
<th>O + CO (+M) $\Leftrightarrow$ CO$_2$ (+M)</th>
<th>$1.80 \times 10^{10}$</th>
<th>0.0</th>
<th>2 385</th>
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<tr>
<td></td>
<td>Low-pressure limit</td>
<td>$3.00 \times 10^{03}$</td>
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<td>52.</td>
<td>$0.602 \times 10^{15} 0.00 \times 10^{00}$</td>
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<td></td>
<td>$\text{H}_2$ enhanced by $2.00 \times 10^{00}$</td>
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<tr>
<td></td>
<td>$\text{O}_2$ enhanced by $6.00 \times 10^{01}$</td>
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<tr>
<td></td>
<td>$\text{H}_2\text{O}$ enhanced by $6.00 \times 10^{00}$</td>
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<tr>
<td></td>
<td>$\text{CO}$ enhanced by $1.50 \times 10^{00}$</td>
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<tr>
<td></td>
<td>$\text{CO}_2$ enhanced by $3.50 \times 10^{00}$</td>
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<tr>
<td></td>
<td>$\text{AR}$ enhanced by $5.00 \times 10^{01}$</td>
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<tr>
<td>53.</td>
<td>$\text{O}_2 + \text{CO} \Leftrightarrow \text{O} + \text{CO}_2$</td>
<td>$2.50 \times 10^{12}$</td>
<td>0.0</td>
<td>47 800</td>
</tr>
<tr>
<td>54.</td>
<td>$\text{CO} + \text{OH} \Leftrightarrow \text{CO}_2 + \text{H}$</td>
<td>$4.76 \times 10^{07}$</td>
<td>1.2</td>
<td>70</td>
</tr>
<tr>
<td>55.</td>
<td>$\text{HO}_2 + \text{CO} \Leftrightarrow \text{OH} + \text{CO}_2$</td>
<td>$4.76 \times 10^{15}$</td>
<td>0.0</td>
<td>23 600</td>
</tr>
</tbody>
</table>

### 1.4 Engine variables

The Chen-Flynn model [2] is widely used to estimate the friction of engines. It assumes that the friction mean effective pressure (FMEP) is a function of the engine speed, the maximum in-cylinder pressure and a pressure constant. The model accounts for the friction caused by engine speed, using the quadratic law of the piston velocity. The effect of engine load is modelled linearly from the maximum in-cylinder pressure. However, the Chen-Flynn friction model does not account for the timing of the maximum in-cylinder pressure. Some discrepancies of the friction prediction have been reported for late fuel injections and increases of the engine load when the cylinder peak pressure is occurring later than 20 CAD after TDCF [3].

The calculation of FMEP can be expressed as follows:

\[
FMEP = C + \left(P_{\text{max}} a\right) + \left(\overline{U}_p b\right) + \left(\overline{U}_p^2 c\right) \quad (A-6)
\]

where C is the constant component of the friction, $P_{\text{max}}$ is the peak cylinder pressure, a is the peak cylinder pressure factor, $\overline{U}_p$ is the mean piston velocity, b is the mean piston velocity factor and c is the mean piston velocity squared factor. The model required the
calibration of the four constants against the experimental data. For the calculations conducted during the study, the coefficients used were: \( C = 0.3, a = 0.006, b = 0.09 \) and \( c = 0 \).

The global heat transfer coefficient depends on the characteristic length \( L(t)^{m-1} \), the transport properties \( \frac{k}{\mu^m} \), the pressure \( P(t)^m \), the temperature \( T(t)^{-m} \) and the characteristic velocity \( V(t)^m \) and can be expressed as:

\[
h_{global}(t) = \alpha_{scaling} L(t)^{m-1} \frac{k}{\mu^m} P(t)^m T(t)^{-m} V(t)^m
\]  

(A-7)

where \( m \) is the exponent and \( \alpha_{scaling} \) is tuned to match the specific engine geometry.

Derived from the global heat transfer coefficient equation, the Woschni heat transfer model can be expressed as:

\[
h_{Woschni} = L^{m-1} P^m T^{0.75-1.62m} \left( C_1 \bar{U}_p + C_2 \frac{V_r T_r}{p_r V_r} (p - p_{motor}) \right)^m
\]  

(A-8)

where \( C_1 \) and \( C_2 \) are constants, \( \bar{U}_p \) is the mean piston speed, \( p_{motor} \) is the pressure at motored conditions and \( r \) denotes a specific crank angle for the variables. For the calculations of this study, the convection multiplier, the head to bore area ratio and the piston to bore area ratio were set at 1, 1.3 and 1, respectively. Some studies investigated variations of the original Woschni model to be applicable for HCCI combustion [4].
The brake mean effective pressure is defined as:

\[ BMEP = \frac{P_{n_r}}{V_d \cdot N} \]  \hspace{1cm} (A-9)

where \( P \) is the engine power output and \( n_r \) is the number of crank revolutions needed for a full cycle. \( n_r \) equals two for four-stroke cycles and one for two-stroke cycles. \( V_d \) is the displacement volume and \( N \) is the engine speed in rpm.

The fuel mean effective pressure can be expressed as:

\[ FuelMEP = \frac{m_f Q_{LHV}}{V_d} \]  \hspace{1cm} (A-10)

where \( m_f \) is the mass of the fuel, \( Q_{LHV} \) is the lower heating value of the fuel.

The net indicated mean effective pressure is defined over the full cycle as:

\[ IMEP_{net} = \frac{\int_{-360}^{360} P \, dV}{V_d} \]  \hspace{1cm} (A-11)

The net indicated work per cycle is integrated from the pressure-volume diagram over the entire cycle.
The net indicated efficiency is defined by:

\[
\eta_{\text{indicated}} = \frac{\text{IMEP}_{\text{net}}}{\text{FuelMEP}} \quad (A-12)
\]

The gross indicated mean effective pressure is defined as:

\[
\text{IMEP}_{\text{gross}} = \frac{\int_{-180}^{180} P \, dV}{V_d} \quad (A-13)
\]

The gross indicated work is integrated from the pressure-volume diagram over the compression and expansion stroke.

The heat release mean effective pressure can be defined by:

\[
Q_{hr \text{MEP}} = \frac{Q_{hr}}{V_d} \quad (A-14)
\]

where \(Q_{hr}\) is the heat released in the cylinder including the heat transfer losses.

The gross indicated efficiency over the compression and expansion stroke can be expressed as:

\[
\eta_{\text{indicated}_{360}} = \frac{\text{IMEP}_{\text{gross}}}{Q_{hr \text{MEP}}} \quad (A-15)
\]
The mechanical efficiency can be defined by:

$$\eta_{\text{mechanical}} = \frac{\text{BMEP}}{\text{IMEP}_{\text{net}}}$$  \hspace{1cm} (A-16)

The pumping mean effective pressure is expressed as:

$$\text{PMEP} = \text{IMEP}_{\text{gross}} - \text{IMEP}_{\text{net}}$$  \hspace{1cm} (A-17)

Finally, the friction mean effective pressure is defined by:

$$\text{FMEP} = \text{IMEP}_{\text{net}} - \text{BMEP}$$  \hspace{1cm} (A-18)
References


