A process for an Efficient Heat
Release Prediction at the Concepts
Screening Stage of Gasoline Engine
Development.

by

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ABSTRACT

In recent years, the exploration of new combustion technologies has accelerated due to new stringent emissions regulations and fuel economy requirements. Virtual engineering tools, that enable the screening of non-traditional hardware and engine calibration at the early stage of engine development, have become imperative to meet new emission regulations. In the current engine development process benchmarking and historical test data, are used to carry out simple 1-D engine system calculations and define the overall engine concept design. Later, to provide a definitive design ready for prototyping, more complex Computational Fluid Dynamics (CFD) calculations are coupled to 1-D engine system codes to optimise initial concept geometries and high-level calibrations. However, to provide meaningful results, 1-D engine system codes often use empirical based combustion models that require an initial input, called engine burn rate. Realistic engine burn rate responses, for the entire engine map and for different design concepts, are also required to provide 3D CFD codes with correct boundary conditions during the design optimisation phase. Thus, the engine burn rate of new combustion technologies, for which little experimental data is available, need to be initially assumed. To improve the predictive capabilities virtual engine development processes, the industry's attention shifted towards Quasi-Dimensional (Q-D) combustion models capable of providing engine burn rate predictions. However, within the Q-D modelling framework, turbulence models, adding extra user-input variables, are required to capture the effect of different combustion chamber geometries on the engine combustion rate. Rigorous validation of Q-D turbulence models for different engine concepts and engine maps is needed to enable Q-D combustion models to predict the engine burn rate. Therefore, an alternative methodology characterised by limited dependency on previous test data is required to enhance the exploration of novel combustion strategies and geometric architectures.

In this thesis, an alternative engine development process that uses a combination of a Q-D combustion Stochastic Reactor Model (SRM), a 1-D engine system model and non-combusting, “cold” CFD calculations, is proposed. The SRM code captures the combustion chemistry in a computationally efficient manner but does not capture in isolation geometric variables such as port and piston geometry. To account for that, the approach uses limited non-combusting CFD baseline calculations to characterise the engine in-cylinder flow of each screened engine concepts. A physics-based scaling factor response was developed and

used to provide the SRM with the correct turbulence input, known as scalar mixing time (τ_{SRM}). The response was assessed against four different engine variants over a variety of engine operating conditions. The same response was used to predict the effect of different bore to stroke ratios (B/S) on the engine combustion rate and knock tolerance. Non-combusting CFD and 1-D engine system simulations have been carried out to investigate the effect of different engine variants and operating conditions on the in-cylinder turbulence. It was shown that τ_{SRM} of different operating conditions can be scaled to the intake flow velocity predicted by 1-D engine system analysis. This allows to predict the engine RoHR at the explored engine variants and operating conditions within the experimental standard deviation. The presented methodology showed augmented predictive capabilities and has potential to move the engine development towards a less hardware dependent approach for the exploration of new engine concepts.

“Tragedy should be used as a source of strength.

If we lose our hope, that is our real disaster.”

Dalai Lama XIV

Planet Earth, MOLAMIA!

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TABLE OF CONTENTS

Abstract	i
Table of Contents	a
List of Equations	f
List of Figures.....	h
List of Tables	o
List of Publications.....	p
Nomenclature.....	q
Acknowledgements	r
Declaration	s
1 Introduction	1
1.1 The Internal Combustion Engine.....	1
1.1.1 The Spark Ignited Combustion Engine	2
1.2 The Early Stage of Engine Development Process	3
1.2.1 Initial engine concept definition.....	4
1.2.2 Initial engine concept review	5
1.2.3 The Current Virtual Engine Development Process	5
1.3 Available Solutions to improve the virtual Engine Development	8
1.3.1 Virtual Engine Development Processes based on CFD Combustion Models.....	8
1.3.2 Virtual Engine Development Processes based on Q-D Combustion Models.....	9
1.3.3 Virtual Engine Development Processed based on Q-D and CFD models.....	9
1.4 The Work Done	10
1.4.1 Terminology	11
1.4.2 Aim & Objectives	12
1.4.3 Research Questions	13

1.4.4	Thesis Contributions	14
1.4.5	Thesis focus and limitations	15
1.5	Future Work	16
1.6	Thesis Structure	17
2	Literature Review	19
2.1	The Problem	19
2.1.1	The Current Rate of Heat Release modelling approach	19
2.1.2	Alternative Solutions to Model the Engine Rate of Heat Release	21
2.2	Introduction to the Flame Front Propagation in SI Engines	25
2.2.1	Laminar Flame Speed	26
2.2.2	Turbulent Flame Speed	28
2.3	The Thermodynamic Quasi-Dimensional (Q-D) Combustion models	29
2.3.1	Mass Burning Rate Sub-Models	32
2.4	Stochastic Reactor Models	37
2.4.1	Flame Propagation Model	38
2.5	In-Cylinder Turbulence Models	39
2.5.1	Q-D Turbulence Models	40
2.5.2	Q-D / CFD Based Approach	42
2.6	Conclusions	44
3	Experimental Data	46
3.1	Engine A	46
3.2	Engine B	48
3.3	Engine C	50
3.4	Engine D	51
4	Numerical models	55
4.1	Non-Combusting In-Cylinder CFD	55

4.1.1	Introduction to Turbulence	56
4.1.2	Turbulence modelling within the RANS CFD framework.....	58
4.2	1-D Engine System Simulation	59
4.3	Q-D Stochastic Reactor Model.....	60
4.3.1	Piston Movement Calculation	63
4.3.2	Flame Propagation Model	63
4.3.3	Turbulence Mixing Model	65
4.3.4	Chemical Reactions Calculation.....	66
4.3.5	Heat Transfer Model	67
4.3.6	Heat Release Calculation	67
4.4	Conclusions	71
5	Methodology.....	73
5.1	Turbulence Scaling Factor Response Assumptions	74
5.1.1	First assumption	74
5.1.2	Second assumption	75
5.2	Procedure to determine the similarity between Turbulent mixing times	75
5.3	SRM Model calibration on Baseline experimental Data	79
5.4	Turbulence Response to Engine Operating Conditions and High-level calibrations.....	82
5.5	Scalar mixing time Response used for Engine Update.....	85
5.6	Conclusions	87
6	In-Cylinder Turbulence Analysis	88
6.1	Engine Operating Conditions and Calibrations Effect	88
6.1.1	Valves Timing.....	88
6.1.2	Engine Speed	95
6.1.3	Start of Injection Timing	98
6.2	Engine Design Effect	102

6.2.1	Engine Variant Effect on In-Cylinder Turbulence	103
6.2.2	Bore to Stroke Ratio Effect on In-Cylinder Turbulence	108
6.2.3	Injector Effect on In-Cylinder Turbulence	113
6.3	Conclusions	116
7	Combustion Predictions Comparison with Experimental Data	119
7.1	Combustion Predictions comparison with Experimental Data from Different Engine Maps	119
7.1.1	Engine A.....	119
7.1.2	Engine B.....	128
7.1.3	Engine C.....	131
7.1.4	Engine D.....	134
7.2	Conclusions	142
8	Conclusions	145
8.1	Simulation Tools Compatible with the Scope of the Thesis	145
8.2	Physics that Governs the RoHR of SI Engines.....	145
8.3	The Developed Methodology	146
8.4	The Non-Combusting CFD analysis	147
8.5	Combustion Predictions Comparison with Experimental Data.....	147
8.6	Future Work.....	148
References		149
Appendix		155
Engine A.....		155
Bore to Stroke Ratio Effect on the In-Cylinder Turbulence Analysis		155
1300rev/min VVT Combustion Prediction		161
1300rev/min Charge Dilution Combustion Prediction		165
2000rev/min VVT Combustion Prediction		168
2000rev/min Charge Dilution Combustion Prediction		170
3500rev/min VVT Combustion Prediction		173

3500rev/min Charge Dilution Combustion Prediction	176
5500rev/min VVT Combustion Prediction	179
Engine B	183
In-cylinder Turbulence analysis	183
2000rev/min Combustion Prediction	185
3000rev/min Combustion Prediction	187
4000rev/min Combustion Prediction	189
5000rev/min Combustion Prediction	191
Engine C	193
In-cylinder Turbulence Analysis	193
Engine map combustion predictions	194
2000rev/min Combustion Prediction	196
3000rev/min Combustion Prediction	198
4000rev/min Combustion Prediction	200
5000rev/min Combustion Prediction	202
6000rev/min Combustion Prediction	204
Engine D	206
In-cylinder Turbulence Analysis	206
Injector A combustion predictions at different engine loads	207
Injector B combustion predictions at different engine loads	208
Injector A combustion prediction at different start of injection timing	209

LIST OF EQUATIONS

<i>Equation 1: Wiebe function.....</i>	<i>20</i>
<i>Equation 2: General formulation for the mass burning rate within SI engines as provided by [42].</i>	<i>33</i>
<i>Equation 3: Entrainment mass burning rate as proposed by Blizard [65].</i>	<i>34</i>
<i>Equation 4: Entrainment model mass burning rate as proposed by Blizard [65].</i>	<i>34</i>
<i>Equation 5: Burning time constant for the entrainment model mass burning rate as proposed by Blizard. ...</i>	<i>34</i>
<i>Equation 6: Mass burning rate in a flame sheet model as proposed in [42].</i>	<i>36</i>
<i>Equation 7: Fractal definition of the wrinkled surface area as provided in [70]</i>	<i>36</i>
<i>Equation 8: Turbulent flame speed according to [6].....</i>	<i>39</i>
<i>Equation 9: Turbulent flame speed according to [86].....</i>	<i>39</i>
<i>Equation 10: Experimental Burn Angle Standard Deviation.....</i>	<i>46</i>
<i>Equation 11: In-cylinder turbulence intensity.....</i>	<i>55</i>
<i>Equation 12: Reynolds number</i>	<i>57</i>
<i>Equation 13: Fluid particles' velocity components</i>	<i>57</i>
<i>Equation 14: Turbulent Kinetic Energy</i>	<i>58</i>
<i>Equation 15: Characteristic length scale</i>	<i>58</i>
<i>Equation 16: Turbulent viscosity</i>	<i>59</i>
<i>Equation 17: Temperature definition between two events.....</i>	<i>60</i>
<i>Equation 18: Random variable corresponding to a normalised temperature definition.....</i>	<i>60</i>
<i>Equation 19: Sample space ψ distribution function for the random variable ϕ.....</i>	<i>61</i>
<i>Equation 20: Sample space probability event</i>	<i>62</i>
<i>Equation 21: Mass distribution function within the SRM code (a) and vector containing the random variable in the MDF (b).....</i>	<i>62</i>
<i>Equation 22: Time evolution of the MDF within the SRM code.....</i>	<i>62</i>
<i>Equation 23: SRM turbulent flame speed calculation</i>	<i>64</i>
<i>Equation 24: In-cylinder turbulence characteristic dictating the turbulent flame speed calculation within the SRM.</i>	<i>64</i>
<i>Equation 25: Change to the PDF due to the mixing of the particles.....</i>	<i>66</i>
<i>Equation 26: Particles mixing calculation steps for gas composition (a) and enthalpy (b).</i>	<i>66</i>
<i>Equation 27: Rate of Heat Release formulation. z is an index representing the model zones.</i>	<i>67</i>
<i>Equation 28: General 4th grade polynomial equation</i>	<i>76</i>
<i>Equation 29: Turbulent Mixing time for the baseline engine</i>	<i>80</i>
<i>Equation 30: Scalar mixing time for the baseline engine</i>	<i>80</i>
<i>Equation 31: Scalar Mixing time multiplier for different operating conditions and calibrations.</i>	<i>84</i>
<i>Equation 32: Scalar Mixing time for different operating conditions and calibrations.</i>	<i>84</i>
<i>Equation 33: Turbulent Mixing time for any engine variant</i>	<i>86</i>
<i>Equation 34: Scalar mixing time for any given engine variant.....</i>	<i>86</i>

<i>Equation 35: Scalar Mixing time at different engine operating conditions and calibrations of any engine variant</i>	<i>86</i>
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LIST OF FIGURES

Figure 1: Major components of an Internal Combustion Engine as reported in [3]	1
Figure 2: The early concepts screening phase of engine development.	3
Figure 3: Gap in the RoHR predictive capabilities in the current virtual engine development process	7
Figure 4: Generic ideal engine development process	8
Figure 5: Schematic of proposed virtual engine development process	11
Figure 6: Overall thesis outline	17
Figure 7: Schematic of the virtual empirical based engine development process.	21
Figure 8: Illustration of the inner structure of a flame front in a stationary, laminar and stoichiometric methane-air mixture accordingly to [43]	27
Figure 9: Wrinkled turbulent flame structure as proposed in [46]	33
Figure 10: Schematic of necessary physical processes to be modelled in the Q-D framework to predict the engine burning rate	41
Figure 11: Engine A Valve Lift	47
Figure 12: Engine A (in blue) and Engine B(in orange) geometry comparison	49
Figure 13: Engine B Valve Lift	50
Figure 14: Engine C Valve Lift	51
Figure 15: Engine D geometry	53
Figure 16: Plan view of injectors holes layout	54
Figure 17: Engine A mesh size without refinement	56
Figure 18: Engine A mesh size with refinement during valve events	56
Figure 19: Sample space ψ for the random variable ϕ	61
Figure 20: Sample space showing the region corresponding to the event A. Filled black dot correspond to the sample point for which A occurred.	61
Figure 21: Overall SRM sub models' layout	63
Figure 22: Schematic representation of the mixing of the particles within the SRM code [106].	66
Figure 23: Engine A's predicted in-cylinder pressure, burnt zone and unburnt zone RoHR at 2000rpm 7.5bar BMEP	69
Figure 24: Engine A's temperature PDF evolution from -35 [CA °ATDC(f)] (graph A) to +27 [CA °ATDC(f)] (graph C) in the burned zone at 2000rpm 7.5bar BMEP.	70
Figure 25: Engine A's temperature PDF evolution from +3 [CA °ATDC(f)] (graph A) to +27 [CA °ATDC(f)] (graph B) in the unburnt zone at 2000rpm 7.5bar BMEP.	71
Figure 26: Schematic of the methodology used to predict the engine RoHR.	73
Figure 27: High-level methodology flowchart. The development process is split into three main phases as follows: models' calibration, engine optimisation and engine update.	74
Figure 28: Turbulent mixing time polynomial fitting using the "least mean square" method.	77

Figure 29: Polynomial coefficients' value of the 4 th grade polynomial curves fitted to the turbulent mixing time from different valve timing. Error bands correspond to the standard coefficients' error calculated with a 95% confidence interval.	78
Figure 30: Comparison between CFD derived τ_t and mixing time values derived using a single 4 th grade polynomial curve, fitted to τ_t from valve timing 1.	78
Figure 31: Flowchart of the initial models' calibration phase. Baseline engine experimental data is used to build a 1-D engine system model that, coupled with single non-combusting CFD calculation, is used to tune the SRM code.	79
Figure 32: Flowchart of the engine optimisation phase. The change in the intake port velocity to engine operating point, captured by the 1-D engine system model, is used to provide the SRM code with the necessary turbulence input.	82
Figure 33: Effect of different engine speeds on the intake port velocity	83
Figure 34: Flowchart of the engine update phase. Non-combusting CFD analysis, one for each explored engine concept, is used to provide the SRM code with the correct turbulence input.	85
Figure 35: Engine A CFD predictions of different valve timing effect on in-cylinder mean flow velocity (graph A), turbulence intensity (graph B) and tumble ratio (graph C). Valve timing data refers to key points 1,2 and 3 in Table 3.	90
Figure 36: Engine A in-cylinder flow speed vectors comparison between different valve timing. Valve timing data refers to key points 1,2 and 3 in Table 3.	91
Figure 37: Engine A 1-D prediction of different valve timing effect on the intake port velocity. Valve timing data refers to key points 1,2 and 3 in Table 3.	91
Figure 38: Engine A CFD prediction of different valve timing effect on the in-cylinder dissipation rate, ϵ (graph A) and the turbulent mixing time, τ_t (graph B). Valve timing data refers to key points 1,2 and 3 in Table 3.	92
Figure 39: Polynomial coefficients' value of the 4 th grade polynomial curves fitted to the turbulent mixing time from different valve timing. Error bands correspond to the standard coefficients' error calculated with a 95% confidence interval	93
Figure 40: Comparison between CFD derived τ_t and mixing time values derived using a single 4 th grade polynomial curve, fitted to τ_t at for valve timing 1. Y-intercept coefficients' values changed for each speed.	94
Figure 41: Predicted scalar mixing time profiles, τ_{SRM} (left axis) vs 3D CFD predicted turbulent mixing time profiles, τ_t (right axis) for different valve timing. Valve timing data refers to key points 1,2 and 3 in Table 3.	94
Figure 42: Engine A CFD prediction of different engine speeds effect on the in-cylinder mean flow velocity (graph A) and turbulence intensity (graph B).	95
Figure 43: Engine A 1-D Intake and Exhaust mass flow for different engine speeds	96
Figure 44: Engine A CFD prediction of different engine speeds effect on the Turbulent Mixing Time	97

Figure 45: Polynomial coefficients' value of the 4 th grade polynomial curves fitted to the turbulent mixing time from different engine speeds. Error bands correspond to the standard coefficients' error calculated with a 95% confidence interval. _____	98
Figure 46: Comparison between CFD derived τ_t and mixing time values derived using a single 4 th grade polynomial curve, fitted to τ_t at 2000rpm. Y-intercept coefficients' values changed for each speed. _____	98
Figure 47: Comparison of the CFD predicted velocity flow vectors for two different SOI timing _____	100
Figure 48: CFD prediction of engine D's turbulent mixing time for different start of injection timing _____	101
Figure 49: Polynomial coefficients' value of the 4 th grade polynomial curves fitted to the turbulent mixing time from different SOI. Error bands correspond to a 95% confidence interval. _____	101
Figure 50: Derived scalar mixing time for different start of injection timing _____	102
Figure 51: CFD prediction of different engine variants effect on in-cylinder mean flow velocity (graph A), turbulence intensity (graph B) and tumble ratio (graph C). _____	104
Figure 52: CFD predicted intake flow velocity vectors comparison of engine A (left graph), engine B (middle graph) and engine C (right graph) at 2000rpm_40Nm. _____	106
Figure 53: 1-D Intake port velocity for different engine variants. _____	106
Figure 54: CFD prediction of different engine variants effect on the turbulent and scalar mixing time, τ_t and τ_{SRM} . _____	107
Figure 55: Change in the engine deck diameter necessary to maintain a constant compression ratio of 11.5:1 for different bore to stroke ratios. _____	109
Figure 56: CFD prediction of different bore to stroke ratios effect on in-cylinder mean flow velocity (graph A) and tumble ratio (graph B) _____	110
Figure 57: CFD prediction of different bore to stroke ratios on in-cylinder flow velocity at vectors at 480 °CA ATDC(F). _____	111
Figure 58: CFD prediction of different bore to stroke ratios effect on the turbulent mixing time τ_t (graph A). Scalar mixing time for different bore to stroke ratios derived using turbulence scaling factor response (graph B). _____	112
Figure 59: Injector A and B' spray patterns comparison _____	114
Figure 60: CFD prediction of the effect of different injector types on the in-cylinder tumble. _____	115
Figure 61: CFD prediction of the effect of different injector types on the turbulent kinetic energy production (graph A), the dissipation rate (graph B) and the turbulent mixing time (graph C) during the closed part of the engine cycle. _____	116
Figure 62: Experimental spark and SRM input timing comparison for different valve timing _____	120
Figure 63: Predicted and experimental CA50 (graph A) and burn duration, CA10-90 (graph B) for different valve timing. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red error bands. _____	121
Figure 64: Predicted and experimental burn duration, CA10-90 for different charge dilution. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red error bands. _____	123

Figure 65: Experimental spark and SRM input timing comparison for different charge dilutions. _____	123
Figure 66: Experimental spark and SRM input timing comparison for different engine speeds and valve timing. _____	124
Figure 67: Predicted and experimental CA10 (graph A) and CA10-90 (graph B) for different engine speeds and valve timing. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red error bands. _____	125
Figure 68: Prediction of different bore to stroke ratios on the engine burn rate and SRM ignition timing (graph A) and engine knock tolerance (graph B). Horizontal dashed line represents the engine knocking area limit. _____	127
Figure 69: Experimental spark (circle symbols) and SRM input ignition input (triangle symbol) timing comparison for different engine speed and load. _____	129
Figure 70: Engine B predicted and experimental burn duration, CA1090 (graph A), 1:1 results prediction line is represented by the dashed line. Error bands represent the average experimental standard deviation (graph A). Burn duration expressed in millisecond is shown in graph B. _____	130
Figure 71: Improved Engine C predicted and experimental burn duration, CA1090 (graph A), 1:1 results prediction line is represented by the dashed line. Error bands represent the average experimental standard deviation (graph A). Burn duration expressed in millisecond is shown in graph B. _____	133
Figure 72: Predicted SRM ignition timing comparison at different speeds between engine B (naturally aspirated) and engine C (turbo-charged) at constant engine load _____	134
Figure 73: Predicted engine combustion rates at 2000rpm_2barBMEP_injector B (left graph) and 2000rpm_8barBMEP_injector B (right graph). Red vertical lines represent the SRM ignition timing and black lines represent the experimental spark time. Black error bands show the experimental standard deviation respectively at CA 10, CA 50 and CA 90. _____	135
Figure 74: Engine D CA10 and CA10-90 prediction at 2000rpm_8bar_BMEP_SOI_420. Red data correspond to injector A. Black data correspond to injector B. _____	136
Figure 75: Prediction of the effect of SRM ignition timing on engine D G-ISFC (top graph) and CA50 (bottom graph) at 2000rpm_8barBMEP_SOI_420. Circles corresponds to a swing of the SRM ignition timing value. Cross data correspond to the predicted SRM ignition timing following the procedure presented in Paragraph 5.5. _____	139
Figure 76: Measured and predicted engine burning rate at 2000rpm_8barBMEP at different SOI timing _____	141
Figure 77: Predicted and experimental burn durations comparison between engine A, B and _____	143
Figure 78: CFD prediction of different bore to stroke ratios effect on in-cylinder turbulent kinetic energy, k (graph a), the in-cylinder dissipation rate, ϵ (graph b). _____	155
Figure 79: 1-D Intake port velocity for different bore to stroke ratios. _____	156
Figure 80: CFD prediction of different bore to stroke ratios on in-cylinder flow velocity at vectors at 360 °CA ATDC(F) (left column) and 370 °CA ATDC(F) (right column). _____	157
Figure 81: CFD prediction of different bore to stroke ratios on in-cylinder flow velocity at vectors at 580 °CA ATDC(F) (left column) and 670 °CA ATDC(F) (right column). _____	158

Figure 82: CFD prediction of different bore to stroke ratios on in-cylinder flow velocity at vectors at 360 °CA ATDC(F) (left column) and 370 °CA ATDC(F) (right column).	159
Figure 83: CFD prediction of different bore to stroke ratios on in-cylinder flow velocity at vectors at 580 °CA ATDC(F) (left column) and at 670 °CA ATDC(F)(right column).	160
Figure 84: Predicted and Experimental CA10 (graph A), CA50 (graph B) (graph C) and CA10-90 (graph D) for different valve timing. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red error bands.	162
Figure 85: Experimental spark and SRM input timing comparison for different valve timing.	162
Figure 86: Predicted pressure and experimental pressure traces for key point 8 (graph A), key point 9 (graph B), key point 10 (graph C) and key point 11 (graph D).	164
Figure 87: Predicted and Experimental CA10 (graph A), CA50 (graph B) (graph C) and CA10-90 (graph D) for different charge dilution. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red error bands.	166
Figure 88: Experimental spark and SRM input timing comparison for different charge dilution	166
Figure 89: Predicted pressure and experimental pressure traces for key point 12 (graph A), key point 13 (graph B) and key point 14 (graph C).	167
Figure 90: Predicted and Experimental CA10 (graph A) and CA90 (graph B) for different valve timing. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red error bands.	168
Figure 91: Predicted pressure and experimental pressure traces for key point 1 (graph A), key point 2 (graph B) and key point 3 (graph C)	169
Figure 92: Predicted and Experimental CA10 (graph A) CA50 (graph B) and CA90 (graph C) for different charge dilution. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red error bands.	170
Figure 93: Predicted pressure and experimental pressure traces for key point 4 (graph A), key point 5 (graph B), key point 6 (graph C) and key point 7 (graph D).	172
Figure 94: Predicted and Experimental CA10 (graph A), CA50 (graph B) (graph C) and CA10-90 (graph D) for different valve timing. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red error bands	174
Figure 95: Experimental spark and SRM input timing comparison for different valve timing	174
Figure 96: Predicted pressure and experimental pressure traces for key point 15 (graph A), key point 16 (graph B) and key point 17 (graph C)	175
Figure 97: Predicted and Experimental CA10 (graph A), CA50 (graph B) (graph C) and CA10-90 (graph D) for different charge dilution. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red bands.	177
Figure 98: Experimental spark and SRM input timing comparison for different charge dilution	177
Figure 99: Predicted pressure and experimental pressure traces for key point 18 (graph A), key point 19 (graph B) and key point 20 (graph C).	178

Figure 100: Predicted and Experimental CA10 (graph A), CA50 (graph B) (graph C) and CA10-90 (graph D) for different valve timing. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red error bands. _____	180
Figure 101: Experimental spark and SRM input timing comparison for different valve timing. _____	180
Figure 102: Predicted pressure and experimental pressure traces for key point 21 (graph A), key point 22 (graph B), key point 23 (graph C) and key point 24 (graph D). _____	182
Figure 103: CFD prediction of different engine variants effect on the in-cylinder turbulent kinetic energy, k (graph A), the in-cylinder dissipation rate, ϵ (graph B) _____	183
Figure 104: CFD prediction of different engine speeds on the turbulent mixing time, τ_t . _____	183
Figure 105: Polynomial coefficients' value of the 4 th grade polynomial curves fitted to the turbulent mixing time from different engine speeds. Error bands correspond to the standard coefficients' error calculated with a 95% confidence interval. _____	184
Figure 106: Comparison between CFD derived τ_t and mixing time values derived using a single 4 th grade polynomial curve, fitted to τ_t at 2000rpm. Y-intercept coefficients' values changed for each speed. _____	184
Figure 107: Predicted and Experimental CA10 (graph A), CA90 (graph B) and CA10-90 (graph C) for different operating points. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red bands. _____	185
Figure 108: Predicted pressure and experimental pressure traces for key point 1 (graph A), key point 2 (graph B) and key point 3(graph C). _____	186
Figure 109: Predicted and Experimental CA10 (graph A), CA90 (graph B) and CA10-90 (graph C) for different operating points. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red bands. _____	187
Figure 110: Predicted pressure and experimental pressure traces for key point 4 (graph A), key point 5 (graph B) and key point 6(graph C). _____	188
Figure 111: Predicted and Experimental CA10 (graph A), CA90 (graph B) and CA10-90 (graph C) for different operating points. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red bands. _____	189
Figure 112: Predicted pressure and experimental pressure traces for key point 7 (graph A), key point 8 (graph B) and key point 9 (graph C). _____	190
Figure 113: Predicted and Experimental CA10 (graph A), CA90 (graph B) and CA10-90 (graph C) for different operating points. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red bands. _____	191
Figure 114: Predicted pressure and experimental pressure traces for key point 10 (graph A), key point 11 (graph B) and key point 12 (graph C). _____	192
Figure 115: CFD prediction of different engine speeds and loads on the turbulent mixing time, τ_t _____	193
Figure 116: Polynomial coefficients' value of the 4 th grade polynomial curves fitted to the turbulent mixing time from different engine speeds. Error bands correspond to the standard coefficients' error calculated with a 95% confidence interval. _____	193

Figure 117: Comparison between CFD derived τ_t and mixing time values derived using a single 4 th grade polynomial curve, fitted to τ_t at 2000rpm. Y-intercept coefficients' values changed for each speed.	194
Figure 118: Engine C predicted and experimental burn duration at different operating points.	194
Figure 119: Experimental spark (circle symbols) and SRM input ignition input (triangle symbol) timing comparison for different engine speed and load	195
Figure 120: Predicted and Experimental CA10 (graph A), CA90 (graph B) and CA10-90 (graph C) for different operating points. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red bands.	196
Figure 121: Predicted pressure and experimental pressure traces for key point 1 (graph A), key point 2 (graph B) and key point 3(graph C).	197
Figure 122: Predicted and Experimental CA10 (graph A), CA90 (graph B) and CA10-90 (graph C) for different operating points. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red bands.	198
Figure 123: Predicted pressure and experimental pressure traces for key point 4 (graph A), key point 5 (graph B) and key point 6(graph C).	199
Figure 124: Predicted and Experimental CA10 (graph A), CA90 (graph B) and CA10-90 (graph C) for different operating points. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red bands.	200
Figure 125: Predicted pressure and experimental pressure traces for key point 7 (graph A), key point 8 (graph B) and key point 9(graph C).	201
Figure 126: Predicted and Experimental CA10 (graph A), CA90 (graph B) and CA10-90 (graph C) for different operating points. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red bands.	202
Figure 127: Predicted pressure and experimental pressure traces for key point 10 (graph A), key point 11 (graph B) and key point 12 (graph C).	203
Figure 128: Predicted and Experimental CA10 (graph A), CA90 (graph B) and CA10-90 (graph C) for different operating points. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red bands.	204
Figure 129: Predicted pressure and experimental pressure traces for key point 13 (graph A), key point 14 (graph B) and key point 15 (graph C).	205
Figure 130: Effect of different Start of Injection (SOI) timing on the in-cylinder turbulent kinetic energy production during the closed part of the engine cycle (graph A) and the turbulence dissipation (graph b).	206
Figure 131: Engine D fitted with injector A predicted (red line) and measured (blue line) pressure and RoHR at 2000rpm_2barBMEP.	207
Figure 132: Engine D fitted with injector B predicted (red line) and measured (blue line) pressure and RoHR at 2000rpm_8barBMEP (top graph) and 2000rpm_2barBMEP (bottom graph).	208
Figure 133: Engine D fitted with injector A measured (blue) and predicted (red) pressure traces for different SOI	209

LIST OF TABLES

<i>Table 1: Overview of the available solutions to model the engine RoHR</i>	25
<i>Table 2: Main Engine A Parameters</i>	46
<i>Table 3: Engine A Operating Points</i>	47
<i>Table 4: Main Engine B Parameters</i>	48
<i>Table 5: Engine B Operating Points</i>	49
<i>Table 6: Main Engine C Parameters</i>	50
<i>Table 7: Engine C Operating Points</i>	51
<i>Table 8: Main Engine D parameters</i>	52
<i>Table 9: Engine D Operating Points</i>	52
<i>Table 10: Non-combusting CFD necessary boundary conditions extracted from the 1-D engine system code</i>	79
<i>Table 11: SRM necessary boundary conditions extracted from the 1-D engine system code</i>	80
<i>Table 12: Data needed to set the 1-D engine system code.</i>	83
<i>Table 13: CFD virtual engine configurations test matrix to study the effect of different bore to stroke ratios on the in-cylinder turbulence</i>	108
<i>Table 14: Summary of the in-cylinder turbulence analysis</i>	118
<i>Table 15: Virtual test matrix</i>	126
<i>Table 16: Engine C predicted burn angles</i>	132
<i>Table 17: Results of the combustion predictions comparison with experimental data</i>	144

LIST OF PUBLICATIONS

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NOMENCLATURE

ATDC(F)	After Top Dead Centre (firing)
BDC	Bottom Dead Centre
BMEP	Brake Mean Effective Pressure
BTDC(F)	Before Top Dead Centre (firing)
CA	Crank Angle
CA10	Crank Angle 10% Mass Fraction Burned
CA10-90	Burn Duration
CA50	Crank Angle 50% Mass Fraction Burned
CA90	Crank Angle 90% Mass Fraction Burned
CFD	Computational Fluid Dynamic
<i>CI</i>	Compression Ignition
EGR	Exhaust Gas Recirculation
EVC	Exhaust Valve Closing
EVO	Exhaust Valve Opening
G-ISFC	Gross Indicated Specific Fuel Consumption
<i>ICE</i>	Internal Combustion Engine
IVC	Intake Valve Closing
IVO	Intake Valve Opening
<i>k</i>	Turbulent Kinetic Energy
<i>l_i</i>	Integral length scale
MBT	Minimum advance for Best Torque
MFB	Mass Fraction Burn
PDF	Probability Density Function
<i>Q-D</i>	Quasi Dimensional
RANS	Reynold Averaged Navier Stokes
RoHR	Rate of Heat Release
<i>SI</i>	Spark Ignited
<i>SI</i>	Spark Ignition
SRM	Stochastic Reactor Model
TDC	Top Dead Centre
<i>TSB</i>	Realisable timescale bound limiter
<i>u'</i>	Turbulence Intensity
VVT	Variable Valve Timing
ε	Turbulent Dissipation Rate
μ_t	Turbulent Viscosity
ρ	Density
τ_{SRM}	Scalar Mixing Time
τ_t	Turbulent Mixing Time

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DECLARATION

I declare that the research contained in this thesis, unless otherwise formally indicated within the text, is the original work of the author. The thesis has not been previously submitted to this or any other university for a degree and does not incorporate any materials already submitted for a degree.

Signed: Christian Rota

Dated: 12/10/2020

1 INTRODUCTION

1.1 THE INTERNAL COMBUSTION ENGINE

The Internal Combustion Engine (ICE) is defined as a machine where the combustion of a fuel mixed with air releases thermal energy, which is then transformed into useful work. ICEs rely on thermodynamic, chemical processes and mechanics principles to deliver their work and are one of the most used and efficient source of power for transportation either commercial or private [1, 2]. The fundamental phenomenon of any ICE is the combustion process, occurring between the fuel and the air, that releases thermal energy. Thus, the main objective of ICEs is to repeatedly and efficiently exploit the energy released from the fuel oxidation [1-3]. Different ICE configurations were proposed over the years. The most used ICE variant is characterised by a slider-crank mechanism that transforms the cyclic motion of a piston into a rotating motion of a crankshaft. The major ICE components are summarised in Figure 1 [3]. Due to the movement of the piston, the volume of the combustion chamber varies from a minimum, when the piston is located at top dead centre (TDC), to a maximum, when the piston is located at bottom dead centre (BDC). The distance travelled by the piston between BDC and TDC is referred to as the engine stroke. There are two main commercially available ICE types: spark ignition (SI) engines, where a spark is required to ignite the fuel, and compression ignition (CI) engines, where a spontaneous ignition is caused by the change of the in-cylinder state during compression [1, 2]. The research reported in this thesis is focussed on the petrol fuelled SI engines.

Figure 1: Major components of an Internal Combustion Engine as reported in [3]

1.1.1 The Spark Ignited Combustion Engine

SI engines are simple, light weighted and cheap to produce [1, 2]. They are very resilient machines and their application can vary from cars and motorcycles, to chainsaws and gardening tools. The main disadvantage of SI engines, compared to other ICEs, is the lower thermal efficiency. However, SI engines are attractive thanks to their power-to-weight ratio, competitive manufacturing cost and very low combustion emissions. In a homogeneous port injected naturally aspirated SI engine, a charge of pre-mixed air and fuel, is drawn in the cylinder through the intake valve during the intake stroke. The term homogeneous refers to the intake charge mixture that, before the combustion process occurs, is characterised by the same proportion of air and fuel. The term port-injected indicates that the fuel is injected in the intake port rather than directly into the combustion chamber through a high-pressure injector. Lastly, the term naturally aspirated is used when the engine draws the fresh intake charge into the cylinder at atmospheric pressure. When a compressor is used to increase the intake charge density, the engine will be referred to as supercharged, if the compressor is driven by the engine crankshaft. Instead, the engine will be referred to as turbocharged, if the compressor is driven by the energy recuperated from the engine exhaust. Regardless the engine configuration, the compression of the intake charge is considered concluded, once the charge is introduced in the cylinder and the intake valve is closed. In SI engines, the final compression temperature remains below the auto-ignition threshold value, so that an ignition spark is required to start the combustion process [4]. Combustion characteristics and resulting engine performance are primarily determined by the flame velocity [4]. The stability of the combustion process is dependent on the ignition system ability to ignite the mixture at a predetermined time (spark timing) during transient operating condition. Unreliable ignition and uneven mixture formation across different cylinders may cause significant variation in the resulting combustion [2, 4]. Initial thermal reactions, occurring due to the external energy of the ignition spark, initiate the kernel development process which leads to the flame development [4]. The energy released during combustion is commonly known as Rate of Heat Release (RoHR). The RoHR of SI engines mainly depends on the combustion regime, the ignition timing and the combustion speed. Combustion speed is determined by diffusion processes in the flame front together with the in-cylinder turbulence [1, 4-6]. In SI engines, turbulence level and flame velocity can be influenced by different factors including the combustion chamber shape, inlet manifolds design and mixture formation. Low fuel consumption and high efficiency are generally promoted by

fast combustion. Moreover, the heat release location in respect to the piston position is also key for the engine performance. For instance, if most of the heat is released too early in the engine cycle, wall heat losses and mechanical losses may increase. On the other hand, if the heat is released too late in the engine cycle, the energy is inefficiently transformed into work [4]. Thus, the engine RoHR and its response to different engine characteristics needs to be known at the early stage of engine development, to allow to design new engines.

1.2 THE EARLY STAGE OF ENGINE DEVELOPMENT PROCESS

In this paragraph, an overview of the early concepts screening phase of a new engine development is proposed. The whole engine development process is not relevant for the scope of the thesis and thus will not be covered. Further details on this topic can be found in [3]. An overall simplified flowchart of the early stage of engine development is shown Figure 2. Firstly, the initial engine concept is defined using experience guidelines and future applications (see Paragraph 1.2.1). The concept design is later reviewed screening different engine geometries and attributes to define the “first build” design (see Paragraph 1.2.2).

Figure 2: The early concepts screening phase of engine development.

1.2.1 Initial engine concept definition

This phase can be split into the following overall steps: concept selection, thermodynamic and mechanical calculations [3].

Concept selection

In this phase of the engine development the engine future applications need to be fully understood before the engine development can begin. Performance targets, including rated power and peak torque are key characteristics to be considered during this phase. Moreover, expected engine life, fuel consumption, cost and weight are among other attributes that need to be accounted in this initial phase of the development [3].

Thermodynamic calculation

Depending on the data gathered in the previous phase the combustion system configuration is selected *e.g. diesel or gasoline engine?* Engine performance targets are used to carry initial analysis to define the required engine displacement. The engine displacement depends on the air flow required to achieve complete combustion and thus, depends on the fuel consumption targets. Therefore, an initial analysis on the fuel efficiency and the engine volumetric efficiency is required. Moreover, comparison between small displacement, coupled with intake air chargers, and larger displacement is necessary. Details on the engine displacement calculation can be found in [1-3]. In this phase of development, the number of cylinders and the bore to stroke ratio must also be determined. The overall future layout and the engine performance are equally important and need to be considered during this phase of development. For instance, any given displacement, may meet the fuel consumption target but not mechanical restrictions imposed by the application (e.g. motorcycles).

Mechanical calculation

This phase of the engine development focusses on the overall engine layout, including cylinders configuration and dimension of the engine compartment. Cost, complexity, engine speed range and serviceability requirements must be considered to finalise the initial engine concept design. The engine displacement and overall configuration *e.g. cylinders layout and bore to stroke ratio* need to be fixed to provide a basis for the next steps of the development

[3]. Moreover, these geometrical features of the future engine need to be definitive to begin the tooling procurement. Changes in the engine displacement and in the bore to stroke ratios are still possible in the next development phase (see Figure 2) but would be not feasible later in the development process.

1.2.2 Initial engine concept review

In this paragraph the second phase of the engine development in Figure 2 will be introduced. It is important to highlight that, the initial engine development phase, in which the first design concept is defined, takes around 4 weeks [3]. Once critical engine dimensions are determined, the review of the concept can start. Discussions with experts in the field and Hoag's work [3] suggest that this stage of development should take between 2 and 3 months.

Thermodynamic layout

This phase of the engine development aims to design the intake and exhaust system, optimising the engine combustion chamber and air handling before the hardware is available. Valve dimensions and timing are also defined at this stage. 1-D engine system tools *e.g. WAVE or GT-Power* are used to carry engine cycle simulations. CFD flow calculations, focussing on specific attributes *e.g. spray patterns* may also be used to aid the design of the new engine [3]. This thesis focusses on improving this part of the engine development process. Further details on the virtual engineering tools used during this phase of engine development can be found in Paragraph 1.3.

Mechanical analysis

In parallel with the previous phase structural tools are used to carry analysis aimed to highlight potential challenges in the future hardware manufacturing process. The main objective of structural analysis in the early concept development is to reduce the overall development time and cost [3]. This part of the engine development is not covered in this thesis.

1.2.3 The Current Virtual Engine Development Process

In this paragraph the engineering tools available and currently used during engine development will be introduced. The main goal of modelling the physics occurring within

ICEs while the hardware is not yet available is to predict their future performance aiding the early concept design process. Later in the development process, modelling tools can also be used to reduce testing efforts during the engine calibration. Therefore, virtual engineering tools have become an imperative for an efficient engine development process. There are different numerical approaches commercially available that allow to model the physics occurring in ICEs. However, depending on the chosen approach the accuracy of the results and the required computational time will vary [7]. Computational methods, that model all the physical 3-D scales occurring in ICEs without any simplification, are known as Direct Numerical Simulation (DNS). DNS can rarely be used during engine development due to the prohibitive computational time. For instance, with current numerical capabilities, a single, full-scale simulation of just a combusting spray with a DNS approach can take up to weeks on a supercomputer [1, 3, 7]. Thus, assumptions, simplifying the physics occurring in ICEs, are necessary to shorten the computational time to a value that can be considered practical during engine development. Simplified numerical approaches such as Large Eddy Simulations (LES) can be used to reduce computational runtimes. However, the computational time related to LES and RANS is still considered unfeasible at the concept stage of engine development (see Paragraph 2.1.2 for further details). Faster analysis can be achieved using the Reynolds-Averaged Navier-Stokes (RANS) framework. However, RANS introduces modelling simplifications that result in increased dependency of models' performance on initial tuning that, at the concept stage of development, cannot be carried out due to the limited experimental data available [1, 2, 7]. RANS CFD analysis can be used later in the development process, once the first concept design is determined, to optimise specific engine attributes (e.g. spray patterns) [8]. Therefore, 1-D engine system codes (e.g. WAVE or GT-Power) characterised by short runtimes (e.g. engine cycles/min [9]) are used to define the overall concept characteristics of new combustion systems during the initial concept design review phase of engine development. However, to provide useful results, 1-D codes require an initial engine rate of heat release (RoHR) input that can be either empirically derived or assumed from historical test data. For a given engine concept the overall performance is influenced by the RoHR that is function of different engine operating conditions and calibrations. Therefore, to predict engine performance using 1-D engine tools, the engine RoHR and the effect of different engine attributes on this characteristic needs to be known in advanced.

Figure 3: Gap in the RoHR predictive capabilities in the current virtual engine development process

Empirical based combustion models within 1-D engine system codes are an often used solution to provide the initial RoHR [1, 7, 9]. Over the years the effect of different engine attributes on the RoHR was investigated and correlations, based on historical experimental data, have been built. Figure 3 shows a high-level schematic of a virtual engine development based on 1-D engine system that uses empirical based combustion models to predict the engine RoHR. Processes similar to Figure 3 can provide useful insights on the effect of known attributes and overall engine concepts on the RoHR. However, these processes fail to predict the burning characteristic of novel engine design due to the initially assumed burning rate characteristic. The assumed RoHR can be reviewed accordingly to the screened concept, only if the effect of the new design on the burning characteristic is already known. Recent emissions regulations have pushed the exploration of new complex engine characteristics, novel overall design, and alternative fuels. Therefore, the RoHR of new products, for which little or no historical experimental data is available, needs to be known. New, fast, and more efficient virtual development processes, capable of predicting the initial RoHR, are required to aid the development of new engines concepts and ensure that customers and new market requirements are successfully met. The physics influencing the engine RoHR need to be captured and modelled to predict the burning characteristics of new combustion systems and decrease the development process dependency on historic test data. Combustion models, to be suitable in the early development stage, should discriminate between different hardware design, operating conditions without the need of tuning at each explore scenarios. Furthermore, due to the shortening of the time to bring product to market, running times comparable to 1-D engine system codes are required (*i.e. minutes per engine cycles*[9]).

1.3 AVAILABLE SOLUTIONS TO IMPROVE THE VIRTUAL ENGINE DEVELOPMENT

1.3.1 Virtual Engine Development Processes based on CFD Combustion Models

Figure 4: Generic ideal engine development process

Figure 4 shows an example of an ideal engine development process for SI engines. Benchmarking and experience-based guidelines on the left-hand side box are used to select initial overall combustion system geometries. The initial proposed engine design is explored targeting the main engine performance parameters. Later, valve events, ports geometries, in-cylinder flows, and intake charging systems are virtually assessed and optimised within the 1-D engine system modelling framework. The change in-cylinder air motion resulting from different engine design (e.g. intake ports) and operating conditions is then analysed through DNS Computational Fluid Dynamics (CFD) calculations and the initially assumed engine concept is updated accordingly. Moreover, for each of the explored engine configurations, DNS combustion calculations are carried out to predict the effect of each explored concept on the engine burn rate. Therefore, the approach shown in Figure 4 is effectively an example of a fully predictive development process. Different simulation frameworks exchange outputs to automatically converge to an optimal solution that meets the desired targets. However, simulation run times and associated costs make the approach in Figure 4 unsuitable [7]. A simplification of the DNS simulation framework, widely known as Reynolds-Averaged-Navier-Stokes (RANS) CFD, have been developed to reduce combustion simulation times but at cost of accuracy[7]. Simulation results within this

framework rely on multiple user-defined variables which need validation to extended operating conditions to be considered predictive. Different studies have tried to enhance RANS simulations predictive capabilities by investigating input-variables sensitivity [10, 11]. Run times and required resources are still unacceptable for virtual hardware screening and calibration at a powertrain system level. Thus, at the time this document was written, a virtual engine development process comparable to Figure 4 couldn't be considered feasible for the scope of this study.

1.3.2 Virtual Engine Development Processes based on Q-D Combustion Models

Q-D combustion sub-models, within the 1-D engine modelling framework, are often adopted to carry out combustion analyses while meeting restrictive development times. Simplified combustion models, adding a level of complexity compared to the empirical approaches, were demonstrated to accurately predict the engine RoHR [12-17]. Within these combustion models the physics influencing the engine RoHR is partially captured to avoid the need of predetermined combustion rates[12]. Most of the currently available Q-D SI combustion models divide the in-cylinder mass into a burned and unburned zone depending on the flame front propagation [12]. In the complete absence of turbulence, the flame front speed, and thus, the engine burn rate, would only be dictated by the fuel laminar flame speed [5, 6]. However, the speed at which the flame front propagates mainly depends on the in-cylinder turbulence. Therefore, combustion predictions with these models rely on an initial turbulence characteristic input that can be either experimentally extracted or derived by extra 0-D turbulence models. However, due to the complex three-dimensional nature of in-cylinder flow, most of the available 0-D turbulence models still fail in correctly predicting the effect of different geometrical effects on the in-cylinder turbulence processes (see Paragraph 2.5).

1.3.3 Virtual Engine Development Process based on Q-D and CFD models

Simplified Q-D combustion models offer run times that are suitable for the virtual screening of engine concepts. However, these combustion models require extra 0-D turbulence models to correctly predict the engine RoHR. An alternative solution, replacing 0-D turbulence models with turbulence data derived from CFD analysis and applied to a Stochastic Reactor combustion Model (SRM), was explored by Pasternak in [18, 19]. Stochastic Reactor Model is a Q-D combustion model that uses probability density functions (PDFs), applied to turbulent flows to capture the flow inhomogeneities [20-25]. PDFs are used in the SRM to account for the turbulence-chemistry interactions and allows the combustion processes to be

predicted [19, 23] (see Paragraph 2.4 for further details). The methodology proposed by Pasternak used an SRM combustion model to capture the combustion chemistry in a computationally efficient manner and CFD analysis to predict the effect of geometric variables on the in-cylinder turbulence. However, due to the high computational time and cost associated with multiple CFD runs, one for each explored scenario, this approach is effectively impractical for virtual engine development. Results in [19] suggested that, if the effect of any given engine geometry on the in-cylinder turbulence was characterised through CFD analysis, simple turbulence responses, comparable to turbulence models, could be used to predict the change in the turbulence characteristics to engine operating points.

1.4 THE WORK DONE

Figure 5 shows the methodology developed to predict the RoHR of SI engines at the concept stage development. The process is split in three different simulation levels as follows:

- Single non-combusting CFD analysis, one for any explored hardware, to characterise geometrical effects on the in-cylinder turbulence.
- A 1-D engine system model that accounts for the engine air handling.
- A Quasi-Dimensional (Q-D) model, specifically, an SRM model, that predicts the key engine performance parameters and the engine RoHR. The SRM combustion model was selected among others due to its capability to account for the in-cylinder inhomogeneities and the use of chemical kinetics library. However, any other combustion model with similar capabilities could be implemented in this methodology.

A new turbulence response was developed to predict the in-cylinder turbulence changes to different engine operating conditions and high-level engine calibrations (see definition in Paragraph 1.4.1). The in-cylinder turbulence characteristics' evolution (see definition in Paragraph 1.4.1) against the crank angle are assumed to be only function of the engine geometry. Different operating conditions and high-level calibrations affect the magnitude of these characteristics. The change in the turbulence magnitude to these engine attributes is consistent across different engine concepts and is assumed to be function of the intake charge flow speed.

The following steps describe how different numerical models and the new turbulence response exchange inputs between each other allowing to predict the engine RoHR for different engine concepts

1. Initial concept design is selected and input for numerical models are gathered.
2. The in-cylinder turbulence of a given concept is derived from a single non-combusting CFD analysis at a given operating condition.
3. Q-D combustion analysis is carried out using the CFD derived in-cylinder turbulence input. This provides boundary conditions (BCs) for the 1-D engine system analysis.
4. 1-D system analysis is carried out at a new given operating condition. The CFD derived in-cylinder turbulence is scaled accordingly to the change in the 1-D intake charge flow speed.
5. Combustion analysis is carried out using the scaled in-cylinder turbulence input and BCs for the 1-D model are reviewed until convergence is reached. Steps 4 and 5 are repeated for any explored operating condition and high-level calibration.
6. If different engine concepts are explored, a new non-combusting CFD analysis is necessary for each explored solution and steps from 3 to 5 are repeated.

Figure 5: Schematic of proposed virtual engine development process

1.4.1 Terminology

The terms engine operating conditions, engine high-level calibrations and turbulence characteristics will be used throughout this thesis. A definition of each of these terms is reported below.

Engine operating conditions

This term refers to any point in the engine operating map defined by engine speed, load. Experimental data used for this thesis is all characterised by $\lambda=1$.

Engine high-level calibration

Different engine attributes can be varied to achieve desired performance and consumption targets at any given engine operating condition. The optimisation of these attributes is called engine calibration. Engine calibration is carried out once the first prototype is available and operating conditions have been characterised [3]. This research focusses on the RoHR prediction at the concept stage of development when the hardware is not yet available. Therefore, complete engine calibration cannot be carried out. However, some attributes, defined here as “high-level calibration” are explored. These attributes are:

- Valves timing
- Spark timing
- EGR ratios
- Fuel injection timing.

In-cylinder turbulence characteristics

In this thesis the following terms are referred to as turbulence characteristics.

- Turbulence intensity
- In-cylinder tumble
- Turbulent kinetic energy
- Turbulent dissipation rate

Explanation of each of these terms can be found in Chapters 4 and 6. In Chapter 6 the mean in-cylinder flow velocity is also referred to as “turbulence characteristic”.

1.4.2 Aim & Objectives

The aim of this thesis is to develop and implement a practical process that predicts the engine RoHR at the concept (*early*) stage of development. During this phase, a methodology that is fast and requires minimum experimental data is required. The objectives of this thesis are listed below:

1. Identify potential simulation tools for the engine RoHR prediction and select those compatible with data and timeframe available during the concept stage of SI engine development.
2. Identify physics (*i.e. flame development and turbulence*) that needs to be modelled to predict the engine RoHR.
3. Define modelling methodology that uses available key inputs and assumptions (*i.e. turbulence modelling*) to predict the RoHR during the concept stage of SI engine development.
4. Verify validity of assumptions (*i.e. turbulence modelling*) through CFD analysis.
5. Implement process and validate predictive capabilities against experimental data for different engine operating conditions, calibrations, and concepts.

Engine burn angles is the industrial units used to analyse engine combustion rates within the automotive industry. Therefore, the two following metrics were used to assess the methodology predictive capabilities. If available, experimental engine RoHR traces can also be used.

- Predicted burn angles, compared to experimental (averaged) values, are expected to fall within the experimental standard deviation.
- Burn angle prediction confidence interval of ± 2 °CA from experimental (averaged) is expected. This interval was defined following industrial guidelines and corresponds to a standard criterion used to assess new modelling frameworks.

1.4.3 Research Questions

Simplified combustion models, that partially capture some of the physics influencing the engine RoHR are commercially available. However, the accuracy of their results depends on an initial turbulence input. Results in [19] showed that, simple turbulence responses can be developed to manipulate an initial CFD derived turbulence characteristic. Such approach would benefit of the CFD capability to account for the geometrical effects on the in-cylinder turbulence. Figure 5 shows that a single non-combusting CFD analysis is used to characterise the in-cylinder turbulence characteristics of a given engine geometry. This assumes that the turbulent characteristics curves against the crank angle are only function of the engine design. The effect of different engine variants on the in-cylinder turbulence was analysed to answer the following question:

“Can the in-cylinder turbulence characteristics be considered bound only to the given engine overall design?”

The effect of different engine operating conditions and high-level calibrations on the in-cylinder turbulence was analysed following research question below:

What are the turbulence characteristics necessary to be numerically resolved to correctly predict the engine RoHR at different engine operating conditions? ”.

1.4.4 Thesis Contributions

In this thesis a new methodology based on three different modelling frameworks was developed to predict the RoHR of different gasoline engine. The process uses a new turbulence response that allows to provide realistic RoHR predictions for different engine variants throughout the engine map. This response scales the key turbulence input of the SRM combustion model to the intake charge velocity. To the authors’ best knowledge, this scaling factor is new and has never been proposed before. The main findings of this research can be summarised as follows.

- 1. The overall shape of the in-cylinder turbulence characteristics, against the crank angle, is bound only to the given engine geometry. Changes in the turbulence characteristics’ shape, against the crank angle, can be neglected when predicting the engine RoHR using an SRM combustion model in response to changes to engine calibration.*

The non-combusting CFD in-cylinder turbulence analysis confirmed that, the main turbulence characteristics’ shape against the crank angle, for a given engine design, *e.g. the Turbulent Kinetic Energy (k)*, can be considered constant for different engine operating points. Engine geometries are the main factors that influence the in-cylinder air motion and, consequentially, the shape of k , or any other considered characteristic, against the crank angle. Thus, the turbulence characteristic needed for the SRM combustion model can be characterised by limited non-combustion CFD calculations for any given engine hardware. Details of the CFD analysis can be found in Chapter 6.

- 2. Different engine high-level calibrations affect the overall turbulence characteristics’ magnitude but not the shape against the crank angle. The change in the turbulence characteristics’ magnitude in response to changes to engine operating conditions and calibrations can be scaled on the intake charge velocity.*

A new turbulence response, based on the changes in the intake port flow velocity to engine operating point, predicted by the 1-D engine system code (WAVE), was developed. The response was used to scale CFD derived in-cylinder turbulence characteristics of any given engine geometry and provide the SRM combustion model with the necessary input to predict the engine RoHR at different engine operating conditions and calibrations. Details of the developed turbulence factor can be found in Chapter 5.

3. *The methodology developed can be extended to any Q-D combustion model with characteristics similar to the code chosen for this research.*

The developed methodology uses CFD calculations to capture the effect of any given engine geometry on the in-cylinder turbulence characteristics. Later, CFD derived turbulence characteristics are scaled on the intake charge speed velocity to provide the Q-D combustion model with the necessary input and predict the effect of any engine operating point at a given engine design. Currently, all commercially available Q-D combustion models require a turbulence input so that the methodology developed in this thesis can also be used with any chosen Q-D model. It is expected that, the initial turbulence multiplier, defined in the initial calibration phase (see Chapter 5), will change with the chosen Q-D combustion model. However, since the physics governing the turbulence is captured, once the Q-D combustion model is correctly calibrated on a baseline engine, the methodology developed in this research can be applied.

1.4.5 Thesis focus and limitations

This thesis focusses on the engine RoHR prediction at the concept stage of engine development (see Paragraph 1.2). Engine characteristics typically investigated during this stage are:

- Ports and manifolds designs
- Charge induction strategy (NA vs Turbo)
- Fuel injection strategy
- Intake/Exhaust valve overall strategy
- Charge dilution

The effect of the above characteristics on engine RoHR and knock is predicted with the developed methodology. However, the effect of engine characteristics explored later in the developments process (e.g. during engine calibration) may not be captured with this

methodology. For instance, engine turbocharging and valve strategies can result in the “blow through” phenomenon [2, 26] that affects the portion of the intake charge that is trapped in the cylinder. This is likely to influence the turbulence characteristics’ curve shape against the crank angle. Further work is required to assess the methodology predictive capabilities outside the scope of applications for which it was designed (*i.e. concept stage of development*). Processes such as [27, 28] can be used for this purpose.

The transient effect of real-life engine operating conditions is not accounted in this methodology. This limitation could be overcome by discretising transient conditions and providing the SRM with AFR and residuals swings that are representative of transient conditions. At the time this document was written this solution had not been assessed.

The computational time associated with CFD analysis can also be considered a limiting factor when runtimes are compared with current empirical base engine development process. CFD representative run times for different applications, indicating the burden of the CFD analysis are available in Paragraph 2.1.2.

1.5 FUTURE WORK

The methodology developed for this thesis is based on a new turbulence response factor that scales CFD derived turbulence characteristics, of any given engine concept, to the intake charge flow velocity, predicted by a 1-D engine system code. Thus, changes in the flow speed, which is the physics governing the turbulence, are used to reproduce the in-cylinder turbulence of any engine operating point. Validation over a wide range of conventional and unconventional engine concepts and high-level engine calibrations is required to consider the developed methodology a practical solution for new engines development. However, non-traditional combustion concepts, attributes and combustion strategies (*i.e. water injection and lean combustion*) were not investigated due to limited experimental data available. The vision is that the solution developed in this thesis will aid the development of the next generation of gasoline ICEs which, unless of a major technological breakthrough, are set to be part of our lives at least until 2050 [29, 30]. Therefore, an interesting expansion of this research would be the exploration of alternative fuels. Detailed chemical kinetics library, available within the chosen SRM, can be used to explore the engine RoHR from different combustion regimes. Depending on the SRM capability to cope with new fuel

mixtures, the developed turbulence response is expected to perform well since the governing turbulence physics are captured.

1.6 THESIS STRUCTURE

Figure 6 shows the overall outline of this thesis highlighting the path followed during the research.

Figure 6: Overall thesis outline

The initial chapter of this thesis introduces the gap in the knowledge covered by this research (*i.e. the engine RoHR prediction in the concept stage of development*). Thesis objectives, scope of applications and research questions are also presented in this chapter. A critical overview of different modelling approaches for the engine RoHR prediction is presented in the following chapter (Chapter 2). Physical processes governing the SI RoHR and fundamental assumptions developed for this research are also presented here. Chapter 3 presents the experimental data used in this research. 1-D and CFD models' characteristics are briefly introduced in Chapter 4. Detailed review of the SRM models is also available in this chapter. The methodology chapter (Chapter 5) presented the modelling workflow and the turbulence scaling factor developed in this research. Chapter 6 presents the non-combusting CFD analysis carried out to verify the hypothesis of this work. The methodology

validated on different engine maps. Combustion prediction comparison with experimental data is shown in Chapter 6

2 LITERATURE REVIEW

2.1 THE PROBLEM

During the early stage of engine development different engine attributes are virtually screened to investigate their effect on the future engine performance. Due to the limited available time, pre-determined RoHR and empirical based combustion models, coupled with 1-D engine system codes (WAVE or GT-Power) are used to predict the engine burning rate response to different engine configurations. However, the following problems are embedded in this approach:

1. 1-D engine simulations are carried out to investigate the effect of different design configuration on the RoHR. However, 1-D codes, to provide useful analysis require an initial RoHR that is derived from previously designed engines. Therefore, the engine RoHR is not predicted and 1-D analysis results depend on the initial assumption.
2. Empirical based combustion models have been developed to accommodate the change in the physics influencing the engine burning rate and to predict the change in the RoHR to known attributes and configurations. However, this approach fails to predict realistic responses when engine design attributes, outside the validated range, are screened. Therefore, an alternative modelling framework which can predict the engine RoHR for different engine configurations and attributes is needed to improve the virtual engine development process.

2.1.1 The Current Rate of Heat Release modelling approach

In this paragraph a review of the approach currently used to model the engine RoHR during the early stage of engine development will be reviewed. Initial questions regarding the accuracy of this methodology will also be raised. To this day, the industrial standard for virtual engine development is carried out within 1-D engine system codes (e.g. WAVE or GT-Power) and empirical based 0-D combustion models (see Paragraph 1.2.3). Figure 7 shows a schematic flowchart of a virtual engine development process based on 0-D combustion models. An initial engine burning characteristic needs to be assumed. Later, the effect of different operating points on the engine burning rate shape is accommodated using

physical data from a previous engine and a suitable empirical correlation. Thus, overall engine performance predictions depend on the initial engine burning rate assumption. Within 0-D combustion models the physics affecting the engine burning characteristic are not modelled [1]. The Wiebe equation reported below (see Equation 1) is the most known example of an empirical SI engine combustion model [1, 2]. Wiebe parameters including the Start of Combustion (SoC) and the burn duration (CA10-90), need to be known in advance for different hardware (*i.e. port, combustion chamber and injector geometry*) and engine characteristics. Therefore, Wiebe constants must be tuned accordingly to achieve accurate combustion predictions. This simplified approach provides good RoHR predictions in situation in which new combustion systems have similar characteristics to existing ones and thus pre-defined combustion rates can be similarly derived in relation to different engine characteristics.

$$x(\theta) = 1 - \exp \left\{ -a \left[\frac{\theta - \theta_0}{\Delta \theta_b} \right]^{m+1} \right\}$$

Equation 1: Wiebe function

Where $x(\theta)$ is the mass fraction burn at crank angle θ , θ_0 is the crank angle at the start of combustion, $\Delta \theta_b$ is the combustion duration and a and m are user input constants. The accuracy of the results of an engine development process based on an empirical based combustion model, depends on the initial assumption regarding the engine burning rate and on the validity of the chosen empirical correlation. In the past years this approach provided good results since most of the engine were derived from experimental data on existing concepts for which pre-existing 0-D combustion models were calibrated [1]. Recent studies, have used alternative 0-D combustion models [31], including neural networks [32], to develop real-time system engine system control. These approaches can provide RoHR prediction within an acceptable error thanks to the initial model calibration on benchmarked test data. However, this kind of experimental data is not available during the early concept screening phase of engine development. Thus, questions related to the accuracy of virtual engine development processes based on 0-D combustion models can be raised and summarised as follows:

1. *How can the initial engine burning rate of new engine concepts be derived with enough accuracy?*
2. *How can the engine burning rate response to new engine calibrations be predicted outside the 0-D empirical combustion model's validation range?*

Figure 7 shows an overall flowchart of an engine development process based on an empirical combustion model, highlighting the problems discussed above.

Figure 7: Schematic of the virtual empirical based engine development process.

2.1.2 Alternative Solutions to Model the Engine Rate of Heat Release

In this paragraph different commercially available modelling approaches for the engine RoHR will be presented. Firstly, CFD combustion models, capable of predicting the engine RoHR with limited assumptions but at cost of computational cost will be discussed. Later the Quasi-Dimensional modelling framework for the engine RoHR prediction will be introduced.

Combustion models, modelling the physics influencing the engine burning rate, are needed to improve the virtual engine development process. Thus, considering the limited time available during the engine development the following question raises:

“Can the RoHR of a gasoline engine be predicted during the early concepts screening phase?”

As explained in Paragraph 1.3, the state of the art for combustion modelling, excluding empirical based models, can be divided into two overall modelling frameworks:

- Three – dimensional Computational Fluid Dynamics (CFD) models

- Zero – Dimensional / Quasi – Dimensional physical (0-D /Q-D) models

CFD models framework

CFD models describe the three-dimensional fluid dynamics of the considered engine. The intake manifolds, the combustion chamber, fuel injection system and exhaust manifolds can be included in a single CFD model [7, 33]. The geometry effects on the in-cylinder charge motion and on combustion processes are considered. Thus, can this framework be used during the concept stage of engine development?

The physics governing combustion processes are fully resolved within the Direct Numerical Simulation (DNS). Therefore, the engine RoHR can be predicted with DNS CFD. However, DNS CFD analysis, applied to industrial-relevant applications, remain unfeasible due to the required computational resources and time [7, 12]. For instance, a single full-scale simulation of a combusting spray with a DNS approach can take up to weeks. A recent DNS analysis simulated a hydrogen-air combustion case and required 40 million CPU hours [34]. Even with the most powerful machine it is easy to see why DNS will not be an option for regular engineering problems. Physical models that simplify combustion processes occurring in the SI engines have been developed to reduce the required computational resources. This led to the formulation of Large Eddy Simulations (LES) [35] and Reynolds Averaged Navier-Stokes (RANS) equations [6]. LES CFD computational requirements [36] are still unacceptable for large-volume industrial applications such as new engine development. Run times for diesel spray simulations reported in [37] suggest that diesel reactive cases can take up to 150hrs and non-reactive cases up to 20hrs. Shorter run times, at cost of result's accuracy, can be achieved using the simplified RANS CFD approach. [37] suggests that reactive diesel spray cases can take around 18hr whereas non-reactive spray cases can take up to 2hrs. Different studies suggested that, once the first engine concept design is defined, RANS CFD analysis could be used during engine development to predict the engine RoHR at different operating points. The combustion processes occurring in a Port Fuelled Injection (PFI) SI engine operating in a pre-mixed charge combustion mode and later upgraded to Direct Injection (DI) were predicted in [38, 39]. Results were achieved thanks to an extensive model calibration that used motored and fuelling data, which are not available during the concept phase of development. A methodology to further reduce RANS computational requirements, achieving computational time as short as 5hrs per engine cycle, was showed in [40]. However, extensive experimental data was necessary to calibrate the model. In [41]

an automated tuning procedure for diesel engines simulations was developed. The methodology showed good combustion predictions at limited operating points for a given engine overall structure. However, even if the limited validity of the developed auto-tuning approach was ignored, the required computational time, necessary to model one single engine cycle, was around 12 hours on an industrial standard cluster. CFD RoHR predictions at multiple operating points for each of the engine design screened during the concept stage of development remain unpractical. This is due to the limited time available to define the first engine concept [3], limited experimental data available to tune CFD models and the lack of consensus on how modelling coefficients should be set [10, 41]. CFD analysis can be used later in the development process, once the concept design is defined [8, 38, 39, 41].

Quasi-Dimensional models framework

Discussion with industrial organisations and Hoag's work [3] suggest that the initial engine design needs to be available between 2-3 weeks from the project kick off to allow different parts to be ordered or manufactured. Thus, computational times, comparable with 1-D engine system codes *i.e. range of minutes per engine cycle*, is a key requirement that needs to be met to solve the problem introduced in Paragraph 2.1. Therefore, to achieve the goal set for this thesis (see Paragraph 1.2.3), a combustion model, that can predict the engine RoHR within minutes and using limited experimental data, at different operating points and engine configurations, is required.

Zero-Dimensional (0-D) / Quasi-Dimensional (Q-D) combustion models are computationally lighter than CFD models and offer a practical and already available solution. Different 0-D / Q-D combustion models, accounting for the closed part of the cycle and offering reasonable computational times (*i.e. range of minutes per engine cycle*) are available in the literature. [12]. The ambiguity in the "0-D/Q-D" name is due to an addition of simplified engine geometrical features that some of these models making them Quasi-Dimensional (Q-D). In the literature there are different examples of Q-D combustion models characterised by different assumptions and overall numerical formulations. All Q-D models, to predict the engine burning rate require to model the physics governing the following characteristics:

- *In-cylinder turbulence (including the effect of different geometries)*
- *Laminar and turbulent flame speeds*

Table 1 shows that, within the Q-D combustion models, there are two overall main modelling approaches. The main differences between the two approaches are the governing equations. The first group in Table 1, labelled as “thermodynamic models”, uses the energy and mass conservation only dependant on time for an open thermodynamic system to predict the engine burning rate. The second modelling framework is known as Stochastic Reactor Model (SRM) which uses the Probability Density Function (PDF) approach applied to turbulent flows to give a statistical description of the state of the fluid at each point in the flow field [25]. A review of the available thermodynamic based Q-D models will be presented in Paragraph 2.3. SRM approach will be introduced in Paragraph 2.4 and further described in Paragraph 4.3.

Table 1: Overview of the available solutions to model the engine RoHR

	CFD	Thermodynamic Models	Stochastic Reactor Models
Governing Equations	3-D mass and energy conservation for an open thermodynamic system	1-D mass and energy conservation for an open thermodynamic system	Probability Density Function (PDF) to solve Navier-Stokes equation
Turbulence Characteristic	Turbulence sub-models (RANS) otherwise calculated	Experimentally derived / turbulence sub-model	Experimentally derived / turbulence sub-model
Geometrical features	CAD geometry	Simplified CAD geometry	Simplified CAD geometry
Laminar Flame	Modelled / chemical kinetics	Modelled / reduced chemical kinetics	Tabulated chemical kinetics
Turbulent Flame	Modelled (RANS &LES) Calculated (DNS)	Modelled	Modelled
Outcome	Burning Rate, Knock, Emissions	Burning Rate, Knock, Emissions	Burning Rate, Knock, Emissions
Computational times	Hours per cycle	Minutes per engine cycle	Minutes per engine cycle

2.2 INTRODUCTION TO THE FLAME FRONT PROPAGATION IN SI ENGINES

The physics of the flame formation and propagation need to be considered, to fully understand how different Q-D combustion models work. Thus, an overview of the flame front propagation occurring in SI engines will be presented.

Combustion processes in ICEs can be split into two main categories depending on the chemical mechanisms occurring during the combustion: auto-ignition and flame front propagation. Diesel engines are characterised by auto-ignition chemical mechanisms that

initiate the combustion processes at the desired time. Liquid fuel is injected into the cylinder and entrains the hot compressed air. Thus, the occurring combustion processes in diesel engines can be described as non-premixed combustion [2]. In this thesis, combustion processes occurring in SI engines are considered. Among different available SI engine variants, the fuel can be either be injected via port or it can be directly injected in the cylinder [2]. In PFI engines the fuel enters in the chamber already mixed with the fresh intake air charge. Depending on the injection timing DI engines can result in complete or partially mixed charge. In this thesis, PFI and DI SI engines, only resulting in a fully mixture of the air and fuel before the combustion will be discussed. The combustion processes occurring in these engines are described as turbulent premixed combustion [2].

2.2.1 Laminar Flame Speed

Premixed flow, by definition, must complete the mixing between air and fuel before the combustion occurs. In SI engines the combustion process is initiated by an external energy, provided by the spark plug, that increases the local temperature above the ignition threshold [42]. Beyond this temperature value, combustion chemical reactions start and lead to a flame that propagates throughout the fresh mixture charge. Peters in [43] investigated the structure of a stationary, laminar, stoichiometric methane-air flame, comparable to a gasoline-air mixture. Peters showed that the flame propagates into the fresh mixture with a laminar burning velocity S_L . This velocity is a thermo-chemical property of any specific oxidant-oxidiser mixture. Moreover, Peters suggested that laminar flame could be split into three different regions as follows: [43, 44] (see Figure 8)

- The chemically inert preheat zone.
- The inner layer reaction zone in which fuel is formed and intermediate species are formed (e.g. H_2 and CO_2).
- The oxidation zone.

Figure 8: Illustration of the inner structure of a flame front in a stationary, laminar and stoichiometric methane-air mixture accordingly to [43]

Referring to Figure 8 the preheat zone, where chemical reactions do not occur, is characterised by the unburnt temperature, T_u . The temperature in this zone increases due to diffusion and convection until it reaches the chemical reactions activation threshold T^0 . When T^0 value is reached the methane-air mixture is effectively in the inner zone, where main chemical reactions occur. Intermediated species, H_2 and CO_2 are formed and later oxidised in the oxidation zone. The rate at which these processes occur is dictated by the laminar flame speed, S_L . At this point the concepts of flame thickness and the thickness of the inner layer can be defined as follow:

- Laminar flame thickness, $l_f = \frac{\left(\left(\frac{\lambda}{c_p}\right)_{t=T^0}\right)}{\rho S_L}$ where c_p is the specific heat capacity value at constant pressure and λ is the thermal conductivity.
- Inner layer thickness, l_δ defined by the chemical time scale of the fuel consumption rate, δ . $\delta = \frac{l_\delta}{l_f}$ is a scale specific of the fuel and decreases with temperature and pressure [44].

In a 3-D space, the flame is subjected to strain which results in a curvature. Thus, the laminar burning velocity changes when a complex 3-D field is considered. Since all combustion

analysis carried out in this research was within a Q-D combustion model, the laminar flame curvature due to 3-D strain stresses will be ignored. In this thesis, the laminar flame propagation will be characterised by a laminar speed S_l normal to the 1-D flame front, as initially proposed by Peters [43]. A thorough review of the laminar flame front propagation, including the flame curvature occurring in a 3-D field is available in [44].

2.2.2 Turbulent Flame Speed

SI engines are characterised by turbulent in-cylinder flows which effectively accelerate the flame velocity. In this Paragraph, an overview of the turbulent flame speed will be presented with the only intent to give the reader a grasp of the processes occurring during the turbulent premixed combustion. A complete review is available in [44].

The turbulent flame speed, in parallel to the laminar flame speed, can be defined as a thin reaction sheet. Locally, each point of the reaction sheet propagates into the fresh mixture with a velocity corresponding to the laminar flame velocity. In SI engines, the reaction sheet is not uniform but it is rather wrinkled due to the entraining turbulent fresh charge [42]. However, the wrinkling of the flame only occurs if certain conditions are met. The concepts of the Kolmogorov scale and molecular viscosity need to be firstly introduced as follows:

- *Kolmogorov scale*: it is the smallest scale considered in a turbulent flow below which the molecular viscosity is not considered. It is defined as the ratio between the kinematic viscosity, ν , and the energy dissipation rate, ϵ .
 - Kinematic viscosity, ν : defined as the ratio between the dynamic viscosity (ratio of shearing stress and shear) of a fluid and its density.
- *Molecular viscosity*: viscosity is a measure a fluid's resistance to deformation. Molecular viscosity is solely caused by internal friction in the fluid due to the random motions of individual molecules not moving together in coherent groups.

The wrinkling of the flame front happens when the Kolmogorov scale, is larger than the laminar flame thickness, l_f [42, 44]. Moreover, until the flame radius is smaller than the integral length scale, the biggest eddy size containing energy in the turbulent flow, the impact of the turbulence on the sheet is negligible. One could argue that, during engine combustion, this portion of the flame development which is not affected by the in-cylinder turbulence is so short, that it can often be ignored. At high engine speed, the laminar flame speed is higher compared to lower engine speed, due to the increased in-cylinder temperature and pressure.

Thus, the time for which the flame radius is not affected by the turbulence eddies would be shorter. However, once the flame radius is larger than the integral turbulent length scale, the flame front start wrinkling with a magnitude that is proportional to this integral length scale and the smallest of the scales [42]. Both these lengths scales reduce their value with increasing engine speed. The speed at which the mean flame front propagates into the fresh mixture charge is known as turbulent flame speed S_T . This characteristic increases with the engine speed since the effect of the turbulent eddies becomes more significant. Peters proposed a diagram showing the relation between the turbulent eddies and the flame eddies to describe all the different turbulent premix combustion regimes that might occur [45]. However, in-cylinder turbulence data highlighted that the wrinkled flame regime, is the case for most SI engines [42, 44, 46]. Moreover, turbulent flame speed sub-models available within the Q-D combustion models all consider a wrinkled flame front. For this reason, all other turbulent premixed combustion regimes, as proposed by Peters, are not described here.

2.3 THE THERMODYNAMIC QUASI-DIMENSIONAL (Q-D) COMBUSTION MODELS

In Paragraph 2.1.1 it was shown that different combustion model approaches, ranging from complex multidimensional models (CFD) to simple quasi-dimensional are available to simulate the combustion processes occurring in SI engines. The choice of the approach depends on the application of each study [1]. Simple approaches are preferable to perform combustion analysis over a wide range of conditions, thanks to the short computational times. Complex modelling frameworks, such as CFD, are instead used for detailed studies over limited conditions [12]. Physical quantities such as in-cylinder state and engine geometry are not expressed in empirical based combustion models, making the engine burn rate prediction challenging for new engine concepts. Therefore, the physics influencing the engine burn rate needs to be modelled to predict the effect of a wide range of engine concepts on the burn rate. More complex Quasi-Dimensional (Q-D) combustion models have briefly presented as a practical solution to improve current virtual engine development process. An initial distinction between Q-D models using thermodynamic equations and Q-D models using the PDF approach was offered in Paragraph 2.1.2. In this Paragraph a review of the general physical sub-models used in all thermodynamic Q-D combustion models is presented. A review of the SRM Q-D models will be offered in Paragraph 2.4.

In the thermodynamic Q-D combustion models the governing equations are based on the energy and mass conservation dependent only on the time. The term Quasi Dimensional (Q-D) derives from the inclusion of simple features to include the geometry's effect on combustion [12]. SI Q-D combustion models are often referred as multizonal due to the presence of a layer, representing the flame front of SI engines. This layer separates the burnt and the unburnt zone inside the cylinder and it is considered as a thermodynamic boundary between two open systems. Different studies have used this approach to investigate the effect of different engine design on the RoHR and to predict engine emissions [47-49]. More complex multi-zones models have also been developed to improve their capability to capture the effect of different geometry on the engine RoHR [50-53]. However, the extra modelling effort related to the addition of extra zones is not justified since the result's accuracy remains similar to simpler models. Moreover, numerical uncertainties, stemming from the heat release calculations in the zones close to the engine walls and from the flame velocity calculation for different burned zones have rather increased the dependency of these approaches on the user-input variables. A general overview of how thermodynamic Q-D models based are used for different engine applications is available in [12].

The objective of the review was to understand how the Q-D modelling framework could be used during the early stage of engine development. Regardless the number of zones implemented in a Q-D combustion model, or the difference in the numerical formulations, the fundamental physics governing the mass and energy conservation need to be modelled to calculate the in-cylinder state evolution during the engine cycle. Moreover, sub-models, accounting for different physical processes occurring in the in-cylinder are necessary to predict the engine RoHR. The followings sub-models are used in all commercially available Q-D combustion models:

- *In-cylinder volume calculation:* the in-cylinder volume as function of crank angle is required to calculate the state of the gas mixture during the power cycle (closed part of the cycle). Main engine geometry: bore, stroke, connecting rod length and compression ratio are required [1].
- *Chemical reactions calculation:* gas mixture composition and chemical properties as a function of temperature are required to calculate the overall chemical reactions necessary to predict the engine emissions. Tabulated data, that allows to define simplified chemical kinetics are widely available [54-56]. To improve the accuracy

of the results, detailed chemical kinetics can also be implemented but at cost of the overall computational requirements.

- *Heat transfer calculation:* this sub-model is used to calculate the amount of heat that is transferred through the walls. The most commonly known models, representing the industrial standard, are Woschni's [57] and Annand's [58].
- *Mass burning rate calculation:* this model is necessary to dictate the velocity at which the mass is transferred between the burnt and the unburnt zones. Within the SI engine the mass burning rate is mainly dependent on the flame propagation and, thus, the turbulent flame velocity, S_T . Often, these sub-models are referred as turbulent flame speed sub-models. An overall review of these sub-models is available in Paragraph 2.3.1.
- *In-cylinder turbulence calculation:* mass burning rate and heat transfer calculations all required in-cylinder turbulence data. If an optical engine is available, this data could be experimentally derived [59, 60]. If new engine concepts are explored, the necessary turbulence characteristic could be defined from extra Q-D turbulence sub-models or non-combusting CFD calculations. An overview of the most known Q-D turbulence model is available in Paragraph 2.5. A broader review is also available in [61].
- *Initial Spark Kernel:* Within the Q-D modelling framework the spark kernel formation and growth are often not modelled. Instead, the start of combustion is initialised at a given chosen point after the experimental spark timing. This is due to the very complex nature of ignition processes. These processes depend, among other factors, on local mixture characteristics around the spark plug and the in-cylinder flow structures [12, 42]. Thus, Q-D kernel models may provide realistic results for some engine operating conditions but not for all. Moreover, the highly turbulent nature of SI engine intake flows makes the initial kernel formation relatively short and, thus, insignificant during the product development phase, when just overall engine performance and burn rate are targeted. Simplified spark kernel models, that related the kernel to a certain mass are available and listed below.
 - Wu [62] assumed the initial ignition kernel to be equal to two percent of the total in-cylinder mass.
 - Verhelst [63] instead, assumed the initial flame radius equal to 1mm.

- Another assumption, and perhaps the most realistic, is available in [64]. In this work the initial kernel radius is defined on the gap distance between the spark plug electrode.

2.3.1 Mass Burning Rate Sub-Models

In the previous Paragraph a list, of the sub-model available in all thermodynamic-based Q-D combustion models, was offered. To predict the RoHR of SI engines the turbulent premixed flame propagation needs to be calculated. Thus, to fully understand the Q-D combustion models' framework, an overview of the mass burning rate sub-models is required.

The fundamental physical factors that affect the mass burning rate in a SI engine combustion processes are:

- Mean flame front area within the combustion chamber
- Bulk in-cylinder turbulent motion and its effect on the flame propagation
- Unburnt mixture gas state that determine the value of the laminar flame speed

If physical-based relations are used to describe the above phenomena then the mass burning rate can be predicted [42]. Therefore, the flame area and the rate at which it propagates through the combustion chamber are fundamental parameters to correctly predict the engine RoHR. As previously explained in Paragraph 2.2 petrol fuelled engines are characterised by turbulent intake flows that, entrains the flame front and wrinkles the laminar flame [6] [46]. Figure 9 provides a schematic of the wrinkled flame front accordingly to Peters [46]. The premixed turbulent flame front can be described as a thin wrinkled reaction layer characterised by a mean flame thickness. Referring to Figure 9 the mean flame front region is obtained by averaging the turbulent scalar fluctuation in the variable G , with G_0 representing the actual flame front [42, 46]. Entraining turbulence eddies are causing the wrinkling of the flame front.

Figure 9: Wrinkled turbulent flame structure as proposed in [46]

Q-D combustion models, to correctly predict the engine RoHR, require modelling the flame initiation and propagation. Therefore, values for the laminar flame and turbulent speeds are necessary. The simplest mass burning rate for a generic Q-D combustion models can be summarised as shown Equation 2 [42]:

$$\frac{dm_b}{dt} = A_f \rho_u S$$

Equation 2: General formulation for the mass burning rate within SI engines as provided by [42].

Where m_b is the mass of charge burnt, A_f is the mean flame area, ρ_u is the density of the unburnt mixture and S is the flame velocity (laminar or turbulent). Within the Q-D engine modelling framework the SI engine flame surface is often assumed to spherically grow with the centre located at the spark plug location. The initial flame speed initially corresponds to the laminar burning velocity (S_L). However, as the kernel grows, the flame becomes turbulent [12, 42]. The initialisation of the flame kernel development is problematic due to the multiple physical factors affecting the phenomenon. Thus, as explained in the previous Paragraph, within the Q-D modelling framework often the spark kernel formation and growth are not modelled. Instead, the start of combustion is initialised at some point after the experimental spark timing. Within thermodynamic based Q-D models the flame front corresponds to a boundary layer for an open thermodynamic system that exchanges heat and mass with the surroundings (unburnt mixture). Initially, the flame speed is equal to the laminar flame speed of the mixture. However, the effect of entraining turbulent eddies gradually becomes more

significant increasing the burning speed. Thus, models for the turbulent flame speed are necessary to correctly predict the SI engine burning rates. Two different turbulent flame models, characterised by a fundamental difference in the flame definition, are implemented in the commercially available Q-D models:

- *Turbulent Entrainment model*
- *Flame Sheet model*

More turbulent flame speed models are available in the literature. However, these models are fundamentally derived from the two approaches listed above. Consequentially, due to the broad similarities across different models only the two approaches listed above will be covered in this thesis.

Turbulent Entrainment Model

This modelling framework was initially developed by Blizard [65] which postulated an entrainment process of the fresh charge mixture into the flame front. The general mass burn rate as described in Equation 2 is modified as shown in Equation 3 and Equation 4.

$$\frac{dm_e}{dt} = \rho_u A_f S_e$$

Equation 3: Entrainment mass burning rate as proposed by Blizard [65].

Where m_e is the entrained charge mass, ρ_u is the density of the unburnt mixture, A_f is the mean flame area (assumed spherical) and S_e is the velocity at which the fresh charge is entraining the flame.

$$\frac{dm_b}{dt} = \left(\frac{d(m_e - m_b)}{d\tau_b} \right) + \rho_u A_f S_L$$

Equation 4: Entrainment model mass burning rate as proposed by Blizard [65].

Where τ_b is defined as the burning time constant, m_b is the mass of charge burnt, A_f is the mean flame area (assumed spherical) and S_L is the laminar flame speed. The burning time constant is defined in Equation 5 where c is a tuning parameter, l_e is the entrained eddies length scale.

$$\tau_b = \frac{cl_e}{S_L}$$

Equation 5: Burning time constant for the entrainment model mass burning rate as proposed by Blizard.

The entrainment model combustion processes can be split into two different stages. Firstly, the unburnt mass charge entrains with a rate defined as Equation 3. The entraining speed, S_e , is dictated by the turbulent eddies. Later, the entrained unburnt charge, burns with a characteristic time, τ_b . This time is a function of the turbulent entraining eddies and the laminar burning rate [12, 42]. Thus, engine combustion rates are affected by the entraining speed and the burning time constant defined in Equation 4. Different model calibrations are required when simulating different combustion regimes [42]. Moreover, it is important to point out that flame models based on the entrainment equations as stated in [65] are not considered phenomenological models. These models are rather numerical expression of observed engine burn rates [12]. Experimental flame studies have yet to confirm the entraining phenomena described in this model. Experimental images show continuous flame front characterised by spots of unburnt gases that burn inwards [12, 42, 66, 67]. However, the entrainment model was extensively used to simulated different engine application. A review of recent developments, tailoring the model's formulation to different application is available in [12]. Equation 3 and Equation 4 show that the model's accuracy depends on the laminar flame speed and the flow turbulence eddies. Therefore, correct values for the two characteristics are critical. Laminar flame speed values can be derived either by empirical correlation based on the fluid physics [54, 55], as proposed in [68], or detailed chemical kinetics is necessary. However, due to the turbulent nature of SI intake charge flows, the amount of time for which the flame is considered laminar is practically insignificant compared to the overall combustion duration. Thus, the turbulent entraining eddies is the process that most affects the engine burning rate within this model. Therefore, turbulence sub-models that provide the flame model with the necessary input are required if experimental in-cylinder turbulence characteristics are not available. A review of turbulence in-cylinder turbulence models is offered in Paragraph 2.5.

Flame Sheet Model

The flame propagating in turbulent flows, typical of SI engines is a thin wrinkled surface [42, 66, 67] as shown in Figure 9. An alternative approach, compared to the previously presented model is to consider the surface area of the wrinkled reaction sheet flame, A_t [42]. Thus, the flame area associated to turbulence combustion regimes, A_t , is increased compared to the flame area, A_l , occurring in a laminar burning process. Therefore, the resulting burning rate is dependent on the ratio between the wrinkled flame area and the laminar, (A_t/A_l) . The

mass burning rate in a flame sheet model can therefore be expressed as shown in Equation 6 [42] in which the ratio (A_t/A_l) is equal to the ratio between the turbulent flame speed and the laminar flame speed, (S_t/S_L).

$$\frac{dm_b}{dt} = \rho_u A_t S_L = \rho_u \left(\frac{A_t}{A_l} \right) A_l S_L$$

Equation 6: Mass burning rate in a flame sheet model as proposed in [42].

Where ρ_u is the unburnt gas density, S_L is the laminar flame speed, A_l is the surface of the laminar flame area (spherically assumed) and A_t is the surface of the turbulent flame area. The turbulent flame speed and, thus, the turbulent burning rate can be calculated once the increase in the flame area is established. However, physical causes that govern the wrinkling of the flame are still not fully understood [69]. Variation of local temperature and turbulence entraining are among the main phenomena that effect the change in the kinetic reaction rate and, thus, in the burning speed. At high engine speeds, turbulence eddies entraining the flame can deform the flame front to a degree at which multiple flame spots in the unburnt mixture start forming. However, it is accepted that, for traditional engine operating points, the flame front behaves similarly to a single flame front, wrinkled by the entraining turbulent flow [69]. Following this assumption, a modelling framework, known as fractal flame model has been developed [12, 42]. This approach states that the flame front can be characterised by a fractal geometry and the wrinkling of the flame is assumed to be within the turbulent length scales L_{max} - L_{Min} interval, defined in Equation 7:

$$\left(\frac{A_t}{A_l} \right) = \left(\frac{L_{max}}{L_{min}} \right)^{D-2}$$

Equation 7: Fractal definition of the wrinkled surface area as provided in [70]

Where L_{max} = corresponds to turbulent length scale which is the biggest scale corresponding to an energy in the in-cylinder turbulence field. L_{min} = corresponds to the Kolmogorov's scale which is the smallest turbulent scale. D = fractal dimension depending on the ratio between the turbulence intensity, u' , and the laminar flame speed, S_L as proposed in [70]. Information of the in-cylinder turbulence flow and laminar flame speed are required to evaluate the magnitude of the wrinkling scales and the fractal dimension. Conclusions regarding the need

of turbulence models, that provide the correct characteristics input to predict the engine RoHR, can be drawn, similarly to the previously presented model.

2.4 STOCHASTIC REACTOR MODELS

Another modelling approach falling within the Q-D combustion modelling frameworks is the Stochastic Reactor Model (SRM). Compared to the previously presented Q-D models, the SRM framework uses the Probability Density Function (PDF) approach applied to turbulent flows as described in [25, 71-73]. Within the SRM in-cylinder mass is treated as a series of particles each with a uniform composition. These particles describe physical quantities of in-cylinder mass thanks to a PDF distribution. Therefore, particles' composition in terms of chemical species, temperature, and mass are described by PDF's changes during the calculation. Detail explanation of the SRM governing equations is available in Chapter 4.

Different studies presented the underlying assumptions of the SRMs and focussed on the models' capabilities to predict burning rates of direct injected diesel engines [23-25]. SRMs were also used to carry pollutants formations analysis of homogeneously charged diesel engines, duel injection engines and natural gas fuelled engines where presented [74-77]. Engine knock prediction and the effect of the engine turbulent mixing on the auto-ignition event were investigated in [78]. Due to more restrictive engine emissions, recent studies have instead investigated the SRMs' capabilities to optimise diesel engines performance based on their emissions [79]. Detailed pre-tabulated chemical kinetics tables together with a turbulence models, tailored for diesel engine simulation, were developed in [80, 81]. Moreover, thanks to the renewed interest in petrol fuelled engines the SRM was also used to predict the RoHR for SI engines [18, 19, 23, 82].

SRMs showed to be capable of carrying combustion analysis for a wide range of engine applications. Moreover, in contrast to the other Q-D models, the in-cylinder inhomogeneities are accounted in the SRM thanks to the statistical nature of governing equations. However, the SRM combustion models, similarly to all the other Q-D models, require the following sub-models to carry the combustion analysis out:

- *In-cylinder volume calculation* – Same as all other Q-D models.
- *Chemical reactions calculation*: due to the PDF based governing equation, the SRM needs to account for the chemical reactions occurring during the combustion. Thus,

pre-tabulated detailed chemical kinetics data to predict the laminar flame speed value of different fuels and to evaluate the engine emissions [83, 84] have been implemented. The engine knock can be also be evaluated as shown in [82]

- *Heat transfer calculation* – Same as all other Q-D models.
- *Flame propagation model*– Flame propagation model based on [85] is used in the SRM. Similarly, to the previously models an analysis of this model will be presented in the next Paragraph.
- *Initial Spark Kernel* – not considered within the SRM framework.
- *In-cylinder turbulence calculation* – the in-cylinder turbulence characteristic is needed to set the frequency at which the PDF particles mix between each other and thus to set the how the PDF changes throughout the simulation. Moreover, the same characteristic is used in the turbulent flame speed calculation. Q-D turbulence models have been applied to the SRM similarly to the other Q-D models. An overview of the most known Q-D turbulence model is available in Paragraph 0.

2.4.1 Flame Propagation Model

In parallel to the other Q-D combustion models, the SRM requires a sub-model to calculate the turbulent flame speed and thus the mass burning rate. In turbulent premixed flames, the mixing of reactants with product at the flame surface is required to sustain the combustion. In a total absent of turbulence, this process, would occur with a rate dictated by the laminar flame speed. Within the SRM the in-cylinder domain is split into particles each with a characteristic composition. Thus, the mixing rate between these particles, can be associated to the mixing of reactants and product occurring during combustion [23, 85]. The simplest turbulent flame speed model that can be used in an SRM requires a user input value for u' to derive the desired turbulent speed. Typical examples of this group of turbulence models are found in [6] (see Equation 8) and [86] (see Equation 9). Similarly, to previously presented models, these two formulations depend on the laminar flame speed value and a turbulence characteristic. A more detailed turbulent flame propagation model, including the scalar dissipation rate occurring during turbulent premixed combustion was developed in [87]. The model was later simplified and applied to a SRM in [23]. Regardless the increased complexity of the flame model, in-cylinder turbulence characteristics remained the crucial input governing the model's results. Further details of the model developed in [23] is available in [88].

$$\frac{s_T}{s_L} = 1 + C \left(\frac{u'}{s_L} \right)^n$$

Equation 8: Turbulent flame speed according to [6]

$$\frac{s_T}{s_L} = 1 + 0.46 \left(\frac{u'}{s_L} \right)^n + 0.2 \left(\frac{u'}{s_L} \right)^{\frac{1}{2}}$$

Equation 9: Turbulent flame speed according to [86]

2.5 IN-CYLINDER TURBULENCE MODELS

Previous Paragraphs showed similarities across different Q-D combustion models. It was shown that, regardless the chosen approach the modelling of the flame, laminar and turbulent is required to predict the RoHR of SI engines. The laminar flame speed can be either be derived by empirical correlation-based approaches [13, 15, 16, 42, 68, 69] or through detailed chemical kinetics libraries [50, 51, 83, 84]. Empirical based approaches offer fast response, but the accuracy of their results depends on the range of engine operating conditions at which they have been validated. Laminar flame speed calculations based on chemical kinetics library, if correctly validated, should offer realistic responses for a wide range of operating conditions and fuels. It is important to point out here that laminar flame speed calculation based on chemical kinetics library can also provide value for alternative fuels where an empirical based laminar flame model has not been validated yet. Irrespective of the chosen approach to determine the laminar flame speed, a turbulent flame speed model is required to predict the effect of the engine in-cylinder turbulence on the laminar flame speed. At a high level all the available turbulent flame speed models simply multiply the laminar flame speed accordingly to a turbulence input. Thus, the physics governing the in-cylinder turbulence needs to be modelled to predict the RoHR in SI engines within the Q-D framework. Therefore, if any Q-D combustion model is used to predict the SI engines RoHR during the early concepts screening phase the following question need to be answered:

“Can the engine in-cylinder turbulence characteristics be predicted during the early concepts screening phase?”

In the next Paragraph available Q-D turbulence models will be reviewed focussing on their capability to predict the effect of different engine structures on the in-cylinder turbulence without the need of model calibration at each explored engine concept.

2.5.1 Q-D Turbulence Models

According to the literature presented in previous Paragraphs, the physical processes that need to be modelled in any Q-D combustion model, to predict the RoHR of SI engines can be summarised as shown in Figure 10. The flame initialisation and growth are necessary to evaluate the engine RoHR. Laminar flame speed values can be determined from empirical correlation or from detailed chemical kinetics. Moreover, the in-cylinder turbulence is a necessary characteristic that needs to be modelled to correctly predict the turbulent flame speed and thus the engine burning rate (see previous Paragraphs). The early concepts screening phase prevent to use empirical derived in-cylinder turbulence characteristics obtained through optical access engines. Thus, two different approaches, similarly to the laminar flame speed calculation, are available to model the turbulent flame speed: 0-D and CFD turbulence model. Figure 10 highlights the existence of a trade-off choice between accuracy and computational time needs is required at this point. 0-D turbulence models are an attractive solution for engine development due to the limited required computational time. CFD calculations instead require higher computational resources but are less dependent on user-input variables.

Figure 10: Schematic of necessary physical processes to be modelled in the Q-D framework to predict the engine burning rate

Currently, there are different available 0-D models that promise to predict the in-cylinder turbulence characteristics: *k-ε models* and *K-k models* are among the most known models. *k-ε models* use 0D equations for the turbulent kinetic energy, k and turbulence dissipation, ε derived from 3-D equations to predict the engine in-cylinder turbulence field. These models were initially proposed by Morel in [89, 90] and later tailored by others to different specific conditions. Overall *k-ε* models used the energy cascade model presented by Morel for which the turbulent kinetic energy, is converted into heat by the flow viscous stresses [89, 90]. A general review of the basic *k-ε* model formulation is available in [61]. Recent improvements have introduced contribution to the turbulence from ordered structured *i.e. tumble* have been introduced in [91]. A different approach describing the energy cascade from the mean flow kinetic energy, K , into turbulent kinetic energy, k , through turbulent dissipation is known as *K-k* model [92, 93]. Within this approach, the integral length scale is related to the instantaneous cylinder volume and piston position through mathematical equations. Once the integral length scale is calculated, the value for the turbulence dissipation is then derived from it. Different improvements of the initially developed *K-k* models are available in the

literature accordingly the application for which they were used. In [94, 95] a tumble model including the geometry of the intake manifold, valves and port inclination is introduced. General issue with this approach is the in-cylinder turbulence characteristics prediction during the compression stroke which was not representative of experimental turbulence data from optical access engine and CFD calculations. Moreover, limited conclusion regarding the model's capability of predicting the effect of different engine geometric features can be drawn. A parametric investigation was carried out without comparing the predicted results with experimental test data. In [96] the two approaches, $K-k$ and $k-\varepsilon$ are merged in a framework which showed good accuracy in the turbulence and tumble ratio prediction. However, the model poor performance to predict intake backflows lead to poor predictions in describing some operating conditions. Regardless the recent general improvements of the predictive capabilities of Q-D turbulence models at different engine operating points, these approaches still fail to reproduce geometrical features of the engine. Different model tunable constants, that accommodate the effect of different geometrical features on the engine in-cylinder turbulence are generally implemented. In his recent work Bozza [15, 16] used a $K-k$ based model to predict the in-cylinder turbulence of six different engine variants including different bore to stroke ratios, compression ratio, valve timing and intake manifold design. A model calibration procedure based on CFD calculations was carried out. The turbulence model was later tested using the calibrated setting for all the available engine variants. However, the 5 calibrated tuning constants had to be adjusted to achieve good results. Thus, an alternative approach to predict the in-cylinder turbulence at different operating points and for different engine concepts is necessary to predict the engine RoHR using Q-D models.

2.5.2 Q-D / CFD Based Approach

Complex CFD calculations, can capture the effect of different engine geometry on the bulk in-cylinder turbulence characteristics [97]. However, the required computational time is prohibitive during engine development. Thus, there is the need of a hybrid approach capable of benefiting of both, the CFD capability of predicting the geometrical effect on the in-cylinder turbulence and the fast calculations of Q-D models [98]. Pasternak [19] presented a new engine development process based on a SRM combustion model and CFD derived turbulence characteristic. The necessary turbulence input was characterised from multiple non-combusting CFD calculations at three different engine speeds and later used to predict the engine RoHR. The in-cylinder turbulence characteristics were time-averaged during the closed part of the cycle resulting in constant turbulence values for different speed. The

engine in-cylinder turbulence was assumed to be only dependant on the engine speed ignoring the effect of different loads and engine calibration on the in-cylinder turbulence. This simplification allowed to develop a correlation, based on the observed operating points, to extract the turbulence number at a different engine speed [19]. Consequentially, a development process, using a combination of CFD derived turbulence characteristics and simple correlations, similar to the one proposed in [19], could provide the correct turbulence input to Q-D combustion models.

It is known that during the closed part of the cycle engine geometries are the main factors that influence the in-cylinder air motion[1, 99]. Moreover, within SI engines, the effect different operating conditions on the in-cylinder can be modelled considering the changes in the intake charge velocity [13-15, 59, 60]. Results suggested that the engine air-motion of a given engine geometry during the closed part can be characterised with CFD calculations. Furthermore, experimental flow results together with the Q-D turbulence models numerical formulation showed that the characterised engine air motion response to operating points could be scaled to the intake charge speed.

The final research question that needed to be answered can thus be split as follows:

- *Can the in-cylinder turbulence characteristics be considered bound only to the given engine overall design?*
- *What are the turbulence characteristics necessary to be numerically resolved to correctly predict the engine RoHR within a Q-D combustion model framework at different engine operating conditions?*

The work carried out for this thesis was based on an SRM. This model was embedded with a pre-compiled detailed kinetic energy library for the laminar flame speed. The model was therefore believed to be capable to provide more realistic RoHR and knock predictions compared to a model based on an empirical based laminar flame table. Moreover, the literature review showed that this SRM model offered realistic RoHR predictions over a wide range on engine applications. In this thesis, during the closed part of the cycle, the overall turbulence characteristics' shape against crank angle was assumed to be bound only to the given engine geometry. For a given engine design, the interaction of the intake charge with the walls, over the closed part of the cycle, would not change for different engine operating points and calibrations. Thus, limited non-combusting CFD can characterise the in-cylinder characteristics of any given engine geometry. Changes in the intake flow velocity

to operating conditions are known to affect the overall in-cylinder turbulence magnitude [13-15] with a rate that is dependent on the intake charge flow speed. The turbulence field, characterised by a single CFD calculation, could therefore be scaled accordingly to changes in the intake flow speed to engine operating conditions, without the need of extra 0-D turbulence models. Following these hypotheses, a turbulence scaling factor correlating the change in the intake port velocity, predicted by the 1-D engine system model, to the turbulence input required by the chosen SRM was developed.

2.6 CONCLUSIONS

A literature review, focussing on how the RoHR of SI can be predicted during the early stage of engine development was presented.

Firstly, the major issue embedded with the current virtual development processes were discussed. It was shown that, current processes use 1-D engine models to analyse the effect of different design configurations and operating conditions on the engine RoHR. However, to provide meaningful results, 1-D codes require a pre-determined engine RoHR characteristic that is based on pre-existing combustion systems. Moreover, empirical based combustion models are used to accommodate the changes in the engine RoHR to operating points. Therefore, 1-D engine analysis results depend on the initial engine burn rate assumption and on the validity of the chosen empirical correlation. Consequentially, alternative modelling approaches to predict the engine RoHR, capturing more of the physics influencing the engine burning rate without the need of empirical correlations, were reviewed. It was shown that, overall, there are two main modelling categories: CFD models and Q-D codes. Due to the limited available time during engine development and the current computational resources, complex CFD calculations were shown to not be suitable for engine development. Therefore, a thorough review of Q-D combustion models, offering computational times compatible with engine development was carried out. It was shown that, regardless the chosen model, the in-cylinder turbulence characteristic needs to be captured to correctly predict the engine RoHR. Consequentially, a review of different modelling approaches for the in-cylinder turbulence was offered. In Paragraph 2.5 it was shown that, similarly to combustion models, modelling frameworks for the in-cylinder turbulence can be split into two main categories: CFD and Q-D models. Q-D models were shown to not be suitable for the screening of different design due to the calibration effort, necessary for each explored concept. CFD turbulence models instead showed to correctly

predict the effect of different hardware on the in-cylinder turbulence but at cost of higher computational time and resources. I

The following gaps in the knowledge were identified:

- The engine burn rate from different engine concepts, fundamental output of the concept stage of engine development is initially assumed rather than predicted (see Figure 7).
- At the early stage of development, the engine combustion rate throughout the operating map of different engine concepts is predicted by empirical based combustion models. This limits the exploration of alternative combustion systems due to the lack of validation data for the empirical model.
- A new process, that can predict the RoHR of different engine concepts and families, throughout the whole operating map using limited experimental data and with a timeframe that is compatible with 1-D engine system models is not yet available.

3 EXPERIMENTAL DATA

In this chapter the experimental data used for this research will be presented. All available data is owned by the project's sponsor and it was collected using their engine test beds. The data was recorded using their instrumentation which corresponds to the industrial standards. Data shown in this thesis corresponds to in-cylinder pressure traces and engine burn angles. The standard deviations of the experimental burn angles for all investigated engines was calculated by the high-speed data logger over 300 engine cycles following Equation 10.

$$\sigma(i) = \sqrt{\frac{\left(n \sum_{j=i-n+1}^i CA_j^2 - \left(\sum_{j=i-n+1}^i CA_j\right)^2\right)}{n*(n-1)}}$$

Equation 10: Experimental Burn Angle Standard Deviation

Where σ is the experimental standard deviation and n is the number of logged cycles. Engine main details will be offered in the following paragraphs.

3.1 ENGINE A

Engine A was a three-cylinder naturally aspirated stoichiometric port-injected gasoline engine capable of achieving Euro 6 emissions targets. Table 2 summarises main engine geometries.

Table 2: Main Engine A Parameters

Displaced volume	650 cc
Bore-to-stroke ratio	0.94
Compression ratio	12.1
Number of valves	4
Number of cylinders	3
Fuel injection system	Port injection
Induction	Naturally aspirated

Table 3 offers the experimental conditions investigated for this research. Four different engine speed points have been selected for this study. A valve timing optimisation was carried out during the testing campaign. Valve timing swings are available at different engine speeds, maintaining CA50 angle constant at around 8 °CA ATDC(F) or at the equivalent angle for Minimum advance for Best Torque (MBT). The maximum external EGR rate achievable combined with ignition timing advance was manually set to maintain CA50 at the desired value. Furthermore, EGR swings at different engine speeds have been carried out

using constant valve timing. The valve lift profiles used for the study are shown in Figure 11.

Table 3: Engine A Operating Points

Key Point	Speed [rev/min]	BMEP [bar]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
1	2000	7.5	21	334	604	121	390
2			18	344	614	111	400
3			16	354	624	141	410
4			29	334	604	121	390
5			17				
6			14				
7			12				
8	1300	6.5	26	329	599	136	405
9			26	349	619	116	375
10			24	339	609	146	415
11			26	349	619	146	415
12			23				
13			20				
14			17				
15	3500	8	8	359	629	136	405
16			17	349	619	146	415
17			18	349	619	126	395
18			18	349	619	126	395
19			14				
20			10				
21	5500	11	3	354	624	116	385
22				344	614	116	385
23				344	614	136	405
24				334	604	126	395

Figure 11: Engine A Valve Lift

3.2 ENGINE B

Engine B was a three-cylinder naturally aspirated stoichiometric port-injected gasoline capable of achieving Euro 6 emissions targets. Engine B is a development variant of engine A. This combustion system was characterised by a more compact combustion chamber geometry characterised by a 3.9% reduction in the bore size compared to engine A's bore. Engine B stroke was increased of 8%, compared to engine A stroke, to maintain the bore to stroke ratio (B/S) and the displacement volume equal to engine A. Main engine geometries are shown in Table 4.

Table 4: Main Engine B Parameters

Displaced volume	650 cc
Bore-to-stroke ratio	0.83
Compression ratio	12.5
Number of valves	4
Number of cylinders	3
Fuel injection system	Port injection (dual injector)
Induction	Naturally aspirated

The main difference between engine A and B corresponds to a different intake manifold port, designed to improve tumble generation during the intake stroke compared to Engine A, was fitted on Engine B (see Figure 12). Main differences between the two ports design are the fuel injector position and the addition of a “belly” feature to maximise tumble formation. Table 5 shows the experimental conditions investigated in this thesis. Thirteen operating points including sweeps in engine load and speed have been selected for this research. The maximum external EGR rate achievable, combined with ignition time advance have been set to maintain the CA50 at MBT value. The valve lift profiles used for the study are shown in Figure 13. The intake valve lift profile was updated compared to the engine A's profile to maximise the engine fuel consumption. Instead, the exhaust valve lift profile was carried over from Engine A.

Table 5: Engine B Operating Points

Key Point	Speed [rev/min]	Brake Torque [Nm]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
1	2000	30	45	330	612	117	417
2		40	30	314	595	122	422
3		50	10	307	588	115	415
4	3000	30	37	335	617	102	402
5		40	27	320	601	102	402
6		55	5	306	588	103	403
7	4000	55	10	324	605	98	398
8		40	5	320	601	102	402
9		30	8	325	606	102	402
10	5000	20	10	315	596	97	397
11		40	8	325	606	99	400
12		55	6	325	606	102	402
13	6000	20	10	315	596	96	397

Figure 12: Engine A (in blue) and Engine B(in orange) geometry comparison

Figure 13: Engine B Valve Lift

3.3 ENGINE C

Engine C was a three-cylinder stoichiometric port-injected gasoline capable of achieving Euro 6 emissions targets. This engine is the turbo charged version of Engine B with the main engine geometries reported in Table 6.

Table 6: Main Engine C Parameters

Displaced volume	650 cc
Bore-to-stroke ratio	0.83
Compression ratio	10.1
Number of valves	4
Number of cylinders	3
Fuel injection system	Port injection (dual injector)
Induction	Turbo Charged

Both engine B and C are fitted with the same intake port geometry. Table 7 shows the experimental conditions studied. Fifteen operating points including sweeps in engine load and speed have been selected for this study. The valve lift profiles used for the study are shown in Figure 14. The exhaust valve timing were fixed across different points (see Table 7).

Table 7: Engine C Operating Points

Key Point	Speed [rev/min]	Brake Torque [Nm]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
1	2000	40	16	280.9	569.1	124.8	380.8
2		60	0	340.9	629.1		
3		95	0	320.9	609.1		
4	3000	40	15	290.9	579.1		
5		60	8	303.9	591.1		
6		100	0	330.9	619.1		
7	4000	40	0	304.9	593.1		
8		60	3	325.9	614.1		
9		95	5	325.9	614.1		
10	5000	90	0	320.9	609.1		
11		60	3	329.9	617.1		
12		40	6	309.9	597.1		
13	5500	85	0	330.9	619.1		
14	6000	75	0	340.9	629.1		
15		40	5	325.9	614.1

Figure 14: Engine C Valve Lift

3.4 ENGINE D

Engine D corresponds to a Ricardo Hydra single-cylinder gasoline engine. The engine was a Euro 6 stoichiometric direct- injection gasoline engine. Table 8 provides the basic engine geometry data.

Table 8: Main Engine D parameters

Displaced volume	500 cc
Stroke	90 mm
Bore	84 mm
Compression ratio	10.2.1
Number of valves	4
Exhaust valve open	140.4 °CA ATDC(F) @ 0.2 mm lift
Exhaust valve close	358.2 °CA ATDC(F) @ 0.2 mm lift
Inlet valve open	361.4 °CA ATDC(F) @ 0.2 mm lift
Inlet calve close	589.2 °CA ATDC(F) @ 0.2 mm lift

Table 9 shows the experimental conditions studied, which included two injector designs, variation in engine load and start of injection time. The engine was run at a knock limit condition for the full load (26 bar) and middle load (8 bar) operating points in Table 9. A schematic drawing of the injectors' holes position is shown in Figure 16. The spray patterns for injector B are designed to be aligned with the bulk intake charge, to maximize the in-cylinder tumbling motion. Injector A spray patterns are instead homogeneously spread into the chamber to ensure an air-fuel mixing.

Table 9: Engine D Operating Points

Operating Point	Speed [rpm]	BMEP [bar]	Fuel Pressure [bar]	SOI [°CA ATDC(F)]	Injector Type
1	2000	26	150	420	A
2		26		390	A
3		26		480	A
4		26		420	B
5		8		420	A
6		8		420	B
7		8		450	B
8		8		480	B
9		8		510	B
10		2		420	B

Figure 15: Engine D geometry

Figure 16: Plan view of injectors holes layout

4 NUMERICAL MODELS

4.1 NON-COMBUSTING IN-CYLINDER CFD

The Ricardo Software CFD package VECTIS was used for this research [33]. Non-combusting RANS CFD analyses were carried out to capture the effect of different operating points and engine geometries, e.g. bore to stroke ratios, on the overall volume averaged in-cylinder turbulence characteristics. Numerical results were used to develop the turbulence scaling factor response and verify the underlying hypothesis of this research. Hypothesis details are offered in Paragraph 5.1. For all simulated cases, a global mesh size of 2 mm was used following VECTIS guidelines for in-cylinder simulations [33] (see Figure 17). Mesh refinements during valves events were defined around the valves and the intake manifold areas reducing the global mesh size from 2mm to 0.5 mm (see Figure 18). The in-cylinder air motion was modelled solving the equations governing turbulent flow motion, energy and mass transfer and using the standard $k-\varepsilon$ RANS turbulence model [33]. Three consecutive engine cycles were simulated to reach model's convergence. Initial turbulent intensity and length scale values, necessary to initialise the CFD turbulence model, resulted in discrepancies between the first and second simulated engine cycle. Analysis showed no difference between third and fourth cycle. Therefore, results presented in this thesis were all extracted from the third engine cycle. The mean flow velocity, at each crank angle, was calculated by averaging the three velocity components in the in-cylinder domain. Moreover, the turbulence intensity, u' , was calculated as presented in Equation 11. u' is considered the characteristic turbulence velocity, representing the speed at which, the large structured tumble eddy performs work on smaller eddies, increasing their motions.

$$u' = \sqrt{\frac{2}{3}k}$$

Equation 11: In-cylinder turbulence intensity

In the next paragraphs a brief introduction to the turbulence fundamentals will be discussed. This only intends to give the background knowledge necessary to understand the CFD analysis results in Chapter 6. For a comprehensive review of the subject, Versteeg's work [7] is suggested.

Figure 17: Engine A mesh size without refinement

Figure 18: Engine A mesh size with refinement during valve events

4.1.1 Introduction to Turbulence

All flows encountered in ICEs modelling are complex 3-D ones that become unstable above a certain Reynolds (Re) number (see Equation 12).

$$Re = \frac{UL}{\nu}$$

Equation 12: Reynolds number

Where U corresponds to the characteristic flow velocity, L corresponds to the characteristic flow length scale and ν corresponds to the kinematic viscosity. The Re dimensionless number is a known metric that measures the importance of inertial forces in respect to viscous forces. Flows with Re values below a critical threshold are characterised by smooth layers of fluid sliding past each other. This regime is known as *laminar*. Flows with Re values above the critical threshold are instead characterised by a random and chaotic behaviour. This regime is called *turbulent*. Within the Reynold Averaged Navier Stokes (RANS) CFD modelling framework the random nature of a turbulent flow, describing the motion of all particles is not fully described. Instead, particles' velocity is decomposed into two components: a steady mean value U and an instantaneous, fluctuating value $u'(t)$ as shown in Equation 13 [7].

$$u(t) = U + u'(t)$$

Equation 13: Fluid particles' velocity components

Flow visualisation studies have shown that turbulent fluctuations have three-dimensional components and are characterised by rotating structures. These structures are usually referred as turbulent eddies and they are characterised by a wide range of length scales [7]. Therefore, flow particles that initially are separated can be brought together by these eddies and exchange heat, mass, and momentum. This phenomenon is referred as *mixing*. Large turbulent eddies interact and extract energy with the mean flow. This interaction results in a stretch of the turbulent vortexes due to velocity gradients [7]. Large eddies have a characteristic velocity and length scales that are the same order as the structured bulk flow scales. At these large turbulent eddies, viscous effects are negligible and the angular momentum is conserved [7]. Consequentially, when large eddies interact with the mean flow, the rotation rate increases while the vortex radius decreases due to the presence of velocity gradients. Therefore, smaller length scales are produced by this phenomenon [7]. These smaller eddies are stretched by the larger eddies. The turbulent kinetic energy, k , is transported down from large eddies to gradually smaller eddies. This phenomenon is referred as *energy cascade* [7]. Viscosity is the main physics that dictates the dimension of smallest scale that can occur in a turbulent flow. The stretching work done by larger scales on smaller scales provides the energy to maintain the turbulence. At a large-scale level, the viscous

effect can effectively be ignored. As the scales become smaller, the viscous stresses effect becomes more significant, so that, work is performed against viscous stresses.

4.1.2 Turbulence modelling within the RANS CFD framework

In a turbulent flow there is the presence of a wide range of length scales. DNS models can resolve all eddies and particles in a turbulent flow, but computational requirements may be unpractical for some industrial applications. Regular engineering problems can be solved with simplified RANS models. These models average the properties of the flow over time and faster turnaround than fully LES and DNS frameworks. Within the RANS modelling approach simplifications to the physics governing turbulence are introduced so that turbulence models are needed.

Introduction to the k - ϵ model

In this thesis the k - ϵ turbulence model was used to derive the in-cylinder turbulence characteristics. An overall introduction of the model's formulation is presented in this paragraph. A more detailed explanation can be found in [7]. The k - ϵ model corresponds to the industrial standard and none of the other available turbulence models was used. However, it is important to point out that, any other turbulence model, characterised by similar predictive performance, can be used to reproduce the research output. Within the k - ϵ turbulence model flow characteristics are expressed by the mass mean values and their fluctuations. The model focusses on the mechanisms that affect the turbulent kinetic energy (per unit of mass) defined as shown in Equation 14.

$$k = \frac{u_i u_i}{2}$$

Equation 14: Turbulent Kinetic Energy

$$l = \frac{k^{\frac{3}{2}}}{\epsilon}$$

Equation 15: Characteristic length scale

Within the RANS k - ϵ turbulence model the characteristic turbulent length scale is defined as Equation 15. The value of ϵ , known as the dissipation rate of k , can thus be derived from Equation 16.

$$\mu_t = \frac{c_\mu \rho k^2}{\epsilon} = c_\mu u' l$$

Equation 16: Turbulent viscosity

Where C_μ is a dimensionless constant=0.09. In this research, default values for all the user-defined model constants available within the chosen turbulence model were used. A review of all constants effect of turbulence, including a sensitivity study, is available in [41]. Only the turbulence limiter, known as the realisable timescale bound limiter (TSB), was tuned. The TSB limiter is tuneable parameter (C_{TSB}) implemented to influence the effect of the turbulent viscosity μ_t in areas of high k/ϵ ratios. [33]. The turbulent viscosity calculation in regions characterised by high kinetic velocity and low dissipation, such as the near nozzle area, is therefore influenced by TSB. The C_{TSB} can effectively be considered as a threshold value for k/ϵ ratios. Therefore, when the k/ϵ ratios are lower than the threshold value set by C_{TSB} , the limiter has no effect on the calculation results. A more detailed explanation of the TSB can be found in [10, 33, 100]. A value corresponding to 0.346 was used during this research. This value was prescribed by internal in-cylinder CFD simulation guidelines and it was mainly applied to improve simulation stability. In this research non-combusting CFD calculations are used to characterise the baseline turbulence input necessary for the SRM for each of the explored engine variants. Raw values of the required turbulence characteristic need to be calibrated to provide the SRM with the correct input. Thus, any other value of the multiplier C_{TSB} is suitable with this methodology.

4.2 1-D ENGINE SYSTEM SIMULATION

The WAVE package developed by Ricardo Software was used to evaluate the overall engine performance[9]. Similar 1-D codes, characterised by comparable capabilities, can be used in the methodology presented in this thesis. Within WAVE, the overall engine structure is discretised into multiple ducts, characterised by their own volume. For each of these ducts mass and energy equations are solved and boundary conditions are calculated through the momentum conservation [9]. 1-D compressible flow equations, governing the conservation of mass, momentum and energy, are used to solve the detail of the engine flows. Engine modelling guidelines, provided by the software developer and corresponding to the industrial standard, were used to build a WAVE model for each of the explored engine variant. Theoretical details of the 1-D engine system model are available in [9]. The boundary conditions, necessary to initialise the SRM code, were manually extracted from the WAVE

(see Chapter 5 for further details). Future work is still required to develop an automatic procedure that would allow to couple the 1-D model to the SRM and feedback the combustion results.

4.3 Q-D STOCHASTIC REACTOR MODEL

The SRM is a simulation tool developed by LOGESoft that uses the Probability Density Function (PDF) approach to investigate the combustion in turbulent flows [20, 24, 25, 88]. Within the SRM code, the in-cylinder mass is discretized into particles (segments) each with its own chemical composition and temperature determining the gas mixture structure through PDFs [74, 75, 101]. During an SRM calculation, the shape of the PDF changes at each timestep, modifying the variables range over the in-cylinder domain (*i.e. temperature*). The initial PDF is characterised by the state mixture boundary conditions. Homogeneity of the particles is assumed to initialise SRM calculations. Within the SRM code, the PDF is discretised by mass into a user input number of segments. Consequentially, the PDF corresponds to a Mass Density Function (MDF).

The sample space concept needs to be introduced to fully understand the SRM modelling approach [25]. Therefore, a simplified explanation of the sample space is offered as follow. If the temperature between two events called “*a*” and “*b*” is defined as shown in Equation 17.

$$T(x, t) = T_a < T(x, t) < T_b$$

Equation 17: Temperature definition between two events

The normalised temperature can be expressed by a random variable ϕ , varying between 0 and 1 as shown in Equation 18

$$\phi(x, t) = (T(x, t) - T_a) / (T_b - T_a)$$

Equation 18: Random variable corresponding to a normalised temperature definition

If we considered an experiment where only a single temperature value was measured, the normalised temperature, ϕ , could be plotted as a point on a ψ axis (see Figure 19).

Figure 19: Sample space ψ for the random variable ϕ

The ψ axis can be called the sample space of the random variable ϕ that, in this example, corresponds to a normalised temperature. Therefore, ψ is an independent temperature variable called temperature space [25, 71]. Any event that is determined by the random variable ψ corresponds to a region of the sample space. Figure 20 shows an example where the event “A” is defined as $A = \left(\frac{1}{3} < \phi < \frac{2}{3}\right)$. The region of the sample space ψ corresponding to the event A is $\frac{1}{3} < \psi < \frac{2}{3}$. In the case that the sample point $\psi = \phi$ falls within this region then the A event occurred [25, 71]. The probability of occurrence of A is $p(A)$ where $0 < p(A) < 1$. If an event cannot occur its probability is zero. Instead, if an event is certain then its probability to occur is 1.

Figure 20: Sample space showing the region corresponding to the event A. Filled black dot correspond to the sample point for which A occurred.

Thus, any event can be associated with a region in the sample space and the probability of the event is equal to the probability of the random variable being in that region of the space. The probability for any region can be determined from the distribution functions defined in Equation 19.

$$F_{\phi}(\psi) = P(\phi < \psi)$$

Equation 19: Sample space ψ distribution function for the random variable ϕ

Therefore, for the random variable ϕ the distribution function increases from zero to one as ψ varies. Equation 20 summarises how the sample space is used to describe the probability of any random event.

$$E = \psi_1 < \phi < \psi_2$$

Where E is a random event and $\psi_1 < \psi_2$

$$P(E) = P(\psi_1 < \phi < \psi_2) = P(\psi < \psi_2) - P(\psi < \psi_1) = F_\phi(\psi_2) - F_\phi(\psi_1)$$

Equation 20: Sample space probability event

Therefore, the MDF within the SRM can be described as reported in (b)

Equation 21

$$F_\phi(\psi_1, \dots, \psi_{S+1}, t) \quad (a)$$

$$\phi(t) = (\phi_1, \dots, \phi_N, t) \quad (b)$$

Equation 21: Mass distribution function within the SRM code (a) and vector containing the random variable in the MDF (b).

Where ϕ corresponds to the vector containing the random variables represented by the MDF, Ψ_i represents the sample space variables of the random variables ϕ_i and N is the number of variables considered in the model [25, 71, 88]. Within the SRM the MDF's time evolution is assumed to be homogeneous across the simulation domain, e.g. *MDF changes with time but not in throughout the space* [22, 88]. The evolution of the initial MDF, within SRM codes follows Pope's formulation derived from the conservation of mass and energy as stated by the Navier-Stokes equations and shown in Equation 22 [77, 88].

$$\frac{\delta}{\delta t} F_\phi(\psi, t) + \frac{\delta}{\delta \psi_i} [Q_i(\psi) F_\phi(\psi, t)]$$

Equation 22: Time evolution of the MDF within the SRM code

Q_i refers to the source term for the sample space variable ψ_i which drives the change of the MDF within the SRM. At each time step the MDF is updated accordingly. Initial boundary conditions are applied at the closing of the intake valve and derived from the 1-D engine system model. Boundary conditions include global pressure and temperature, air fuel ratio (AFR), EGR rate and other main engine parameters. The chosen SRM code used for this thesis was tailored for engine combustion modelling. Consequentially, the source term Q_i can be split into the following physical processes: *piston movement, flame propagation, turbulence mixing, chemical reaction* and *heat transfer* [88, 102] Each of these processes corresponds to a sub model available within the chosen SRM code. Figure 21 shows a simplified flowchart of the different calculations, needed within the chosen SRM, to update the PDF at each timestep. The initial PDF is defined by setting the flow state boundary condition derived by the 1-D engine code. Later the MDF is define based on the number of particles set by the user. In this research the value of particles was set to 1000 for all investigated cases. The value was chosen following software developer best-practice

guidance provided in [88]. Higher number of particles was reported to increase the computational time without significant improvements in the results accuracy. Calculations in the chosen SRM code follow the order presented in the blue area in Figure 21. Following paragraphs will offer the high-level explanation of each of the sub models available within the chosen SRM.

Figure 21: Overall SRM sub models' layout

4.3.1 Piston Movement Calculation

The chosen SRM code is used to simulate the closed part of the engine cycle. The remaining part of the cycle needs to be modelled by any of the commercially available 1-D engine system codes. The effect of the piston moving on the in-cylinder volume during the late part of compression, combustion and initial expansion is modelled [88]. Main geometries, including the piston pin offset need to be defined to initialise the SRM calculation.

4.3.2 Flame Propagation Model

In the chosen SRM code the in-cylinder domain is split into two different zones: unburned and burned with mass exchanged between the particles of each of the two zones. The rate at which this exchange occurs is dictated by the flame propagation model. Within the chosen SRM code, the flame front propagation, is calculated through a model developed by Bjerkborn [23] and initially provided by Kolla [87] which defines the turbulent flame speed as in Equation 23. The turbulence element shown in Equation 23 is an external user input

that is defined as Equation 24. In this thesis a methodology to correctly define the C_{SRM} value was developed and will be presented in Chapter 5.

$$S_t = f(S_L, \tau_{SRM})$$

Equation 23: SRM turbulent flame speed calculation

Where S_L is the laminar flame speed defined by the chemical kinetics. The turbulence input is defined as

$$\tau_{SRM} = C_{SRM} * \tau_t = C_{SRM} * \frac{k}{\epsilon} \approx C_{SRM} \frac{l_l}{u'}$$

Equation 24: In-cylinder turbulence characteristic dictating the turbulent flame speed calculation within the SRM.

Where τ_t is the turbulent mixing time expressed in [s]. k is the turbulent kinetic energy expressed in [m^2/s^2]. ϵ is the turbulent dissipation expressed in [m^2/s^3]. l_l is the integral length scale expressed in [m], as defined in Paragraph 4.1.1. u' is the turbulent intensity expressed in [m/s]. C_{SRM} is a user input multiplier explained in Chapter 5. The main limitation of Kolla's flame propagation model is the spherical flame growth assumption which is not valid for all engine applications and combustion regimes. However, due the simplified nature of the SRM code, this assumption can be considered effective, since the actual in-cylinder flow field is not fully resolved. Moreover, Kolla's formulation showed good combustion predictions over a considerably wide range of combustion applications [85]. Equation 24 shows that, the turbulent flame speed calculation is only function of the laminar flame speed, provided by the chosen chemistry library, the integral length scale and turbulence intensity. The turbulence term is an external turbulence input that needs to be provided by the user. This characteristic can be derived by experimental data (e.g. optical engine), or CFD calculations and is defined as the ratio between the Turbulent Kinetic Energy, k , and its dissipation, ϵ [103]. Further details on the turbulence term will be presented in Chapter 5. l_l in Equation 24, corresponds to the largest turbulence scale (see Paragraph 4.1.1) and is known as the integral length scale. Thus, l_l depends on the position of the piston during the engine cycle. However, it was shown that, during the IVC and EVO timing, l_l was shown to slightly change due to the reduced movement of the piston [15, 19]. Moreover, Bozza [13] showed that, overall l_l can be considered independent on the engine operating conditions but is rather driven by the engine geometries e.g. bore to stroke ratio. In this research, for the closure of Equation 24 a constant value of l_l , equal to half of the engine bore, was assumed for each of the simulated engines. In Chapter 5 the procedure followed to calculate the correct value of C_{SRM} for different engine operating points and high-level calibration will be

explained. One last user input needs to be set to initialise the flame propagation model. Within the chosen SRM code, the spark kernel formation and growth, depending on the mixture state, type of ignition systems, 3-D flow field, etc. are not considered. Consequentially, a user-input variable, known as “SRM ignition timing”, that sets the time at which the flame starts propagating is therefore available in the code’s settings. This user-input multiplier effectively indicates the crank angle at which the flame propagation sub models start calculating the turbulent flame speed. Direct comparison with the experimental spark timing is therefore not possible. A procedure to automatically set the SRM ignition timing value was developed. Details of this procedure will be presented in Chapter 5.

4.3.3 Turbulence Mixing Model

The turbulence generating during the intake stroke is the main physical process that characterises the S.I. combustion and the mixing of the air-fuel charge. Within the SRM modelling framework, the mixing of the particles throughout the simulation is modelled through the so-called mixing models. Different models are available in the literature covering different applications. Among the most popular models, design to perform engine simulations, there are: the Interaction by Exchange with the Mean Square (IEM) [25, 104], the Linear Mean Square Estimation (LSME) [105]. Both models, when applied to SRM codes, at each timestep, relax the scalar particles’ values to the mean with a characteristic mixing time which depend by a user input constant C_{SRM} . These two models are relatively simple to implement and give reliable results for engine combustion application [88, 104]. Different modification of the IEM and LMSE mixing models’ have been developed accordingly to the application for which they were used. In this thesis the coalescence /dispersal model (C/D model), available within the chosen SRM code, was used to account the turbulence mixing occurring during the engine combustion following the software developer guidelines and relative literature [72, 73, 88, 103]. The C/D mixing model, requires the same external input as the flame propagation model, called turbulent mixing time, τ_t (see Equation 24). Following the formulation of the C/D model, the change in the MDF due to the particles mixing be expressed as Equation 25. The underlying assumption of this model is that randomly selected segment pair mix to their mean [73, 106]. The frequency at which the scalars, *mass fraction and species enthalpy*, in the random variable vector, ψ mix is dictated by τ_{SRM} [106]. A user multiplier C_{SRM} available in the SRM suite and set to a default value of 1. C_{SRM} values used in this thesis and the procedure followed to tune the value will be explained later in Chapter 5. A non-continuous PDF distribution,

represented by delta function, close to a Gaussian distribution is obtained with this model [106]. The C/D mixing steps for the gas composition and the enthalpy scalars are presented in Equation 26. Figure 22 shows a how a pair of particles mix with time determining the change of the PDF [88, 106].

$$\tau_t * C_{SRM} \left(\int_{\Delta\phi} F_\phi(\psi - \Delta\psi, t) F_\phi(\psi + \Delta\psi) d(\Delta\psi) - F_\phi(\psi, t) \right)$$

Equation 25: Change to the PDF due to the mixing of the particles.

$$Y_i^j(t + t_{sub}) = Y_i^k(t + t_{sub}) = \frac{w^j Y_i^j(t) + w^k Y_i^k(t)}{w^j + w^k} \quad (a)$$

$$h_i^j(t + t_{sub}) = h_i^k(t + t_{sub}) = \frac{w^j h_i^j(t) + w^k h_i^k(t)}{w^j + w^k} \quad (b)$$

Equation 26: Particles mixing calculation steps for gas composition (a) and enthalpy (b).

Where i corresponds to any given species in the system, Y is the mass fraction of each species, h is the system enthalpy, w is the chemical production or consumption rate of all species in the system and t_{sub} is a randomly selected sub time step

Figure 22: Schematic representation of the mixing of the particles within the SRM code [106].

4.3.4 Chemical Reactions Calculation

Within the chosen SRM code detail chemical kinetics libraries can be used to determine the particles' rate of change due to chemical reactions. A new chemical composition and state

for each particle is set at each time step. In this thesis, chemical reactions, defined in the 200 species NICE 4.02 PRF mechanism for n-heptane and iso-octane were used.

4.3.5 Heat Transfer Model

In this thesis, the Woschni heat transfer model available within the SRM code [57] was used to calculate the amount of energy lost through the walls. A stochastic approach was applied to the standard Woschni mode to decide the distribution of the heat transfer [74]. Depending on the number of particles, a user-input variable is available to set the ratio of heat distribution over the engine walls. An initial sensitivity study was carried out to investigate the effect of the heat transfer user input variable on the combustion results. Default value equal to 1 was used for this thesis as the variable resulted to have little significant on the results. Standard Woschni's coefficients were as well used [57].

4.3.6 Heat Release Calculation

The engine RoHR within the SRM is calculated as shown in Equation 27.

$$RoHR(z) = \sum_{n(z)=1}^{N_p(z)} \frac{m_{nz} (H_{nz}^f - H_{nz}^i)}{\Delta CAD}$$

Equation 27: Rate of Heat Release formulation. z is an index representing the model zones.

The heat release of each model's segment is calculated in both zones. The heat released in the unburnt zone is an important indicator of pre-ignition and knock. Detailed chemistry is solved in both zones to predict the main emissions formation and end gas auto-ignition [82]. The end gas ignition event for hydrocarbons blends consist of two stages: low temperature pre-reactions and later the main auto-ignition event due to high temperature excitation [82]. The two reaction phases in the end gas can be characterised by the heat released in the unburnt zone. The low temperature pre-reactions heat release is characterised by a peak of energy released before the spark. This increases the likelihood of combustion pre-ignition. The energy released in the unburnt zone due to the high-temperature auto-ignition processes result in a steep rise in the heat release, towards the end of combustion [82]. To detect whether these phenomena decrease the engine knock tolerance the detonation diagram proposed in [107] can be used. However, this diagram may not be easy to read to a non-expert user; so that, a simplified index to evaluate the engine knock was used for this thesis. A knock index, defined as the ratio between the heat release from the unburnt and burnt zone was selected [18, 19]. A value corresponding to 15% was selected as the knock limit. Knock

index values above the limit are likely to result in abnormal combustion. Predicted engine RoHR overall traces resulting in engine knock index values above the chosen threshold were characterised by initial abnormal rises after the ignition timing. Figure 23 shows an example of predicted in-cylinder pressure and RoHR traces from both zones. Figure 24 and Figure 25 show the corresponding burn and unburnt temperature PDF evolution at 2000rpm 7.5bar BMEP for different crank angles. At this operating point the SRM ignition timing was set at -14 [°CA ATDC(f)] corresponding to the experimental spark timing at -24 [°CA ATDC(f)] (procedure followed to set the SRM ignition timing is explained in Chapter 5). In the example the initial pre-reactions in the unburnt zone, due to low-temperature reactions, can be seen in the initial “bump” in the unburnt zone RoHR trace at -15 CA °ATDC(f). Moreover, the unburnt RoHR is characterised by a steep increase towards the end of the combustion, at around 20 CA °ATDC(f). A value of 16% for the knock index was calculated in this instance, suggesting an increase sensitivity of the engine to knock when operated at this condition. The increased of the knock likelihood can also be noticed in the temperature PDF evolution (see Figure 24 and Figure 25). The initial PDF at $t=0$ is defined by the gas state boundary conditions at IVC, derived by the 1-D engine system code. Thus, particle at $t=0$ of the first simulated cycle are assumed to be homogeneously distributed. At -35 CA [°ATDC(f)], before the SRM ignition timing, the particles’ temperature PDF, is characterised by a homogeneity towards 630K (see Figure 24a). Since the main combustion process has not started at this crank angle, changes in the particles’ temperature are mainly due to the compression work done by the piston. Later, at 3 CA [°ATDC(f)] the particles’ temperature PDF is characterised by a wider range with most of the particles having a value of around 900K (see Figure 24b). Later in the cycle, at 27 CA [°ATDC(f)] the particles’ temperature PDF is characterised by a cluster with a temperature value of around 2250K (see Figure 24c). This increased in the overall temperature of the in-cylinder gas is due to the auto ignition processes that started in the unburnt zone (see Figure 25).

Figure 23: Engine A's predicted in-cylinder pressure, burnt zone and unburnt zone RoHR at 2000rpm 7.5bar BMEP

Figure 24: Engine A's temperature PDF evolution from -35 [CA °ATDC(f)] (graph A) to +27 [CA °ATDC(f)] (graph C) in the burned zone at 2000rpm 7.5bar BMEP.

Figure 25: Engine A's temperature PDF evolution from +3 [CA °ATDC(f)] (graph A) to +27 [CA °ATDC(f)] (graph B) in the unburned zone at 2000rpm 7.5bar BMEP.

4.4 CONCLUSIONS

In this Chapter an introduction on the CFD RANS modelling framework and an overview of the turbulence modelling physical principles was initially offered. Later, the 1-D code, used to carry out engine system analysis, was introduced. Finally, a thorough review of the chosen SRM code was offered. The objective of the review was to describe the sub-models available within the SRM framework. It was shown that, the chosen SRM can capture the engine knock limit. Moreover, it was highlighted that both, the flame propagation and the heat release sub-models require the same external turbulence characteristics: the turbulent mixing time. The methodology developed to provide the SRM with the required turbulent mixing

time characteristic at different engine attributes and variants will be described in the following chapter.

5 METHODOLOGY

In this chapter the methodology developed to predict the in-cylinder turbulence characteristic, necessary for the SRM to predict the RoHR, will be presented. For clarity, the overall schematic of the methodology is reported below in Figure 26. Firstly, the initial concept design inputs derived from a baseline engine are used to build the 1-D engine model and the CFD models. Secondly, a non-combusting CFD calculation, at any chosen operating point, is used to evaluate and capture the in-cylinder turbulence characteristics, necessary to initialise the SRM combustion model. 1-D engine system simulations are later used to evaluate the engine overall performance at the explored conditions. SRM boundary conditions at IVC are extracted from the 1-D engine system model. The developed turbulence response is used to provide the SRM code with the turbulence input at any operating point. Later, a non-combusting CFD calculation, at any explored engine variant, is used to capture the effect of different engine design on the in-cylinder turbulence characteristic. Finally, the SRM code and the developed turbulence response are used to predict the engine RoHR at the explored engine variants.

In this research non-combusting CFD, 1-D engine system analysis and SRM simulations were run independently. Ideally, these different modelling frameworks should run simultaneously. An automatic procedure, to feedback engine burn rates predicted by the SRM in the 1-D engine system code, has still to be developed.

Figure 26: Schematic of the methodology used to predict the engine RoHR.

Figure 27: High-level methodology flowchart. The development process is split into three main phases as follows: models' calibration, engine optimisation and engine update.

5.1 TURBULENCE SCALING FACTOR RESPONSE ASSUMPTIONS

In this paragraph the underlying assumptions made to develop the turbulence response are reported.

5.1.1 First assumption

The turbulence characteristics' evolution i.e. the shape of the curve against the crank angle, during the closed part of the cycle, is considered only bound to the given engine geometry.

The main assumption made in this research was to consider the overall shape of turbulence characteristics against crank angle only bound to a given engine geometry. Numerical studies showed that, the overall evolution of turbulence characteristics during the closed part of the engine cycle and consequentially the characteristics' shape against the crank angle, can be considered constant for a given engine geometry [13-15, 18, 19]. In his work, Achuth [95] showed the effect of different engine calibrations *e.g. different valve lifts* on the in-cylinder tumble. Results highlighted an increased tumble magnitude but limited changes in the characteristic profile against the crank angle. Instead, different pentroof angles showed a significant effect on the tumble profile against crank angle. This was due to the large

turbulent eddies' formation caused by the interaction of the intake charge and the combustion chamber geometry (see Paragraph 4.1.1).

In this research non-combusting CFD analysis on different engine design was carried out to investigate the effect of different engine attributes, including changes in the engine design, on the in-cylinder characteristics. Numerical results showed that, during the closed part of the cycle, the turbulence characteristics' profile against the crank angle can be considered constant for a given geometry. Detailed analysis results are presented in Chapter 6.

5.1.2 Second assumption

At a given engine geometry, during the closed part of the cycle, the effect of different engine calibrations on the in-cylinder turbulence characteristics, can be scaled on the intake flow charge speed.

Different engine calibrations, *e.g. valve timing*, are known to affect the engine in-cylinder turbulence [1, 13, 15, 95]. In Paragraph 2.5 it was shown that Q-D turbulence models, can capture the effect of different engine attributes on the in-cylinder turbulence. However, initial tuning is required to calibrate the model on a specific engine geometry. Within Q-D turbulence model, changes in the turbulent kinetic energy, k , in response to operating condition and engine calibrations, are function of the mean intake flow charge velocity. Q-D turbulence prediction results in [13, 14] showed that, for a given engine geometry, different engine operating condition and calibrations affect the in-cylinder turbulence characteristics' magnitude but not the shape against the crank angle. The development against the crank angle of turbulent eddies related to k is affected by larger eddies that depend on the combustion chamber geometry. Thus, to predict the effect of different engine calibrations, the turbulence information of any engine design, characterised by a non-combusting CFD calculation can be scaled to the intake charge speed.

5.2 PROCEDURE TO DETERMINE THE SIMILARITY BETWEEN TURBULENT MIXING TIMES

The following procedure was used to prove that, for a given engine geometry, different operating conditions and high-level calibrations affect the magnitude of the turbulent mixing time (τ_t) but not the shape against the crank angle during the closed part of the engine cycle.

The similarity between the two turbulent mixing times can be determined following the steps below.

1. The turbulent mixing (τ_t) of different operating conditions and calibrations is derived from CFD analysis. τ_t curves from key point 1 and 3 of engine A will be used here as an example. The main difference between the two points is a change in the valves calibration with key point 3 characterised by retarded valve events (see Table 3). Key point 1 will be referred to as “valve timing 1” whereas key point 3 as “valve timing 2”.
2. Each τ_t curve, defined as $\tau_t = f(CA)$, is fitted to “n” degree polynomial function using the least mean square error method [108]. Trial error showed that 4th polynomial curve resulted in the best fit for all explored cases. The chosen SRM combustion model, similarly to all other available Q-D models, accounts for the closed part of the engine cycle. Therefore, τ_t should be fitted between IVC and EVO timing. However, due to the valve events effect on the in-cylinder turbulence *i.e.* *sudden increase in k and ε production* (see Figure 38) τ_t curves were fitted over a smaller crank angle interval. In this example a crank angle interval between 640 °CA ATDC(F) and 800 °CA ATDC(F), was chosen. Figure 28 shows two 4th grade polynomial functions used to fit the chosen turbulent mixing times. Time step equal to zero corresponds the first crank angle in the fitting interval. Polynomial equations are characterised by coefficients that determine the shape of a dependent variable (y) as a function of the independent variable (x) (see Equation 28). However, the y-intercept coefficient “e” only defines the value of y when x=0 but not the shape. Therefore, the similarity of two polynomial curves can be determined by comparing a, b and c’ coefficient values.

$$y = ax^4 + bx^3 + cx^2 + dx + e$$

Equation 28: General 4th grade polynomial equation

Figure 28: Turbulent mixing time polynomial fitting using the “least mean square” method.

3. The polynomial coefficients values of the two fitted curves are compared as shown in Figure 29. Results shows that coefficients fitted to τ_t of “valve timing 1” are adequate to fit τ_t of “valve timing 2”. Error bands correspond to the standard coefficient error calculated using a 95% confidence interval. Overlapping coefficient values indicate that the trend of two curves, over the considered interval, is similar. Therefore, different valve calibrations do not affect the shape of the turbulent mixing time shape against the crank angle. Changes in the engine operating conditions or calibrations affect the in-cylinder turbulence characteristics magnitude (see Chapter 6). Changes in the “y-intercept” values represent the change in the magnitude.
4. Figure 30a shows the comparison between the CFD derived τ_t of “valve timing 2” (red curve), the fitted 4th grade polynomial fitted (red dotted curve) and the curve resulting using the fitted polynomial equation of “valve timing 1” and the y-intercept value of “valve timing 2” (black curve). Figure 30b shows the linear regression line, between the CFD derived τ_t of valve timing 2, treated as independent variable, and the fitted turbulent mixing time using valve timing 1 coefficients, treated as depended variable .

Coefficients	a	b	c	d	e
Valve timing 1	-4.25E-07	1.20E-05	-8.57E-05	6.08E-05	2.32E-03
Valve timing2	-4.85E-07	1.36E-05	-9.84E-05	8.64E-05	2.86E-03

Figure 29: Polynomial coefficients' value of the 4th grade polynomial curves fitted to the turbulent mixing time from different valve timing. Error bands correspond to the standard coefficients' error calculated with a 95% confidence interval.

Figure 30: Comparison between CFD derived τ_t and mixing time values derived using a single 4th grade polynomial curve, fitted to τ_t from valve timing 1.

5.3 SRM MODEL CALIBRATION ON BASELINE EXPERIMENTAL DATA

In this paragraph, the initial calibration, corresponding to the first phase shown in Figure 27 will be explained. Figure 31 shows the steps necessary to initially calibrate the SRM model. Initial baseline experimental data collection is required to build a validated 1-D engine system model that will provide necessary input to the SRM and the CFD models. In this research, geometrical characteristics of the baseline engines in Table 2 (engine A) and Table 8 (engine D) were used to initially calibrate the models. For each baseline engine, experimental data in Table 3 and Table 9, including burn angles, were used to calibrate the 1-D model. Calibration procedure, available in [9] was followed. Once the 1-D model was built the data shown in Table 10 was extracted and used as port boundary condition in the CFD model.

Fuel air residual ratio	Liquid fuel mass fraction	Mass flow	Mass fraction fuel vapor
Mass fraction of air	Pressure	Residual mass fraction	Temperature

Table 10: Non-combusting CFD necessary boundary conditions extracted from the 1-D engine system code

Figure 31: Flowchart of the initial models' calibration phase. Baseline engine experimental data is used to build a 1-D engine system model that, coupled with single non-combusting CFD calculation, is used to tune the SRM code.

Later, a non-combusting CFD calculation at any single operating point is carried out to characterise the initial turbulent mixing time (see Equation 29).

$$\tau_{t_{BaselineEngine}} = \frac{k_{Baselineengine}}{\epsilon_{Baselineengine}} \approx \frac{l_{BaselineEngine}}{u'_{BaselineEngine}}$$

Equation 29: Turbulent Mixing time for the baseline engine

Once the baseline turbulent mixing time, $\tau_{BaselineEngine}$, is derived from the non-combustion CFD calculation, the boundary conditions, necessary for the SRM calculation, are extracted from the 1-D engine system code (see Table 11).

Engine geometries	Engine speed	Equivalence ratio	Pressure at IVC
Residual	Temperature at IVC	Walls temperature	

Table 11: SRM necessary boundary conditions extracted from the 1-D engine system code

In Paragraph 4.3.3 a user-input multiplier, $C_{SRMBaseline}$, was introduced. $C_{SRMBaseline}$ is a variable available within the PDF modelling approach that allows to counterbalance uncertainties stemming from CFD derived turbulence input characteristics and the simplified 0-D nature of the model (see Equation 30).

$$\tau_{SRMBaseline} = \tau_{t_{BaselineEngine}} * C_{SRMBaseline}$$

Equation 30: Scalar mixing time for the baseline engine

The scaled turbulent mixing time, known as scalar mixing time, τ_{SRM} , affects the scalar particles' PDF mixing frequency [25, 71]. In [25], Pope reviewed findings from different studies focussing on turbulent flows analyses using the PDF approach. Pope showed that, the value of $C_{SRMBaseline}$ cannot be considered universal. However, $C_{SRMBaseline}$ can be considered constant for a given experimental configuration, but its value depends on the initial conditions. Within the chosen SRM code, the scalar mixing time is used to calculate the flame front propagation and the mixings of the PDF particles. Therefore, the value of $C_{SRMBaseline}$ was effectively treated as a tuning variable used to calibrate the SRM code and consequentially, initial model tuning, matching experimental burn angles and load, is required to define the value of $C_{SRMBaseline}$. Moreover, the SRM ignition timing input introduced in Paragraph 4.3, necessary to initialise the flame propagation sub model, needs to be calibrated accordingly. Due to the lack of a spark kernel sub model, the SRM ignition timing needs to be always set later in the combustion stroke compared to the experimental spark timing. The difference between spark and SRM ignition timing can be referred as to the mixture ignition delay period. Therefore, the SRM ignition timing was constrained to occur after the experimental spark and iteratively calibrated with C_{SRM} to match the chosen baseline operating points burn angles and engine load as follows:

1. The initial turbulence mixing time, τ_t , is derived from a non-combusting CFD calculation at any chosen baseline point (see Equation 29).
2. An initial value of C_{SRM} corresponding to 1 is assumed. At the condition explored for this thesis and according to the available literature C_{SRM} values are always greater than 1 [19, 25].
3. An initial value of the SRM ignition timing, retarded of 1 °CA from the spark timing is assumed.
4. All boundary conditions (see Table 11), derived from the 1-D engine system model, are applied to the SRM code.
5. Once the SRM code is set, the combustion analysis at the chosen baseline operating point is carried out. Depending on the end results the two following options can be taken.
 - a. If predicted burn angles and load matched the chosen baseline experimental data go to step 11.
 - b. If predicted burn angles and load did not match the chosen baseline experimental data go to the next step.
6. Delay the SRM ignition timing of a further 0.5 °CA compared to the experimental spark timing.
7. Combustion analysis is carried out using the SRM code set with a delayed SRM timing. Depending on the end results the two following options can be taken
 - a. If predicted burn angles and load matched the chosen baseline experimental data go to step 11.
 - b. If predicted burn angles and load did not match the chosen baseline experimental data go to the next step.
8. Repeat steps 6 and 7 until combustion does not start due to late ignition timing. If that happens go to the next step.
9. At this point, a greater value of C_{SRM} , needs to be assumed. Increase previous C_{SRM} value of 0.1.
10. Go back to step 3.
11. Tuned SRM model.

A value for $C_{SRMBaseline}$ of 9.5 and an SRM ignition input timing at 14 °CA BTDC(F), retarded of 10 °CA, compared to the experimental spark timing, matched engine A burn angles at 2000rpm_40Nm. Engine D resulted in a $C_{SRMBaseline}$ value of 11.4 and SRM ignition

input timing at -4°CA BTDC(F), retarded of 2°CA , compared to the experimental spark timing at 2000rpm_26Bar_BMEP. SRM ignition timing results (see Chapter 7) are comparable to experimental ignition delays found in [109, 110] for similar engine operating conditions.

5.4 TURBULENCE RESPONSE TO ENGINE OPERATING CONDITIONS AND HIGH-LEVEL CALIBRATIONS

Figure 32: Flowchart of the engine optimisation phase. The change in the intake port velocity to engine operating point, captured by the 1-D engine system model, is used to provide the SRM code with the necessary turbulence input.

In this paragraph the steps of the engine optimisation phase will be presented (see Figure 32). This phase focusses on the effect of different engine operating conditions and calibrations on the engine burning rate. Consequentially, engine design changes are not considered. The evolution of the turbulent mixing time against the crank angle during the closed part of the cycle is considered function of the given engine geometry. The effect of different high-level engine calibration can be predicted by scaling the in-cylinder turbulence on the intake charge speed. Referring to Figure 32 the following steps need to be taken:

1. An initial data collection at desired operating points is needed to define boundary conditions for the 1-D engine system model – Table 12 shows the data required by the 1-D code.

AFR (desired)	EGR (desired)	Exh. T. (assumed)	FMEP (calculated)
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Intk. T. (assumed)	Torque (desired)	Valve timing	Valve profiles
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Table 12: Data needed to set the 1-D engine system code.

2. 1-D engine system analyses are carried out focussing on the effect of different engine operating conditions on the intake flow charge velocity as shown in Figure 33.

Figure 33: Effect of different engine speeds on the intake port velocity

3. Since the SRM code and the 1-D code do not run in co-simulation an extra combustion model, within the 1-D engine model, is required for the closure of the code. Estimated burn angles and targeted performance are therefore necessary.
4. Changes in the in-cylinder turbulence characteristics to engine operating points, are scaled to the intake charge speed. A multiplier, C_{SRM_i} , defined as the ratio between the intake port velocity integral value within IVO and IVC timing, predicted by the 1-D engine system code at any operating point, and the intake port velocity integral value of the baseline operating point, can be calculated (see Equation 31a). Therefore, any engine attribute that results in changes in the intake port velocity during the intake stroke, *e.g.* IVC timing, or, higher overall intake port velocity *e.g.* different engine speeds, result in different values for the multiplier (see Equation 31a and Figure 33). When the start of injection (SOI) timing, in a direct injected engine (DI), is the solely investigated

characteristic, Equation 31b must be used to calculate the $C_{SRM_{OP_i}}$. In a DI engine, the energy associated with the fuel injection affects the in-cylinder flow momentum (refer to Paragraph 6.1.3 for further details). However, this effect cannot be predicted by a 1-D engine system code. The engine intake air flow is not influenced by the injection timing, while all other operating factors are held constant. Thus, a linear correlation, relating the time at which the fuel is injected in the chamber and the resulting in-cylinder turbulence is used (see Equation 31b). This correlation assumes that, late injection timing, due to the shorter time available to dissipate the energy associated with the injection event, result in higher in-cylinder turbulence, compare to a chosen baseline SOI.

$$C_{SRM_i} = \frac{\int_{IVO_{OP_i}}^{IVC_{OP_i}} Intake\ Port\ Velocity_i}{\int_{IVO_{Baseline}}^{IVC_{Baseline}} Intake\ Port\ Velocity_{Baseline}} \quad (a)$$

$$C_{SRM_i} = \frac{SOI_i}{SOI_{Baseline}} \quad (b)$$

Equation 31: Scalar Mixing time multiplier for different operating conditions and calibrations.

With i is any given engine calibration, C_{SRM_i} is the scaling factor at any given calibration and SOI = Start of Injection [$^{\circ}$ CA ATDC(F)]. Equation 31b needs to be used only on DI engines, when the SOI is the solely investigated characteristics.

5. Once $C_{SRM_{OP_i}}$ multiplier is calculated, the corresponding scalar mixing time for any given engine operating point can be calculated scaling the baseline turbulence characteristic derived during the initial tuning phase can be scaled as shown in Equation 32. Details of the non-combusting CFD analysis that showed similarities between CFD and 1-D results is presented in the Chapter 6. For instance, retarding IVC timing further from the BDC result in greater negative intake velocity due to the piston moving towards TDC while the intake valve is still open. This reduces the resulting in-cylinder turbulence level during combustion due to higher energy being dissipated into heat. Higher scalar mixing time are therefore associated with late IVC timing.

$$\tau_{SRM_{OP_i}} = \frac{(\tau_{tBaselineEngine} * C_{SRM_{Baseline}})}{C_{SRM_i}} \quad (Equation\ 32)$$

Equation 32: Scalar Mixing time for different operating conditions and calibrations.

6. Combustion analysis is carried out using the SRM code. Necessary IVC boundary conditions for the SRM are extracted from the 1-D engine system model for each engine operating condition tested (see Table 11). Once all the necessary model input, for any given operating point, were defined, the SRM ignition timing were set to achieve the desired engine load and a knock index below the threshold value (see Paragraph 4.3.6).

5.5 SCALAR MIXING TIME RESPONSE USED FOR ENGINE UPDATE

Figure 34: Flowchart of the engine update phase. Non-combusting CFD analysis, one for each explored engine concept, is used to provide the SRM code with the correct turbulence input.

In this paragraph details of the steps characterising the engine update stage will be offered. This final phase focusses on engine developments that include changes in the overall design. Thus, non-combusting CFD calculations capturing the effect of different geometrical features are required to define the in-cylinder characteristic for each explored engine variant. Referring to Figure 34 the following steps need to be taken to predict the engine RoHR:

1. An initial data collection at desired operating points, for each of the explored engine variant, is needed to define boundary conditions for the 1-D model. Table 12 shows the required data.
2. A new 1-D engine system model is required to be built for each of the explored engine variants. In this thesis, the standard procedure describe in [9] was followed.

3. A non-combusting CFD calculation, one for each of the explored engine variant, is carried out to characterise the effect of different engine design on the evolution of the turbulence characteristics against crank angle. The turbulent mixing time for any engine variant is derived as shown in Equation 33. The same speed against load operating point between the baseline engine and the engine development variants needs to be simulated. This allows to solely compare the effect of different engine variant on the turbulent mixing time.

$$\tau_{EngineVariant_i} = \frac{k_{EngineVariant_i}}{\epsilon_{EngineVariant_i}} \approx \frac{l_{EngineVariant_i}}{u_{EngineVariant_i}} \quad (\text{Equation 33})$$

Equation 33: Turbulent Mixing time for any engine variant

4. Once the in-cylinder turbulence characteristic, τ_t , is predicted for each of the engine variant, Equation 34 is used to define the scalar mixing time at each engine variant. If different engine development variants are explored (e.g. Engine B and C compared to engine A) the value of $C_{SRM_{Baseline}}$ in Equation 34 is held equal to the value defined during the tuning phase. Pope showed that, the value of C_{SRM} can be considered constant for a given experimental configuration [25]. Thus, the turbulent mixing time, calculated at the same engine speed and load condition, can be scaled using the same $C_{SRM_{Baseline}}$ multiplier.

$$\tau_{SRM_{EngineVariant_i}} = \tau_{t_{EngineVariant_i}} * C_{SRM_{Baseline}} \quad (\text{Equation 34})$$

Equation 34: Scalar mixing time for any given engine variant

5. The same procedure described in the previous Paragraph is used to characterise the effect of different engine operating points on the in-cylinder turbulence characteristics (see Equation 31a)
6. The scalar mixing time for each of the explored engine variants can now be calculated. To capture the effect of different engine geometry, a different turbulence characteristic for of each explored engine hardware needs to be scaled (see Equation 35)

$$\tau_{SRM_{OP_i}} = \frac{(\tau_{t_{EngineVariant_i}} * C_{SRM_{Baseline}})}{C_{SRM_{OP_i}}} \quad (\text{Equation 35})$$

Equation 35: Scalar Mixing time at different engine operating conditions and calibrations of any engine variant

7. Combustion analysis is carried out using the SRM code. IVC boundary conditions for the SRM were extracted from the WAVE model of each engine variant. Once all the necessary model input, for any given operating point, were defined, the SRM ignition

timing was set to achieve the desired engine load and a knock index below the threshold value.

5.6 CONCLUSIONS

In this chapter the methodology developed to predict the turbulence characteristic required by the SRM code to predict the engine RoHR was presented. Firstly, the two underlying assumptions were introduced and discussed. Later, the main phases of the methodology were described. The calibration phase, necessary to tune, the 1-D engine system and the SRM was presented. It was shown that, experimental data, including burning angles, is necessary to correctly calibrate the SRM models and the CFD derived turbulence characteristic. Later, the second overall phase of the methodology, tailored for a specific engine optimisation was discussed. A thorough “step-by-step” guide was offered. It was shown that, to predict the turbulence input necessary to initiate the SRM code, the CFD derived turbulence characteristic of a specific engine design, calculated at any chosen operating point, can be scaled on the intake charge flow velocity. Finally, the last phase of the methodology, tailored for the screening of different engine concept design, was described. It was shown that, the non-combusting CFD calculations, one for any screened hardware, can be used to capture the geometrical effect on the engine in-cylinder turbulence characteristics. Later, to predict the effect of different engine operating points on the in-cylinder turbulence, the CFD derived characteristic of any engine design, was scaled on the intake charge flow velocity as described in the previous phase of the methodology. Details of the CFD study, carried out to verify assumptions necessary to develop the methodology described here, can be found in the following Chapter.

6 IN-CYLINDER TURBULENCE ANALYSIS

6.1 ENGINE OPERATING CONDITIONS AND CALIBRATIONS EFFECT

6.1.1 Valves Timing

Figure 35 shows non-combusting CFD predictions of the in-cylinder mass-averaged turbulence characteristics, for different valve timing at constant engine speed. Engine A experimental data, corresponding to Key Points 1, 2 and 3 in Table 3, was used. Results labelled as “Valve timing 1”, are characterised by the most advanced intake valve opening (IVO), occurring at 334 °CA ATDC(F). The intake valve events of the other available cases in Figure 35, were retarded respectively of 10 °CA, for data labelled as “Valve timing 2”, and 20 °CA, for “Valve timing 3”. Exhaust valve timing were shifted accordingly to the intake valve events, resulting in a constant overlapping duration for all three cases. For clarity, detailed valve timing are reported in all figures. Moreover, data corresponding to “Valve timing 1” will be considered the baseline data for this discussion.

Figure 35a shows that, the mean in-cylinder velocity is generated during the initial part of the intake stroke, after the piston has reached TDC. The most retarded IVO timing (valve timing 3) results in the highest velocity formation, due to a more favourable intake valve pressure condition at IVO. Since the engine speed, load, fuelling and valve overlap duration were held constant, retarded exhaust valve closing timing, compared to the baseline data, result in higher exhaust backflow during the valve closing event. This is due to the piston moving downwards towards BDC, resulting in the mean in-cylinder flow velocity deceleration, occurring close to EVC timing. The increased pressure difference, between the cylinder volume and the exhaust manifold, draws the exhaust flow back, while the valve is still open. Figure 36 shows the predicted in-cylinder flow vectors of the three different analysed valve timing during the valve overlapping period. Results show that, later EVC timing, corresponding to a higher-pressure difference between the exhaust manifold and the in-cylinder volume, result in higher exhaust backflow. Consequentially, the exhaust bulk flow performs work on the low-pressure and low-velocity in-cylinder flow, increasing the motion of the in-cylinder flow smaller scale eddies. As the piston continues moving towards BDC, the in-cylinder velocity starts decreasing for all cases at around 450 °CA ATDC(F),

due to reduced intake charge flows. This is caused by the reduced difference between the atmospheric pressure, available in the intake manifold, and the relative vacuum, created by the piston moving downwards.

The effect of the valve strategy on the turbulence intensity, u' , is shown in Figure 35b. Results show that, during the intake stroke, u' follow the mean in-cylinder flow velocity, with peak values occurring at the same crank angle. Therefore, higher u' peak values, are related with later IVO timing. The exhaust backflow, characterised by disordered small eddies (see Figure 36) increases the effect of viscous stresses in the cylinder volume (see Equation 16 in Chapter 4). Thus, part of the energy associated to the large eddy intake flow, is used to perform work against the actions of the exhaust flow. Afterwards, u' slowly decreases due to the overall flow deceleration caused by the increasing volume.

Figure 35c shows that, the intake tumble motion starts forming during the intake stroke, before TDC, following the mean flow velocity results. After the piston has passed TDC, results follow the mean in-cylinder velocity and turbulence intensity's trends, throughout the initial part of the intake stroke. Afterwards, tumble profiles decay, due to the combination of the following effects: in-cylinder volume variation, reduced intake flow rates and increased dissipative effects caused by the higher turbulent viscosity. During the compression stroke, the tumble vortex increases after the piston reached BDC, until around 650 °CA ATDC(F). This effect is due to the momentum conservation, which increases the tumble vortex's velocity while the vortex's radius is reduced, due to the decreasing in-cylinder volume. As the piston approaches TDC, the tumble vortex breaks up into several smaller eddies, resulting in a tumble decay. As the structured tumble eddy collapses, the motion at the smaller scales increases, and the action of viscous stresses becomes more significant, resulting into more energy dissipation.

Figure 35: Engine A CFD predictions of different valve timing effect on in-cylinder mean flow velocity (graph A), turbulence intensity (graph B) and tumble ratio (graph C). Valve timing data refers to key points 1,2 and 3 in Table 3.

Figure 36: Engine A in-cylinder flow speed vectors comparison between different valve timing. Valve timing data refers to key points 1,2 and 3 in Table 3.

Figure 37: Engine A 1-D prediction of different valve timing effect on the intake port velocity. Valve timing data refers to key points 1,2 and 3 in Table 3.

Figure 37 shows the 1-D predicted intake port velocity for the three different investigated valve timing. The negative pressure difference, calculated subtracting the pressure in the cylinder volume and the corresponding pressure in the intake port, causes the negative velocity occurring during the initial part of the compression stroke. For clarity, the negative flow velocity convention corresponds to the flow moving from the in-cylinder volume back to the intake port velocity. Results show that, late IVC timing correspond to greater negative intake flow, compared to the baseline case. Thus, higher dissipative effect, compared to the baseline case, are related to higher negative intake backflows which further destroy the structured tumble motion.

Figure 38: Engine A CFD prediction of different valve timing effect on the in-cylinder dissipation rate, ϵ (graph A) and the turbulent mixing time, τ_t (graph B). Valve timing data refers to key points 1,2 and 3 in Table 3.

Figure 38a shows the in-cylinder turbulent dissipation rate, ϵ , during the compression and expansion strokes. The latest IVC timing shows the highest in-cylinder dissipation rate while the intake valve is open. The effect of different valve timing, on the turbulent mixing time, τ_t , during the compression and the expansion strokes, is shown in Figure 38b. The turbulent mixing time defined in Equation 29 (see Paragraph 5.2) corresponds to the turbulence characteristic that the SRM code requires to perform the combustion calculation. The initial drop in the turbulent mixing time profiles results, at around 585 °CA ATDC(F), is due to the IVC timing and the significant ϵ generation caused by intake backflows (see Figure 38a). Increased k and ϵ at EVO timing are instead the reason of the sudden drop in the turbulent mixing time profiles, occurring during the late part of the expansion stroke. The most retarded IVC timing, results in the highest turbulent mixing time profile's magnitude, τ_t , which corresponds to the lowest in-cylinder turbulence level during the combustion. Since

the turbulent flame speed within the SRM is proportional to τ_t , greater turbulent mixing time's magnitude corresponds to slower engine combustion rate [19, 88, 100]. The turbulent mixing time response to valve timing, can be explained by looking at u' values. Since all attributes, but valves timing, were held constant, the energy introduced in the engine, during the intake stroke, is equal for all three cases. However, difference valve timing showed a variation in the turbulence production during the intake stroke, as shown by u' values. Consequentially, a change in the flow energy, associated to the large tumble eddy after IVC timing, is observed. Results show that u' converges to a single value of about 1.4 m/s at TDC. Therefore, the observed difference in τ_t 's magnitude, is due to the increased viscous effect in the cylinder volume, caused by different intake backflow magnitudes. Moreover, results show that the turbulent mixing time shape against the crank angle, is not significantly affected by different valve timing. This can be verified using the procedure presented in Paragraph 5.2. Figure 39 shows that, polynomial coefficients' value of the 4th grade polynomial curves fitted to τ_t from different valve timing are comparable. Error bands correspond to the standard coefficients' error calculated with a 95% confidence interval. Figure 40 shows a comparison between turbulent mixing time values, predicted using a single 4th grade polynomial fitted to the CFD derived turbulent mixing time of “valve timing 1”, and the CFD derived mixing time values for each explored valve calibration.

Figure 39: Polynomial coefficients' value of the 4th grade polynomial curves fitted to the turbulent mixing time from different valve timing. Error bands correspond to the standard coefficients' error calculated with a 95% confidence interval

Figure 40: Comparison between CFD derived τ_t and mixing time values derived using a single 4th grade polynomial curve, fitted to τ_t at for valve timing 1. Y-intercept coefficients' values changed for each speed.

Figure 41: Predicted scalar mixing time profiles, τ_{SRM} (left axis) vs 3D CFD predicted turbulent mixing time profiles, τ_t (right axis) for different valve timing. Valve timing data refers to key points 1,2 and 3 in Table 3.

Figure 41 shows the scalar mixing time response to valve timing, predicted by using Equation 30, Equation 31a and Equation 32.

6.1.2 Engine Speed

Figure 42: Engine A CFD prediction of different engine speeds effect on the in-cylinder mean flow velocity (graph A) and turbulence intensity (graph B).

Figure 42 shows the non-combusting CFD prediction results of the main in-cylinder mass-averaged turbulence characteristics, for two different engine speeds, at constant valve timing for Engine A. Data at 2000rpm corresponds to Key point 1 in Table 3, while data at 5500rpm do not represent any available test data. To investigate solely the effect of different engine speeds, on the in-cylinder turbulence, it was decided to carry out a CFD calculation characterising Key point 1 valve timing but with higher engine rotational speed. For clarity, detailed valve timing used in the analysis, are reported in all figures. Results show that, the in-cylinder turbulence characteristics proportionally change with the engine speed. In-

cylinder turbulence intensity, u' , and mean flow velocity are expected to increase with engine speed, due to higher intake charge flow [13, 15].

Figure 43: Engine A 1-D Intake and Exhaust mass flow for different engine speeds

The effect of different engine speeds, on the 1-D predicted intake port velocity, is shown in Figure 43. Intake flow port velocity start increasing after IVO timing for all engine speeds. Results characterised by the higher engine speed show an initial velocity drop before 450 °CA ATDC(F). This is caused by the flow fluctuations in the intake manifold due to the pressure difference between the cylinder and the manifold [1]. The same drop can be noticed in the CFD predicted mean flow velocity and turbulent intensity, u' . The intake port velocity, at the higher engine speed case, showed lower intake backflows occurring at IVC timing. At a given crank angle, higher engine speed, results in an intake charge flow characterised by a higher momentum, and, thus, in lower intake backflows. The effect of different engine speeds on the turbulent mixing time is shown in Figure 44. Higher engine speeds correspond to lower τ_t 's magnitudes, which result in faster engine combustion rates [100]. The turbulent mixing time's shape at 5500rpm, against the crank angle, compared to the lower engine speed, does not show the sudden drop close to IVC timing. This is due to the lower intake

backflow, which result in lower turbulence dissipation, ϵ , during the closing of the valve. Instead, the same drop, occurring at EVO timing, is shown at all engine speeds.

Figure 44: Engine A CFD prediction of different engine speeds effect on the Turbulent Mixing Time

Results show that engine speed, has an insignificant effect on the overall turbulent mixing time shape against the crank angle. This can be verified following the procedure presented in Paragraph 5.2. Figure 45 shows that, polynomial coefficients' value of the 4th grade polynomial curves fitted to τ_t from the two engine speeds are comparable. Error bands correspond to the standard coefficients' error calculated with a 95% confidence interval. Figure 46 shows the comparison between CFD derived τ_t and mixing time values derived using a single 4th grade polynomial curve, fitted to τ_t at 2000rpm. Y-intercept coefficients' values changed for each speed. The effect of different engine speeds, on engine B and C's

turbulent mixing time, τ_t can be found in the appendix. Results show that, the observed changes in the turbulence characteristics are proportional to the engine speed.

Figure 45: Polynomial coefficients' value of the 4th grade polynomial curves fitted to the turbulent mixing time from different engine speeds. Error bands correspond to the standard coefficients' error calculated with a 95% confidence interval.

Figure 46: Comparison between CFD derived τ_t and mixing time values derived using a single 4th grade polynomial curve, fitted to τ_t at 2000rpm. Y-intercept coefficients' values changed for each speed.

6.1.3 Start of Injection Timing

The Start of Injection (SOI) timing corresponds to the time at which the fuel is injected in the cylinder in respect to the piston position. Phasing the injection timing in a gasoline engine, is a key attribute that governs the combustion efficiency and pollutant emissions. Often, in port fuelled engines, due to the low fuel rail-pressure, the injection starts prior the

intake valve opens and continues through the intake stroke, improving the air and fuel mixing.

The data presented in this paragraph correspond to key point 2 and 3 in Table 9. All engine parameters, including fuelling and valve timing, with the exception for the SOI, were held constant. Figure 47 shows the effect of different SOI timing on the CFD predicted flow velocity vectors. Late injection timing results highlight the flow acceleration due to the fuel injection at BDC. This is caused by the fuel injection continuing after BDC. Later, at 590 °CA ATDC(F), retarded SOI timing results in higher in-cylinder flow speed. This is due to the shorter time available to dissipate the energy associated with fuel injection. Therefore, during the closed part of the engine cycle, greater intake flow momentum is associated with retarded SOI timing. Engine fuelling, including the fuel injection period, was held constant for investigated SOI timing. Thus, the same energy is introduced in all analysed cases. Consequentially, during the closed part of the cycle, increased turbulence production, is necessary to dissipate the higher air-fuel charge flow momentum resulting from retarded SOI timing.

Figure 48 shows the predicted effect of different SOI timing, on the turbulent mixing time, τ_t . The effect on the turbulent kinetic energy, k , and the turbulence dissipation, ε is available in the appendix. Results show that, retarded SOI timing, at a given engine speed, load, valve timing and fuelling including duration, result in higher turbulence production. Thus, at the explored conditions, retarded SOI timing result in lower turbulent mixing time's magnitude, which corresponds to higher in-cylinder turbulence production. However, since the fuel injection characteristics *e.g. the spray pattern*, are held constant, the overall in-cylinder flow development, against the crank angle, is not influence by different SOI. Figure 49 shows coefficients' values of the 4th grade polynomial curves fitted to the turbulent mixing time from different SOI timing (see Paragraph 5.2). Results show the similarity between different coefficients indicating that the shape of the two curves, against the crank angle, can be described with the same curve. The effect of different SOI timing is described by the difference in the “y-intercept” coefficient.

Figure 47: Comparison of the CFD predicted velocity flow vectors for two different SOI timing

Figure 48: CFD prediction of engine D's turbulent mixing time for different start of injection timing

Figure 49: Polynomial coefficients' value of the 4th grade polynomial curves fitted to the turbulent mixing time from different SOI. Error bands correspond to a 95% confidence interval.

The developed scaling factor correctly predicts the change in the turbulence characteristics for engine attributes that affect the intake charge velocity, predicted by the 1-D engine system code. However, in a direct injected engine, such as engine D, the 1-D intake port velocity prediction results are not affected by different SOI timing. For given engine operating condition and fuelling, 1-D engine system codes do not capture the difference in the mixing process due to different SOI. Thus, if the SOI timing effect on the engine performance is the only attributes analysed, Equation 31b, must be used to predict the in-cylinder turbulence change to SOI. CFD in-cylinder velocity vector analysis results showed that, for given operating conditions, including the injection duration, different SOI timing affect the air and fuel mixing process. Difference the in-cylinder turbulence is due to the shorter time available to dissipate the energy associated with the fuel injection. The

correlation assumed in Equation 31b empirically reproduces the effect of reduced time on the energy dissipation. Scalar mixing times, τ_{SRM} , at different SOI timing show the same trend shown in the CFD derived turbulent mixing times. However, it is important to point out here that, the empirical correlation described in Equation 31b, does not model but accommodates the change in the physics governing the turbulence formation. The correlation is used to predict solely the effect of different SOI timing on the in-cylinder turbulence which are not captured by 1-D engine system codes. Moreover, the fuel injection timing is a characteristic that is investigated during late phases of engine development and not during the early concepts screening phase. If the SOI timing are explored, engine fuelling data and burning from the first prototype are available and can be used as input for the 1-D engine system code to improve the model's results accuracy.

Figure 50: Derived scalar mixing time for different start of injection timing

Figure 50 shows the effect of different SOI timing, on the scalar mixing profiles derived with Equation 31b and Equation 32. Results show that, at a given engine operating point, retarded injection timing are related to lower scalar mixing time's magnitude. Thus, faster engine combustion rates will be predicted when retarding the injection timing from a baseline value.

6.2 ENGINE DESIGN EFFECT

The effect of different intake manifold design, air induction systems, bore to stroke ratios and injector types, on the in-cylinder turbulence characteristics, predicted by the 1-D engine system and CFD codes, will be presented in the following paragraphs.

Firstly, in Paragraph 6.2.1 engine A's turbulence characteristics will be compared with engine B and C's characteristics. The intake port design is a factor known to influence the generation of tumble during the intake stroke [111]. For instance, the inclination of the intake charge flow, in respect to the engine crank axis, can change with the port geometry and influence the angular momentum associated to the intake charge. Thus, the effect of different engine design, on the in-cylinder turbulence generation, is a key factor that need to be considered during engine development. Later, in Paragraph 6.2.2 engine A's design will be used as baseline to investigate the effect of different bore to stroke (B/S) ratios on the in-cylinder characteristics. For instance, recent SI engines, to increase the engine knock tolerance, are designed with B/S ratios below the unity [112, 113]. Smaller bore sizes shorten the distance to be covered by the flame to consume the fresh charge, resulting in less time available to the autoignition chemical reactions. Lastly, in Paragraph 6.2.3, the effect different injectors on engine D's in-cylinder turbulence characteristics will be shown. Different injection patters can enhance the air-fuel mixing and thus change the in-cylinder turbulence.

6.2.1 Engine Variant Effect on In-Cylinder Turbulence

In this paragraph, the in-cylinder turbulence characteristics of three different engine concepts, will be discussed. Engine A, B and C experimental data will be used for this analysis. The major difference between engine A, and the other two engine concepts, is a bore reduction while holding the B/S ratio constant, and a change in the intake manifold design. Full engines geometrical details are available in Chapter 3. Operating points, characterised by constant engine speed and load, were used for this analysis (see Key point 1 in Table 3, Table 5 and Table 7). Experimental valve timing, corresponding to the selected operating points, are reported in all figures.

Figure 51: CFD prediction of different engine variants effect on in-cylinder mean flow velocity (graph A), turbulence intensity (graph B) and tumble ratio (graph C).

Figure 51 shows the mean in-cylinder velocity, turbulence intensity and tumble of all engine variants. Engine A's turbulence characteristics analysis was previously presented in

Paragraph 6.1. CFD predicted in-cylinder mean velocity results show that, engine B and C's velocity are characterised by a rapid acceleration, after IVO timing and before TDC. The increased velocity shown in the results, is due to the intake backflow occurring towards the final part of the exhaust stroke, while the piston is moving towards TDC and the intake valves open. Once the piston reached TDC, engine B and C intake backflow's magnitude decreases due to the piston moving downwards. This causes a balance in the relative pressure difference between the intake manifold and the in-cylinder volume, resulting in a sudden drop of the in-cylinder tumble's magnitude. Moreover, the higher mean piston speed (MPS), caused by engine B and C's stroke (8% longer compared to engine A) results in a faster intake charge flow acceleration after TDC. The difference in engine A's mean velocity formation of engine A, compared to the other two engine variants, is determined by a difference in the intake valve opening event. Engine A has the most retarded IVO, therefore, the sudden velocity formation after IVO timing, followed by a steep flow deceleration, occurs later compared to the other two engine variants. As the piston moves downwards towards BDC, the in-cylinder mean velocity of all engine variants, start decreasing with a similar rate between the three cases. Results show that, the higher MPS has a clear effect during the compression stroke, with engine B and C having greater flow acceleration, compared to engine A.

The turbulence intensity results, u' , available in Figure 51b show that, engine B and C are characterised by a lower turbulence intensity generation during the initial part of the intake stroke. This suggests that the intake port design fitted on engine B and C, promotes the organised, large eddy tumble structure. Lower u' values during the initial part of the intake stroke, indicate a more structured motion of the charge flow. This effect can also be seen in the intake flow velocity vectors, shown in Figure 52. Results highlight a more structured tumble flow for engine B and C. Results shown in Figure 51c confirms that, the intake port design has a significant effect of the tumble generation. Engine B and C intake port layout, compared to engine A's, was designed to maximise tumble generation. Tumble decay, during the last stage of the intake and the initial part of compression strokes, is mainly driven by the piston movement, and no clear effect of the different intake port design is shown.

Figure 52: CFD predicted intake flow velocity vectors comparison of engine A (left graph), engine B (middle graph) and engine C (right graph) at 2000rpm_40Nm.

Figure 53: 1-D Intake port velocity for different engine variants.

Figure 53 shows that the 1-D engine code predicts similar intake port velocity for all the three engine variants, during the intake stroke. Engine B and C results show initial intake backflow, occurring before non-firing TDC, due to early IVO timing. Moreover, results show negligible intake backflow, compared to engine A values, occurring during the intake valve closing. This difference can also be seen in the tumble formation during the compression stroke. Peak tumble levels, generated during the compression stroke for engine B and C, show similar values to their corresponding peaks, generated during the intake. Engine A, instead, generates lower peak tumble values during compression, due to the intake backflow, occurring close to the IVO timing. Thus, the higher-pressure difference at the

intake valve of engine A, generates greater intake back flows and increased viscous stresses. This causes the dissipation of the flow energy which destroys the intensity of the tumble vortex. The effect of different engine variant, on the average turbulent mixing time, defined in Equation 29, during the compression and expansion strokes, is shown in Figure 54.

Figure 54: CFD prediction of different engine variants effect on the turbulent and scalar mixing time, τ_t and τ_{SRM} .

In-cylinder turbulent kinetic energy, k , increases with the piston moving towards TDC, following the turbulent intensity profile (see Figure 51c). As the piston moves towards firing TDC, viscous stresses become more significant, increasing the dissipation of flow energy into heat. Engine B and C are characterised by steeper tumble decays. Thus, greater turbulence is generated during the compression stroke [7]. The steeper tumble decay, of engine B and C, is due to the more compact engine head geometry, compared to engine A, which increase the tumble vortex stretching. The effect the smaller bore size, associated to higher tumble stretching, can also be seen in the increased engine B and C's turbulent intensity during the intake stroke. Modern SI engines generate a bulk in-cylinder tumble motion with a given vortex radius larger than the engine clearance. Thus, the bigger tumble vortices generated by engine B and C, result in greater in-cylinder turbulence formation and consequentially, lower turbulent mixing time profile, τ_t (see Equation 29). Moreover, since the in-cylinder flow development has changed due to the different intake port design, the resulting turbulent mixing time's shape, against crank angle, changed between engine A and B. Instead, the turbulent mixing time's shape difference between engine B and C is due to the boosting system which impact on the in-cylinder turbulence development. Thus, the 3-D effect of different geometry and boosting systems need to be captured.

Figure 54 compares CFD predicted turbulent mixing times and the corresponding scalar mixing times.

6.2.2 Bore to Stroke Ratio Effect on In-Cylinder Turbulence

In this section the effect of different B/S ratios on the in-cylinder turbulence characteristics is analysed. Table 13 shows the virtual test matrix used to analyse the effect of different bore to stroke ratios on the average in-cylinder turbulence characteristics.

Table 13: CFD virtual engine configurations test matrix to study the effect of different bore to stroke ratios on the in-cylinder turbulence

Case	Operating Point	Δ Stroke [%]	Δ Bore [%]	Bore to Stroke	C.R.	Swept Vol.[l]	Δ Swept Vol. [%]	Δ Vol. @TDC. [%]	Intk. Port variant
1	2000rpm_40Nm	-	-	0.94	11.5:1	0.22	-	-	A
2		+13		0.83	11.5:1	0.25	+13%	+14%	
3		+34		0.70	11.5:1	0.29	+32%	+23%	
4		-	-3.9	0.94	11.0:1	0.20	-9%	-	
5		+8		0.83	11.6:1	0.22	-	-	
6		+27		0.70	12.8:1	0.26	+18%	-	

The investigation was carried out with engine A's geometry (see Table 2). The piston top height at TDC position was kept constant for all the cases in Table 13. Three different B/S ratios equal to 0.94, 0.83 and 0.70 were investigated. The compression ratio for case 1, 2 and 3 was kept equal to 11.5:1 while the stroke length was increased resulting in a volume change at TDC. To maintain a constant compression ratio, the engine deck diameter for case 2 and 3 needed to be adjusted at each investigated stroke as shown in Figure 55. Furthermore, the effect of different strokes was investigated on a more compact combustion chamber, corresponding to a 3.9% reduction in engine bore compared to case 1. The compression ratio for case 4,5 and 6 in Table 13 was varied while the volume at TDC was held constant for each explored stroke.

Figure 55: Change in the engine deck diameter necessary to maintain a constant compression ratio of 11.5:1 for different bore to stroke ratios.

Case 1 in Table 13 is the equivalent of Key point 1 of engine A. All other cases do not correspond to any commercially available combustion system. The non-combusting CFD analysis was carried out to investigate the sensitivity of different bore and stroke lengths on the in-cylinder turbulence and the resulting effect on the engine combustion rate. The engine speed, load, valve timing and all other CFD model inputs but geometrical features were held constant for all cases. Results in Figure 56a show that, similar mean flow velocities are generated during the intake stroke for all the investigated cases. After an initial decay corresponding to EVC timing, the mean flow velocity of all cases, starts increasing until around 420 °CA ATDC(F). Albeit valve timing were the same for all the cases, velocity profiles of Case 2 and Case 3 start increasing later, at around 380 °CA ATDC(F). Velocity vectors analysis showed initial intake backflows occurring at 360 °CA ATDC(F) (see the Appendix). Prolonged intake backflows, until around 370 °CA ATDC(F) are generated for Case 2 and Case 3, due to bigger clearance volume, which resulted in a pressure difference between cylinder volume and the intake manifold port. This causes the initial delay in the mean flow velocity formation, shown in the results in Figure 56a. Increased stroke lengths, result in higher MPS values, that, for given engine clearance volume, contrast the effect of negative backflows, occurring close to IVO and EVC, and promote the in-cylinder intake flow acceleration. Thus, the increased clearance volume of case 2 and 3, compared to the baseline case 1, reduce the longer stroke positive effect. Comparison between case 4,5 and 6, characterised by constant clearance volume, shows earlier velocity formation as the stroke is increased (see Figure 56a). Mean flow velocity increases for all cases, as the piston moves closer to firing TDC, with peak values around 660 °CA ATDC(F).

Figure 56: CFD prediction of different bore to stroke ratios effect on in-cylinder mean flow velocity (graph A) and tumble ratio (graph B)

Higher peak velocity values are reached with longer strokes due to higher MPS. Results in Figure 56b show that tumble profiles broadly follow the mean in-cylinder velocity trends during compression and intake strokes. The negative back flow, occurring at EVC due to bigger clearance volume for Case 2 and Case 3, is affecting the initial tumble formation. Negative flow occurring with increased stroke, cause an initial reduction in the mean flow velocity along the tumble axis. Case3 shows a significant lower tumble formation throughout the intake stroke. Similar effect can be noticed comparing Case 2 with Case1. Increased clearance volume of Case 2 and 3, necessary to keep the CR constant with different B/S ratios, causes this effect. The intake port layout was held constant during this part of the study. The layout was designed to contribute in the intake tumble motion generation. Thus, the bulk in-cylinder tumble motion is generated with the same given radius but within a bigger clearance volume for case 2 and 3. This, results in a less structured tumble vortex as shown in Figure 57.

Case1, 480 CA °ATDC(f)

Case3, 480CA °ATDC(f)

Figure 57: CFD prediction of different bore to stroke ratios on in-cylinder flow velocity at vectors at 480 °CA ATDC(F).

The same effect of increased clearance volume can also be noticed in k and u' formation during the intake stroke (see the Appendix). However, comparison for cases with constant

clearance volume (cases 4,5 and 6), show that longer stroke advances tumble generation during the initial part of intake stroke, increasing the rate of tumble formation (see Figure 56b). Furthermore, results show that longer stroke, associated to higher MPS, generates overall higher tumble level towards firing TDC. The effect of different B/S ratios on the turbulent mixing time defined in Equation 29, during compression and expansion strokes, is shown in Figure 58a.

Figure 58: CFD prediction of different bore to stroke ratios effect on the turbulent mixing time τ_t (graph A). Scalar mixing time for different bore to stroke ratios derived using turbulence scaling factor response (graph B).

Initial drop seen in the τ_t profiles results, at around 580 °CA ATDC(F) is due to the IVC timing and the corresponding ε generation [114]. Increased k and ε at EVO timing are instead the reason of the sudden drop in the turbulent mixing time profiles, occurring during the late part of the expansion stroke. Results show that, different B/S ratios modify the τ_t shape profile since the overall engine design changed with different B/S ratios. Moreover, comparison between cases with constant bore size (e.g. Case 1,2 and 3) shows that increased stroke results in lower τ_t profiles, corresponding to greater level of in-cylinder turbulence during the combustion. The SRM turbulent flame speed calculation is proportional to τ_t . Thus, as expected, longer strokes would result in faster combustion duration while the engine bore is held constant thanks to higher MPS [114, 115]. Moreover, cases with smaller bore (Case 4,5 and 6) show higher τ_t profiles compared to the baseline Case1. Those, for given

engine operating condition, the turbulent mixing time profiles, derived from CFD calculations, will result in higher engine knock tolerance for the engine cases with smaller bore [88, 100, 112]. The main objective of this analysis was to assess the capability of the turbulence scaling factor response to provide the SRM with correct input for different B/S ratios during the early screening of different combustion system configurations. Non-combusting CFD results in Figure 58a confirmed that turbulence characteristics are dependent to the given engine geometry. Non-combusting CFD calculation at each of the explored engine variant is therefore required to capture turbulence characteristics changes as explained in Chapter 5. However, a hypothetical scenario, for which only a single CFD engine variant model was available, was carried out. Engine A Key point 1 turbulent mixing time profile was used as baseline turbulence characteristic to derive the necessary turbulence input for different B/S ratios. Figure 58b shows the corresponding scalar mixing times calculated with Equation 30, Equation 31 and Equation 32. 1-D intake port velocity profiles for different B/S ratios, used to manipulate baseline τ_t profile are available in the appendix. Necessary pre-defined burn rates within the 1-D engine system model, calibrated to match engine performance of Case 1, were not changed for different B/S ratios. Results in Figure 58b show similarities across CFD predicted turbulent mixing times and corresponding scalar mixing times. Increasing the stroke length, while holding the bore size constant results in greater in-cylinder turbulence, thus, lower τ_{SRM} profile. Moreover, comparing cases with similar B/S ratios (e.g Case 2 and Case5) shows that more compact engine variant result in lower in-cylinder turbulence during combustion, thus, higher τ_{SRM} profile. Thus, improved engine knock tolerance, compared to cases with bigger bore would be predicted by the SRM [19, 100].

6.2.3 Injector Effect on In-Cylinder Turbulence

In this paragraph, the effect of different spray patterns, at constant engine speed, load and fuelling, on the in-cylinder turbulence of a Direct Injected gasoline engine, will be investigated. Key point 1 and key point 4 presented in Table 9 will be used. Differences in the two injector designs is available in Paragraph 3.4. Injector labelled as “injector B”, due to the fuel spray patterns, designed to be aligned to the main bulk in-cylinder charge flow, is expected to increase the flow momentum, and consequentially, the in-cylinder turbulence production. Figure 59 shows the predicted CFD spray patterns for the two injectors during the intake stroke. Injector B introduces the fuel along the bulk intake charge flow axis,

increasing the intensity of the structured tumble motion. (see Paragraph 3.4 for injectors' holes layout)

Figure 59: Injector A and B' spray patterns comparison

Results in Figure 60 show that, engine D fitted with injector B, reaches higher tumble levels during the intake stroke, after the SOI timing, compared to injector A. Moreover, injector B is associated to higher tumble peak levels, during the compression stroke. However, tumble levels of both injectors, converge to a similar value towards firing TDC. During the closed part of the cycle, the higher flow energy associated with injector B, is dissipated faster than the flow energy associated with injector A.

Figure 60: CFD prediction of the effect of different injector types on the in-cylinder tumble.

Results in Figure 61 show the resulting effect of the different spray patterns on the turbulent kinetic energy production (see graph A) and the turbulence dissipation rate (see graph B), during the closed part of the engine cycle. To ensure that the observed change in the turbulence characteristics was only caused by the different injector hardware, CFD boundary conditions, including fuelling, were kept constant between the two injectors. For a given engine speed and load, injector B shows higher k production and consequentially, higher turbulence dissipation rate, ε . The turbulent mixing time profile of injector B, compared to injector A, will therefore have a different shape against the crank angle (see Figure 61c). Following the procedure presented in Chapter 5, faster engine combustion rates, will therefore be predicted for injector B, compared to the engine burning characteristic of injector A at any given operating condition.

Figure 61: CFD prediction of the effect of different injector types on the turbulent kinetic energy production (graph A), the dissipation rate (graph B) and the turbulent mixing time (graph C) during the closed part of the engine cycle.

6.3 CONCLUSIONS

Results presented in Paragraph 6.1 showed that, the turbulence characteristics' shape of a given engine geometry, against the crank angle, was not significantly affected by different

operating points. Moreover, it was shown that, different operating conditions affect the turbulence characteristics' magnitude. The change in the characteristic' magnitude was shown to be proportional to the intake port velocity. Later, in Paragraph 6.2, the effect of different engine design on the in-cylinder turbulence characteristics was discussed. It was confirmed that the turbulence characteristics' shape, against the crank angle, is function of the engine geometry. Moreover, it was shown that the intake flow charge speed is the physic that governs the change in the in-cylinder turbulence. A summary of the CFD analysis results is shown in Table 14.

Table 14: Summary of the in-cylinder turbulence analysis

Change in	Effect on in-cylinder turbulence during intake and compression	Effect on turbulent mixing time (τ_t) during closed part of the cycle	Conclusions
Valve timing	<ul style="list-style-type: none"> Increased valves backflows result in greater in-cylinder flow viscous stresses Viscous stresses increase turbulence generation Higher turbulence generation reduces the bulk flow energy 	<ul style="list-style-type: none"> τ_t magnitude is function of the energy in the flow Changes in the flow energy are function of the intake flow speed The large-scale air-motion, that characterises the shape of τ_t against the crank angle of is not affected by different valve timing 	<ul style="list-style-type: none"> The intake flow speed is the physics that governs the in-cylinder turbulence generation The large-scale in-cylinder motion is not affected by valve timing during the closed part of the cycle The effect of different valve timing on τ_t can be predicted scaling a known τ_t curve on the intake flow velocity derived from a 1-D analysis.
Engine Speed	<ul style="list-style-type: none"> Turbulence generation is proportional to the engine speed Higher engine speeds correspond to higher flow kinetic energy 	<ul style="list-style-type: none"> τ_t magnitude decreases as the engine speed increases The large-scale air-motion is not affected by different engine speeds 	<ul style="list-style-type: none"> The large-scale in-cylinder motion is not affected by the engine speed during the closed part of the cycle The effect of different engine speeds on τ_t can be predicted scaling a known τ_t curve on the intake flow velocity derived from a 1-D analysis
SOI	<ul style="list-style-type: none"> The bulk flow kinetic energy is affected by SOI Retarded SOI increase the intake charge momentum 	<ul style="list-style-type: none"> Higher kinetic energy is available in the bulk flow when SOI is retarded τ_t magnitude decreases as SOI is retarded The large-scale air-motion is not affected by different SOI 	<ul style="list-style-type: none"> The large-scale in-cylinder motion is not affected by different SOI during the closed part of the cycle Empirical correlation to predict changes in τ_t to SOI developed
Engine variant: <ul style="list-style-type: none"> Bore to Stroke Intake manifold Injector Turbocharger 	<ul style="list-style-type: none"> The large-scale air motion is affected by the engine variant Port design can improve tumble motion and reduce the energy dissipation Longer stroke generates more turbulence due higher MPS Turbocharger has no clear effect on the in-cylinder turbulence 	<ul style="list-style-type: none"> Change in all investigated engine variants affect the large-scale air flow motion 	<ul style="list-style-type: none"> Changes in all investigated engine variants affect the large-scale air motion throughout the engine cycle CFD analysis required to derive τ_t for each explored engine variant

7 COMBUSTION PREDICTIONS COMPARISON WITH EXPERIMENTAL DATA

In this chapter, burn angle results, predicted by the SRM code will be presented. Firstly, the SRM code will be tuned on a single operating point from engine A's map. Later, engine B and C, development concepts of the baseline engine A, will be used to assess the methodology capabilities to predict the engine RoHR for different engine design. Lastly, the SRM code will be tuned on a single operating point of engine D's map. Combustion prediction results for two different injectors, at different operating conditions, will be compared with experimental combustion data. Predicted combustion results were assessed using the two metrics presented in Paragraph 1.4.2. Black error bands, showing the experimental standard variation, are applied to all the figures. Red error bands represent the ± 2 °CA confidence interval.

7.1 COMBUSTION PREDICTIONS COMPARISON WITH EXPERIMENTAL DATA FROM DIFFERENT ENGINE MAPS

7.1.1 Engine A

Valve Timing Effect on the Engine Burn Angles

In this part of the paragraph experimental test data corresponding to Key points 1, 2 and 3 in Table 3 are compared to the engine burn angles predicted by the SRM. The chosen experimental data corresponds to a valve timing optimisation sweep, carried out at constant engine speed and load. The same data was previously used for the CFD analysis presented in Paragraph 6.1.1. Experimental data corresponding to Key point 1 (2000rpm_40Nm) will be considered as the baseline operating point for the following analysis. Engine A's burn rate predictions, at different engine speeds are reported in the appendix.

Boundary conditions at IVC timing and engine fuelling were extracted from the 1-D engine system code and applied to the SRM. In this thesis the 1-D and the SRM codes were not run in co-simulation. Thus, an extra combustion model, within the 1-D code, needed to be selected to initialise the 1-D analysis and derive the initial boundary conditions for the SRM code. Burn angles predicted by the SRM were later manually imposed as input to the extra

combustion model. In the future, the two codes would run in parallel and the extra combustion model will be no longer necessary. The chosen combustion model within the 1-D code was based on the empirically derived Wiebe equation (presented in Paragraph 1.2.3). Experimental burn angles from key point 1 in Table 3 were used to tune the combustion model and allowed to provide the SRM with the initial boundary conditions.

The turbulent mixing time, τ_t , derived from the non-combusting CFD calculation at Key point 1 was scaled accordingly to the methodology presented in Paragraph 5.2. The initial $C_{SRMBaseline}$ multiplier and the SRM ignition timing were iteratively calibrated to match the engine load at the chosen operating point. A value of the $C_{SRMBaseline}$ multiplier equal to 9.5 was found. This resulted in a difference between the experimental spark and the chosen SRM ignition timing of 10 °CA (see Figure 62). The SRM ignition timing physically corresponds to the crank angle at which the flame kernel is fully developed, and the actual flame front starts propagating. This difference can be referred to the mixture ignition delay period (see Paragraph 4.3.6). Once the SRM was tuned, the in-cylinder turbulence response to different valve timing was predicted following the procedure presented in Paragraph 5.4 and briefly reported here. The engine burn rate at different valve timing, necessary to initialise the combustion model within the 1-D code, was held constant throughout the sweep.

Figure 62: Experimental spark and SRM input timing comparison for different valve timing

Figure 62 shows the difference between the experimental spark and the predicted SRM ignition timing, at different valve events. Results are comparable to experimental ignition delays found in [109, 110] at similar operating conditions. Late intake valve events, such as key point 3, compared to the baseline valve timing, corresponded to retarded experimental spark timing. The non-combusting CFD analysis showed that late intake valve events result

in higher τ_{SRM} magnitudes. Consequentially, late intake valve events result in slower combustion rates. This is due to the direct relation between the τ_{SRM} and the flame propagation calculation in the SRM code. Results in Figure 62 show a discrepancy in the experimental spark and the SRM ignition timing. The experimental spark timing at key point 3 was retarded of about 2 °CA compared to key point 1. Instead, at key point 3, the SRM ignition timing was advanced of 1 °CA compared to the baseline SRM ignition timing. This is due to experimental uncertainties in the combustion results of key point 3. Since the engine was operated at the Maximum Brake Torque (MBT) timing, at a given engine speed and load operating point, retarded experimental spark timing should correspond to longer engine burn duration (CA 10-90) [1, 4]. Instead, key point 3 burn duration was shorter than the baseline key point.

Figure 63: Predicted and experimental CA50 (graph A) and burn duration, CA10-90 (graph B) for different valve timing. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red error bands.

Results in Figure 63 show that, the predicted SRM ignition timing allowed to predict engine burn rates at different valve timing within the experimental standard deviation (black error bands) and the ± 2 °CA confidence interval from the experimental burn angle target (red error bands). The experimental data, selected for this analysis, was characterized by small valve timing adjustments, for given engine speed and load. Small changes in the predicted CFD bulk turbulence characteristics and 1-D intake port velocity profiles were observed for different valve timing. Despite this, the methodology successfully discriminated the engine burn rate for different valve timing. Moreover, the experimental data was acquired over a two days test campaign, aimed to optimise the engine valves phasing. Therefore, the influence of others external parameters, (e.g. hardware replacements), and possible experimental sources, (e.g. sensors re-calibration), on the observed burn angles can be considered minimised. A good in-cylinder pressure match for all investigated key points was achieved (results are available in the appendix).

Intake Charge Dilution effect on the Engine RoHR

In this part of the paragraph the experimental data corresponding to Key points 4, 5 and 6 in Table 3 is compared to the engine burn angles predicted by the SRM. Test data selected for this analysis corresponds to an intake charge dilution (EGR rate) sweep, characterised by constant engine speed fuelling and valve timing. Reported EGR rates refer to total EGR rates extracted from the 1-D engine system code. Engine burn rate predictions, for the other available intake charge dilution sweeps in Table 3 are available in the appendix.

Figure 64: Predicted and experimental burn duration, CA10-90 for different charge dilution. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red error bands.

The predicted burn angle response to charge dilution, for given constant engine speed and valve timing, are shown in Figure 64. Predicted results show that higher EGR ratios correspond to longer burn durations, CA 10-90. The experimental spark timing, at different EGR rates, were adjusted to keep the CA 50 angle constant. Thus, the SRM ignition timing had to be adjusted accordingly to keep CA 50 close to a constant value and to match the desired engine load (see Figure 65). Results show that predicted burn durations followed the experimental data trend and fell within the two assessment criteria.

Figure 65: Experimental spark and SRM input timing comparison for different charge dilutions.

Engine Speed effect on the Engine RoHR

In this part of the paragraph, experimental test data corresponding to Key Points 3, 11, 16 and 21 in Table 3 are compared to the engine burn angles predicted by the SRM. The data reported here is characterised by changes in engine speeds, load, valve timing and EGR rates. Engine burn rate predictions, of all other operating points in Table 3 is available in the appendix.

Figure 66: Experimental spark and SRM input timing comparison for different engine speeds and valve timing.

The difference between the experimental spark and SRM ignition timing for different engine speeds is shown in Figure 66. SRM ignition timing followed the experimental spark timing trend, with a constant difference between the two values of around 7.5 °CA. Results show that, at 3500 rev/min the difference between the experimental spark and the SRM ignition timing was reduced to 5.5 °CA. The SRM ignition time at 3500 rev/min (Key Point 16) had to be further advanced to match the targeted engine load. This earlier SRM ignition timing resulted in an early CA10 prediction, falling outside the experimental standard deviation (see Figure 67a). Nonetheless, CA10 prediction for Key Point 16 falls within the ± 2 °CA confidence interval target. The effect of advanced ignition timing can also be seen for the CA10-90 prediction (see Figure 67b). Results for different speeds and valve timing show good agreement with test data suggesting that the assumed correlation between intake port velocity and τ_{SRM} is valid at the explored engine conditions.

Figure 67: Predicted and experimental CA10 (graph A) and CA10-90 (graph B) for different engine speeds and valve timing. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red error bands.

Engine burn rate prediction for different Bore to Stroke ratios

In this part of the paragraph, the effect of different B/S ratios on the engine burn duration (CA 10-90) and knock tolerance, will be discussed. Among the various parameters that can be explored during development, the bore to stroke (B/S) ratio, is one of the most important characteristics affecting the fuel efficiency of SI engines [112]. Depending on the engine application an optimum B/S ratio can be determined [1, 3, 112, 115]. For instance, large B/S ratios improve the engine breathing and, at a given engine speed, reduce the mean piston speed (MPS) increasing the engine operating range. Increasing the stroke length results in faster MPS. Therefore, due to the higher mixture speed reached during the compression stroke, greater in-cylinder turbulence intensity is generated reducing the combustion

duration [115]. High-performance engines, characterised by elevated specific power output and high engine speeds, have B/S ratios that are greater than the unity. Small B/S ratios reduce the heat losses when the piston is close to TDC thanks to reduced piston surface to volume ratios. Moreover, the distance to be covered by the flame is shortened resulting in reduced engine heat losses. Reducing the bore diameter is an effective mean to suppress abnormal combustion processes. A more compact chamber geometry shortens the distance to be travelled by the flame front reducing the time available to the auto-ignition chemical reactions [13, 112, 115].

Table 15: Virtual test matrix

Case	Operating Point	Δ Stroke [%]	Δ Bore [%]	Bore to Stroke	C.R.	Swept Vol.[l]	Δ Swept Vol. [%]	Δ Vol. @TDC. [%]	Inlk. Port variant
1	2000rpm_40Nm	-	-	0.94	11.5:1	0.22	-	-	A
2		+13		0.83	11.5:1	0.25	+13%	+14%	
3		+34		0.70	11.5:1	0.29	+32%	+23%	
4		-	-3.9	0.94	11.0:1	0.20	-9%	-	
5		+8		0.83	11.6:1	0.22	-	-	
6		+27		0.70	12.8:1	0.26	+18%	-	

Case 1 (see Table 15) was used as baseline case for the following analysis. To replicate a real-life scenario, where one single CFD model is available due to the limited time, changes in the turbulence characteristics' shape, against the crank angle, were ignored. Thus, the turbulent mixing time shape of Case 1 was used as baseline shape to derive the scalar mixing time for the other cases. Predefined burn angles, necessary to initialise the 1-D engine system code, were left constant and equal to Case 1.

Figure 68: Prediction of different bore to stroke ratios on the engine burn rate and SRM ignition timing (graph A) and engine knock tolerance (graph B). Horizontal dashed line represents the engine knocking area limit.

Figure 68 shows the effect of different B/S ratios on the engine burn angles and SRM ignition timing (graph A) and load and knock index (graph B). The knock index is defined as the ratio between the heat release from the unburned and the burned zone, as proposed in [18, 19]. A value of around 15% was selected as threshold value. Index values above the chosen threshold would result in abnormal combustion [100] (see Paragraph 4.3.6). The SRM ignition timing of each explored B/S ratios was initially held constant at -14 °CA ATDC(F), corresponding to the ignition timing of Case 1. Later, for each B/S ratios, the SRM ignition timing was calibrated to operate the engine at the knock limit (see Figure 68). Results show that, shorter combustion durations are predicted by the SRM code when the stroke is increased, while the bore is held constant (e.g. burn duration comparison between Cases 1,2 and 3 Figure 68a). A combustion duration reduction, of about 25%, compared to the baseline

case, was observed when the stroke was increased of 34% (see combustion duration of Case 1 against Case 3). The shorter CA 10-90 is due to the higher MPS that is associated to longer stroke lengths and resulting in greater in-cylinder turbulence (see Paragraph 6.2.2). Moreover, to keep the knock index below the threshold value, the SRM ignition timing had to be retarded, as the stroke was increased. For instance, SRM ignition timing for Case 3, had to be retarded of 3 °CA compared to the baseline Case 1. Increased engine knock tolerance and burn duration comparable with the baseline case, was predicted when the bore length was reduced while holding the stroke constant (e.g. combustion duration comparison between case 1 and case4). The SRM ignition timing of case 4 had to be advanced of 1 °CA to maintain the engine at knock limit conditions. This is due to the more compact engine combustion chamber that suppress abnormal combustion processes thanks to the shorter time available for the auto-ignition reaction that is related to shorter distance to be covered by the flame to burn the fresh charge. Comparison between cases with the same B/S ratios (e.g. Case 3 and 6) shows improved engine knock tolerance for the case with smaller bore size. For instance, Case 6 is characterised by a longer stroke length and a smaller bore compared to the baseline Case 1. No adjustment to the SRM ignition timing for Case 6 was required to operate with the same knock index as Case 1. Moreover, cases with reduced bore to stroke ratios correctly predicted improved engine knock tolerance and faster combustion duration when the SRM ignition timing was adjusted accordingly. Results in Figure 68 follow the expected burn angles and knock tolerance trends for different B/S ratios. Heat transfer and friction losses changes to different B/S ratios were not considered.

7.1.2 Engine B

In this paragraph the experimental data shown in Table 5 (see Paragraph 3.2) will be compared to the engine burn angles predicted by the SRM code. The experimental data used for this analysis was characterised by relatively small burn duration variations going, from a minimum CA 10-90 of around 16 °CA, to a maximum value of around 26 °CA. Despite this limited variation, the methodology successfully discriminated the engine burn rate for different key points across the engine map. A single CFD calculation, at key point 1 in Table 5, was used to characterise the turbulent mixing time's shape against the crank angle. The value of the $C_{SRMBaseline}$ multiplier was held equal to the value previously defined during the tuning phase of engine A. Later, similarly to engine A, the 1-D engine system model of engine B, was used to analyse the change in the intake charge port flow velocity to the engine operating point (see Paragraph 5.4, Equation 31). Expected burn angles response to engine

speed and load, derived from previously developed engines, was used to impose necessary input to the Wiebe based combustion model necessary to initialise the 1-D code and derive the boundary condition for the SRM code. Finally, Equation 35 was used to predict the in-cylinder turbulence change throughout the engine map and derived the scalar mixing time input of engine B.

Figure 69: Experimental spark (circle symbols) and SRM input ignition input (triangle symbol) timing comparison for different engine speed and load.

Figure 69 shows the difference between the experimental spark and the predicted SRM ignition timing for different key points in Table 5. Results showed that the difference between the two scales is inversely proportional to engine speed and load. At high speed and load key points, shorter delay periods, and thus lower difference between the spark and the SRM timing, are expected due to higher in-cylinder turbulence [109, 110]. For instance, at 2000rpm_30Nm a difference of 10 °CA, between the experimental spark timing and the model ignition timing, was reduced to 0.5 °CA at 2000rpm_50Nm. This is due to the increased engine intake charge mass, necessary to achieve higher loads at a given engine speed, that results in greater in-cylinder turbulence. Thus, increased engine loads result in lower time for the spark kernel to develop into flame. Moreover, for a given engine load, increased engine speeds correspond to retarded experimental spark timing compared to the corresponding values at lower speeds. This is due to the increased overall in-cylinder turbulence, related to the higher engine mean piston speed, that draws more intake mass into the cylinder, as shown in the CFD analysis in Paragraph 6.1.2. Therefore, the engine speed

affects the spark kernel formation similarly to the engine load. A difference of 10 °CA, between the spark and the ignition timing, at 2000rpm_30Nm, was reduced to 4 °CA, at 3000rpm_30Nm. Chosen ignition timing in Figure 69, resulted in good agreement with the experimental burn duration CA10-90 as shown in Figure 70.

Figure 70: Engine B predicted and experimental burn duration, CA1090 (graph A), 1:1 results prediction line is represented by the dashed line. Error bands represent the average experimental standard deviation (graph A). Burn duration expressed in millisecond is shown in graph B.

Predicted combustion duration (CA 10-90) results, expressed in crank angles, for different key points in Table 5 are shown in Figure 70a. Burn angle predictions and predicted in-cylinder pressure traces, for difference operating conditions, are available in the appendix. Combustion duration predictions expressed in milliseconds are shown in Figure 70b. Expressing error between predicted and experimental data, at different engine speed, in crank angles, may lead to data misinterpretation (*i.e. a hypothetical error of 2 °CA between experimental and predicted data at 2000rpm is bigger than the equivalent 2 °CA error at*

5000rpm). A simple linear regression line, between the experimental burn duration, treated as independent variable, and the SRM predicted burn duration, treated as depended variable, can be built to analyse the significance of the predicted results. The linear correlation resulted in a R^2 value equal to 0.98. Regression line characterised by R^2 equal to 1 would correspond to SRM combustion duration predictions that perfectly reproduce the experimental data. Thus, only the 2% of the experimental data shown in Figure 70 is not correctly predicted by the developed methodology.

7.1.3 Engine C

In this paragraph the experimental data available in Table 7 (see Paragraph 3.3) will be compared to the engine burn angles predicted by the SRM code. A single CFD calculation at key point 1 was used to characterise the effect of the turbo charger on the turbulent mixing time shape against the crank angle. At the chosen operating point, the engine was operated at similar conditions (2000rpm_40Nm) to the other two analysed engines. Initial results showed that, holding the $C_{SRMBaseline}$ equal to 9.5, corresponding to the value found by calibrating the SRM on engine A at 2000rpm_40Nm, allowed the prediction of burn angles within the experimental standard deviation (see Table 16 below). This confirmed the validity of the assumptions presented in Chapter 5. The procedure presented in Paragraph 5.2 was used to confirm the similarity in the shape of the turbulent mixing time shape against the crank angle at 2000rpm and 5000rpm following (see Figure 115, Figure 116 and Figure 117 in the appendix). However, results in Table 16 show that combustion predictions for engine speeds above 4000rpm did not fall within the more restrictive ± 2 °CA confidence interval target. The discrepancy in the combustion duration predictions between high and low engine speeds is likely due to the turbocharger effect on the in-cylinder flow state. Therefore, to improve result's accuracy, the SRM model was calibrated at a higher engine speed. Engine A test data at 5000rpm_55Nm was chosen as second calibrating operating point and a second value for the initial $C_{SRMBaseline}$ was determined. The $C_{SRMBaseline}$ value changed from an initial 9.5, found calibrating the model at 2000rpm, to 7. The scalar mixing time for engine speeds above 4000rpm was derived using the new $C_{SRMBaseline}$ value, Equation 33, Equation 35 and τ_t at 5000rpm. The turbulent mixing time at 2000rpm, together with the firstly found value of $C_{SRMBaseline}$ were instead used to characterise the turbulence input for engine speeds lower than 4000rpm.

Table 16: Engine C predicted burn angles

Speed	Load	CA 10 [°CA ATDC(F)]		CA 90 [°CA ATDC(F)]		CA 10 90 [°CA ATDC(F)]				
		Exp.	Predicted	Exp.	Predicted	Exp.	Predicted	Δ%	Within Std. Dev	±2 °CA confidence interval
2000	95	23.34	23.66	38.88	40.12	15.53	16.52	6.4	😊	😊
2000	60	13.33	13.47	27.45	27.72	14.12	14.24	0.8	😊	😊
2000	40	6.67	6.68	25.92	25.81	19.24	19.13	0.6	😊	😊
3000	100	25.21	24.35	42.02	41.74	16.81	17.38	3.4	😊	😊
3000	60	10.71	10.82	26.26	27.18	15.55	16.32	5.0	😊	😊
3000	40	5.00	4.73	22.03	23.31	17.02	18.57	9.1	😊	😊
4000	95	27.76	28.55	46.87	48.51	19.10	19.96	4.5	😊	😊
4000	60	14.73	13.92	30.87	31.15	16.5	17.22	4.4	😊	😊
4000	40	6.55	5.54	20.62	22.14	14.06	16.60	18.1	😊	😞
5000	90	20.18	20.41	42.62	38.67	22.43	18.45	17.7	😊	😞
5000	60	13.21	14.56	34.61	33.9	21.4	19.34	9.6	😊	😞
5000	40	6.73	7.91	26.54	25.38	19.84	17.46	12.0	😊	😞
6000	75	18.80	20.75	40.85	39.74	22.06	18.93	14.2	😊	😞
6000	60	13.2	13.94	33.68	32.35	20.48	18.41	10.1	😊	😞
6000	40	8.38	9.15	28.55	27.02	20.17	17.87	11.4	😊	😞

Figure 71 shows that a linear R^2 coefficient, between the experimental predicted burn durations, of 0.97 was found, compared to a 0.95 obtained with a single calibration (see Figure 118 in the appendix) achieving a 3% improvement. All other burn angle predictions, the comparison between the experimental and the predicted in-cylinder pressure traces and the SRM ignition timing are available in the appendix.

Figure 71: Improved Engine C predicted and experimental burn duration, CA1090 (graph A), 1:1 results prediction line is represented by the dashed line. Error bands represent the average experimental standard deviation (graph A). Burn duration expressed in millisecond is shown in graph B.

Figure 72 shows the comparison of the experimental spark and the SRM ignition timing between engine B and C. The high intake charge density, due to the turbocharger, affects the engine knock tolerance. At the same operating point, the effect of the turbocharger can be noticed in the different experimental spark timing between the naturally aspirated variant (engine B) and the turbo charged variant (engine C). At a given engine speed against load operating point, reduced engine knock tolerance, due to faster engine combustion rates corresponds to retarded experimental spark timing. Results in Figure 71 showed that, the predicted SRM ignition timing of engine B and C followed the same trend as the experimental spark timing. Thus, engine C was characterised by retarded SRM ignition timing, compared to engine B. For instance, at 3000rpm, the experimental spark timing of engine C was retarded from -22 °CA ATDC(F), corresponding to engine B spark timing, to

-11 °CA ATDC(F), resulting in a 50% change in the spark timing between the two engine variants. The same relative change between the SRM ignition timing of the two engine variants was predicted. At 3000rpm the SRM ignition timing of engine C was retarded to -10 °CA ATDC(F) from -18 °CA ATDC(F), corresponding SRM ignition timing of engine B. This corresponded to a change of 55% in the SRM ignition timing between the two engines. Thus, the reduced engine knock tolerance of engine C, due to the turbo-charger, was correctly predicted by the methodology.

Figure 72: Predicted SRM ignition timing comparison at different speeds between engine B (naturally aspirated) and engine C (turbo-charged) at constant engine load

7.1.4 Engine D

Engine Load Effect on the Engine RoHR

In this section, key point 1 in Table 9 (see Paragraph 3.4) is used as baseline test data to tune the SRM code. At the chosen operating point, the engine was fitted with injector A and operated at 2000rpm_26bar_BMEP. Engine D was calibrated at MBT (Maximum Brake Torque) which corresponds to the most achievable advanced spark timing without decreasing the likelihood of abnormal engine combustion regimes [1]. Thus, the SRM ignition timing was set to tune the combustion model to the engine knock limit (for further details on the knock index see Paragraph 4.3.6). A value of the $C_{SRMBaseline}$ multiplier equal to 11.4 and an SRM ignition input timing occurring at 4 °CA ATDC(F), corresponding to a delay of 2°CA from the experimental timing, were found during the SRM tuning phase (see

Paragraph 5.2). Later, Equation 31a and Equation 32 were used to derive the scalar mixing time input of any chosen operating point, with engine fitted with injector A in Table 9. Pressure and RoHR predicted results are available in the appendix and will be no further discussed here. A second CFD calculation was carried out to investigate the effect of injector B on the turbulence mixing time's shape against the crank angle. The engine, with exception of the injector, was operated at the same condition as the previously chosen baseline point (see Key point 4 in Table 9). Following the methodology presented in Paragraph 5.5, the value of $C_{SRMBaseline}$ was held constant between engine fitted with injector A and B (see Equation 34). The SRM ignition input was set at 10 °CA ATDC(F), corresponding to a delay of 3 °CA from the experimental spark timing and resulted in good agreement with the experimental load, in-cylinder pressure trace and burn angles. Later, Equation 31a and Equation 35 were used to derive the scalar mixing time, necessary to initialise the SRM code at any chosen operating condition.

Figure 73: Predicted engine combustion rates at 2000rpm_2barBMEP_injector B (left graph) and 2000rpm_8barBMEP_injector B (right graph). Red vertical lines represent the SRM ignition timing and black lines represent the experimental spark time. Black error bands show the experimental standard deviation respectively at CA 10, CA 50 and CA 90.

The effect of different engine loads, while the engine speed is held constant, on the engine combustion rate is shown in Figure 73. Results show that, the difference between the experimental spark timing, represented by a black vertical line, and the predicted SRM ignition timing, represented by a red vertical line, decreases with engine load. A difference between spark and SRM timing of 8 °CA was predicted at 2bar BMEP. The difference between the two values is reduced to 2 °CA at 8bar BMEP due to the lower scalar mixing time' (τ_{SRM}) magnitude at higher engine load. Higher in-cylinder turbulence levels result in

shorter mixture ignition delays that consequentially, reduce the time necessary for the spark kernel to develop into flame. Figure 73 shows that, predicted SRM ignition timing, together with the derived scalar mixing time at different engine loads, result in good agreement with the measured 10%, 50% mass fraction burned (MFB) crank angles and 10-90% MFB duration.

Fuel Spray Patterns Effect on the Engine RoHR

The effect of different spray patterns on the turbulent mixing time shape against the crank angle, was previously described in Paragraph 6.2.3. It was shown that, injector B, due to the different spray patterns, increases the in-cylinder tumble motion which results in increased turbulence levels during the closed part of the cycle. This resulted in a change in the turbulent mixing time shape, against the crank angle, at a given engine operating point. Due to the increased turbulence level injector B, at a given operating point, a shorter combustion duration, compared to injector A, is expected.

Figure 74: Engine D CA10 and CA10-90 prediction at 2000rpm_8bar_BMEP_SOI_420. Red data correspond to injector A. Black data correspond to injector B.

The effect of the two difference injectors at 2000rpm 8bar BMEP, on the engine combustion duration (CA 10-90) and CA 10, is shown in Figure 74. To investigate the sole effect of the injector on the engine combustion, all engine attributes, including fuelling, were held constant. Thus, all SRM boundary conditions and inputs, except for the scalar mixing time and the SRM ignition timing, were held constant between the two injectors. To operate the engine at the same operating conditions that included the burn angles, the experimental spark timing of injector B had to be retarded of 3 °CA compared to injector A (see Figure 74). This

was due to injector B's spray patterns that increase the in-cylinder turbulence and therefore, increased the flame propagation speed. Thus, since engine D was operated at MBT, at a given operating point, the knock tolerance of the engine fitted with injector B was reduced compared to the resulting knock tolerance of injector A. Results in Figure 74 show that, the SRM ignition input, predicted following the methodology described in Chapter 5, had to be retarded when the engine was fitted with injector B instead of injector A. Thus, the SRM ignition timing of injector A was retarded from $-16.5^{\circ}\text{CA ATDC(F)}$ to $-13.5^{\circ}\text{CA ATDC(F)}$. This difference in the predicted SRM ignition timing is due to the CFD predicted change in the turbulent mixing time between the two injectors (see Paragraph 6.2.3). Thus, to keep the knock index below the chosen threshold value, the SRM ignition timing of engine D fitted with injector B had to be retarded compared to injector A. Moreover, the SRM combustion model should predict reduced mixture ignition delays, defined as the difference between the SRM ignition timing and the experimental spark timing, when engine D is fitted with injector B instead of injector A. However, since all boundary conditions were held constant between the two injectors, the mixture state, determining the value of the laminar flame speed and thus, the ignition delay, are not significantly affected. At 2000rpm the change in the mixture state between $-16.5^{\circ}\text{CA ATDC(F)}$ and $-13.5^{\circ}\text{CA ATDC(F)}$ corresponds to a 12% difference in pressure and a 1.5% change in the temperature. This results in only a 2% increase in the laminar flame speed at the ignition timing between the two injectors which does not affect the mixture ignition delay. The SRM ignition timing of injector B, retarded of 3°CA from the ignition timing of injector A, resulted in CA 10 and CA 10-90 comparable between the two injectors. Thus, if the ignition timing were held constant between the two injectors, the SRM would predict faster combustion rates and shorted combustion duration when engine D is fitted with injector B. This, again, is due to the higher in-cylinder turbulence level generated by injector B (see Paragraph 6.2.3) and the SRM turbulent flame calculation (see Paragraph 4.3.2).

Figure 75 shows the effect of different SRM ignition timing on the engine Gross Indicated Specific Fuel Consumption (GISFC) [1] against the crank angle and the CA 50. The best engine performance can be achieved when the entire combustion process takes place around TDC with the initial part of the combustion occurring while the piston is moving upwards. If the spark timing is retarded, combustion processes start when the piston is moving downwards losing part of the compression work previously done. Thus, retarded ignition timing result in lower combustion efficiency which increases the engine fuel consumption.

Moreover, advancing the spark timing, result in earlier start of the combustion, while the piston is moving upwards. Thus, higher work is required to compress the gas inside the cylinder, resulting in lower combustion efficiency and consequentially the fuel consumption. Furthermore, if spark timing occur too early during the compression stroke, high pressure and temperature gas conditions trigger unwanted auto-ignition reactions. Results in Figure 75 show that, the expected “u-shape” of the GISFC at different ignition timing was correctly predicted by the SRM code [1]. To operate the engine at the same burn angles the SRM spark timing of injector B had to be retarded compared to injector A. Moreover, advancing SRM ignition timing of injector B, from the predicted matching value at $-13.5^{\circ}\text{CA ATDC(F)}$ (x-marked in Figure 75), results in higher fuel consumption and advanced CA 50 timing. However, lower GISFC is predicted with the same SRM ignition timing for injector A. This is due to autoignition processes in the un-burn zone predicted by the SRM when simulating injector B. Moreover, injector B shows lower predicted engine fuel consumption retarding the ignition times compared to the predicted injector A fuel consumption, due to the faster predicted combustion rate.

Figure 75: Prediction of the effect of SRM ignition timing on engine D G-ISFC (top graph) and CA50 (bottom graph) at 2000rpm_8barBMEP_SOI_420. Circles corresponds to a swing of the SRM ignition timing value. Cross data correspond to the predicted SRM ignition timing following the procedure presented in Paragraph 5.5.

Start of Injection Timing Effect on the Engine RoHR

Key point 6,7,8 and 9 in Table 9, corresponding to the engine operated at 2000rpm_8barBMEP with different SOI timing will be used for this analysis. 420 °CA ATDC(F) (key point 6) SOI was chosen as baseline timing. Predicted burn angles for different SOI timing are shown in Figure 76. The non-combusting CFD analysis showed that, retarded SOI times, compared to the baseline SOI 420°CA BTDC(F), correspond to higher production of turbulent kinetic energy, k , and ε during the closed part of the engine cycle. This is due to the energy that is related to the fuel injection that, for given fuelling parameters, has less time to dissipate during the intake stroke, when the injection is retarded. Therefore, higher turbulence is generated to dissipate the remaining energy associated with

the injection. Moreover, due to the direct correlation between turbulent speed and in-cylinder turbulence magnitude, faster engine combustion rates are predicted by the SRM when the SOI is retarded from the baseline timing. The predicted combustion duration is reduced by 13% when the SOI is retarded to 510 °CA ATDC(F) (see Figure 76). Thus, to operate the engine at the same operating conditions, retarded ignition timing are predicted due to the faster engine combustion rate. The predicted SRM ignition timing of the baseline case, occurring at -13.5 °CA ATDC(F), was retarded to -9.5 °CA ATDC(F) for the most retarded fuel injection timing. This corresponds to a change in the ignition event of 30%. The predicted change in the SRM ignition timing, followed the experimental spark timing trend. The spark timing for the baseline case, occurring at -16 °CA ATDC(F) was retarded to -12 °CA ATDC(F) for the most retarded fuel injection timing. This corresponds to a change in the spark event of 25%. Predicted burn angles in Figure 76 fall within the experimental standard deviation. Thus, the empirical correlation used to predict the scalar mixing time at different SOI (see Equation 31b in Paragraph 5.4), showed to be valid at the explored conditions. However, further delay the injection event in the compression stroke may result in inefficient mixing of the air and the fuel. This could result in reduced engine knock tolerance due to the formation of zones characterised by a high fuel concentration which enhance the likelihood of autoignition reaction. Moreover, the efficiency of the combustion will be also affected. Thus, further assessment of the empirical correlation (Equation 31b) is necessary to increase the injection timing range in which it can be considered valid.

Figure 76: Measured and predicted engine burning rate at 2000rpm_8barBMEP at different SOI timing

7.2 CONCLUSIONS

Results showed that, the methodology can provide RoHR predictions falling within the experimental standard deviation and the $\pm 2^\circ CA$ confidence interval from the experimental data. A summary of all combustion results is available in Table 7 below.

Results shows that the engine geometry is the most influencing factor that affects the formation of the large-scale tumble motion. This confirms the turbulence modelling background presented in Chapters 2, 4, 6 and answered the thesis' first research question. Predicted burn angles results show that, for a given engine geometry, the in-cylinder charge speed is the physics that governs changes in the in-cylinder turbulence to operating conditions and calibrations. This answers the second research question of this thesis.

Figure 77 shows that, the difference in the engine combustion duration between the baseline engine A and the two variants: engine B and C. The methodology predicted the engine burn rate within the set criteria for different valve timing, engine speeds and charge dilutions. Results show that the methodology can offer a practical solution for the RoHR prediction during the engine development limiting the number of necessary CFD calculation to a minimum and moving towards a fully predicted and less experimental data dependent development process. Engine C combustion results showed that two non-combusting CFD calculations at different operating conditions, were necessary to achieve prediction within $\pm 2^\circ CA$ from experimental (averaged) confidence interval. This is due to the turbocharger that affects the in-cylinder charge state and consequentially challenges the first hypothesis of this thesis. Combustion predictions within the experimental standard deviation were achieved with a single non-combusting CFD calculation. Further validation on turbocharged engines is therefore required.

Figure 77: Predicted and experimental burn durations comparison between engine A, B and

Table 17: Results of the combustion predictions comparison with experimental data

Change in	Assessments criteria	Criteria met?	Comments
Valve timing	Burn angles prediction within: <ul style="list-style-type: none"> exp. standard dev. ± 2 °CA from exp. data Spark timing trends to evaluate <ul style="list-style-type: none"> SRM ignition timing Knock tolerance 	Y	<ul style="list-style-type: none"> Engine A, B and C burn angles and spark maps predicted within targets. SRM calibrated with a single non combusting CFD. Limited valve timing explored – further validation required.
EGR		Y	<ul style="list-style-type: none"> Engine A burn angles and spark maps predicted within targets. SRM calibrated with a single non combusting CFD
Engine Speed		Y	<ul style="list-style-type: none"> Engine A, B and C burn angles and spark maps predicted within targets.
SOI		Y	<ul style="list-style-type: none"> Engine D map burn angles and spark timing maps predicted within targets. SOI effect predicted using an empirical correlation – further validation required.
Bore to Stroke ratio	Expected burn duration and knock trends from literature	Y	<ul style="list-style-type: none"> B/S ratio virtually explored on engine A. Expected burn duration, ignition timing and knock limit trends predicted.
Intake manifold	Burn angles prediction within: <ul style="list-style-type: none"> exp. standard dev. ± 2 °CA from exp. data 	Y	<ul style="list-style-type: none"> Engine A and B burn angle maps compared. Effect of intake manifold on burn angles predicted (faster combustion for engine B). At given engine operating point, SRM ignition timing difference between variants predicted consistent with spark timing (change in engine knock).
Turbocharger	Burn angles prediction within: <ul style="list-style-type: none"> exp. standard dev. ± 2 °CA from exp. data 	Y	<ul style="list-style-type: none"> Engine B and C burn angles maps compared Two CFD runs needed to achieve predictions within ± 2 °CA interval at high engine speed (engine C) Effect of turbocharger on burn angles predicted (faster combustion for engine C) Effect of turbocharger on engine knock tolerance (retarded SRM ignition timing for engine C)
Injector	Spark timing trends to evaluate <ul style="list-style-type: none"> SRM ignition timing Knock tolerance 	Y	<ul style="list-style-type: none"> Engine D burn angles map predicted within targets for two injectors. SRM calibrated with a single non combusting CFD for each explored injector. Faster combustion predicted with injector generating more turbulence At given engine operating point, injector characterised by greater turbulence resulted in retarded SRM ignition timing.

8 CONCLUSIONS

The goal of providing reliable prediction of heat release rates at the concept stages of development for gasoline engines, has led to a new process proposed, which incorporates 1-D and 3-D CFD tools with a Q-D SRM. A new turbulence scaling factor response that scales the CFD derived turbulent mixing time (τ_t), to the intake charge flow velocity was developed. The scaling of τ_t allows to predict the effect of different engine operating conditions and high-level calibrations on the in-cylinder turbulence. To the author's best knowledge, the response developed for this thesis has never been proposed before.

8.1 SIMULATION TOOLS COMPATIBLE WITH THE SCOPE OF THE THESIS

The aim of the thesis was to develop and implement a practical virtual engine development process that predicts the engine RoHR at the concept (*early*) stage of development, when different concepts and attributes are virtually screened. The literature reviewed carried out in Chapter 2 showed that there are two modelling frameworks that can predict the engine RoHR: CFD and Q-D models. CFD models, solving the 3-D in-cylinder fluid dynamics, can predict the effect of different hardware on the engine RoHR. However, due to the high computational requirements, CFD screening of different engine operating conditions and calibrations for each explored engine concept is not feasible at the concept stage of development. Instead, Q-D models, meet the necessary computational requirements in terms of both, time and predictive capability at different operating conditions but fails to predict the effect of different engine concepts. Therefore, an hybrid process, based on CFD and Q-D models, such as [18, 19, 98], was proposed.

8.2 PHYSICS THAT GOVERNS THE ROHR OF SI ENGINES

SI engine combustion rates depend on the flame front propagation that is function of the laminar and turbulent flame speeds. In the complete absence of turbulence, the flame front speed, would only be dictated by the fuel laminar flame speed. However, the turbulent nature of SI engines in-cylinder flows needs to be considered to provide realistic RoHR predictions. The in-cylinder turbulence generation is defined by the *energy cascade* phenomenon that describes how different in-cylinder eddies mix between each other (see Paragraph 4.1.1).

The bulk in-cylinder motion (*i.e. large turbulent eddies*) is function of the engine geometry. The in-cylinder flow kinetic energy (*i.e. energy that dissipates moving from large to smaller eddies*) is instead function of the intake charge speed. Therefore, intake flow speed and the geometrical effects on the in-cylinder flow need to be modelled to predict the RoHR of SI engines.

8.3 THE DEVELOPED METHODOLOGY

The following assumptions were developed to simplify the modelling of the in-cylinder turbulence:

- The in-cylinder turbulence characteristics' evolution, *i.e.* the shape against the crank angle, during the closed part of the cycle, is considered only bound to the given engine geometry.

The engine geometry is the most influencing factor that affects the formation of the large-scale tumble motion. Therefore, single CFD analysis can be used to define the in-cylinder turbulence of each of the explored engine concepts.

- At a given engine geometry, the effect of different engine calibrations, on the in-cylinder turbulence characteristics, during the closed part of the cycle, is scaled on the intake charge speed.

The intake charge speed is the physics that governs the formation of the small-scale eddies. Therefore, the CFD derived in-cylinder turbulence can be scaled accordingly to the change in the intake charge flow speed.

The developed methodology uses non-combusting CFD calculations to characterise the in-cylinder turbulence characteristics of each explored engine concept, a 1-D engine system code (WAVE) to predict the overall engine performance and an SRM combustion model (LOGESoft) to predict the engine RoHR. A scaling factor response, relating the change in the average turbulent mixing time to the intake port velocity was used to manipulate the CFD characterised turbulence of each of the explored engine variants. The developed process is split into three main stages as follows:

- Models' calibration
- Engine optimisations
- Engine update.

Baseline experimental data, including burn angles, is necessary to carry the initial models' calibration phase. Once all models are calibrated, the CFD derived turbulence characteristic of a baseline engine design is scaled to the intake charge flow velocity, predicted by the 1-D engine system code. Later, the turbulence scaling factor is used to provide the SRM code with the necessary input for any operating conditions and high-level calibration. Lastly, to predict the effect of different engine design on the in-cylinder turbulence, non-combusting CFD calculations, one for any screened design, are carried out.

8.4 THE NON-COMBUSTING CFD ANALYSIS

A non-combusting CFD analysis was carried out to capture the effect of different engine variants, operating conditions, and calibrations on the in-cylinder turbulence. It was shown that, for each of the explored engine variants, the shape of the turbulent mixing time against the crank angle, key input to the chosen Q-D model, can be characterised by a limited number of 3-D CFD calculation. Moreover, it was shown that different engine operating conditions affect the overall magnitude of the turbulent mixing time but not the shape of the curve against the crank angle. These findings confirmed the validity of the assumptions presented previously.

8.5 COMBUSTION PREDICTIONS COMPARISON WITH EXPERIMENTAL DATA

Results presented in this thesis showed good combustion predictions meeting targets set in Paragraph 1.4.2. Combustion predictions were compared with experimental data from four different engine maps investigating the following characteristics:

- Change in engine speed
- Change in valve timing
- Change in charge dilution
- Discrimination between two intake port designs
- Discrimination between two charge induction systems
- Discrimination between two injector designs

Results for the turbo charged engine variant (engine C) showed combustion duration predictions within the experimental deviation but outside the $\pm 2^\circ CA$ confidence interval at high engine speed operating points *e.g. above 4000rpm*. This discrepancy between

predictions and experimental combustion duration is due to the turbo charger effect on the in-cylinder gas state. Improved accuracy, resulting in combustion duration predictions falling within the confidence interval, was achieved characterising the turbo-charged engine in-cylinder turbulence with an extra non-combusting CFD calculation at a speed higher than 4000rpm. Further validation on turbocharged engines is required to assess the validity of the developed process. The approach was also able to predict the effect of different bore to stroke ratios on the engine burn duration and knock tolerance through the application of a knock index. Results show that the methodology can be used to provide insights that can guide the design of new engines.

8.6 FUTURE WORK

Further analysis over a wider range of engine variants and unconventional combustion technologies is necessary to thoroughly validate the developed methodology. For instance, combustion prediction within the $\pm 2^\circ CA$ confidence interval for the turbo charged engine (engine C) could not be achieved with a single non-combusting CFD calculation. Therefore, engine attributes, that may affect the in-cylinder state, will challenge the fundamental hypothesis of the methodology.

Future research should focus on alternative fuels and combustion strategies (*e.g. water injection [116] and split cycle engines [117]*). Due to detailed chemical kinetics libraries available within the chosen SRM combustion model, it is expected that the developed methodology will predict the effect of different fuels. However, the accuracy of the combustion predictions will depend on the validity of the chosen chemical kinetics library and on the CFD capability to provide the SRM with realistic turbulence inputs.

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APPENDIX

ENGINE A

Bore to Stroke Ratio Effect on the In-Cylinder Turbulence Analysis

Figure 78: CFD prediction of different bore to stroke ratios effect on in-cylinder turbulent kinetic energy, k (graph a), the in-cylinder dissipation rate, ϵ (graph b).

Figure 79:1-D Intake port velocity for different bore to stroke ratios.

Case1, 360 CA °ATDC(f)

Case1, 370 CA °ATDC(f)

Case2, 360 CA °ATDC(f)

Case2, 370 CA °ATDC(f)

Case3, 360 CA °ATDC(f)

Case3, 370 CA °ATDC(f)

Figure 80: CFD prediction of different bore to stroke ratios on in-cylinder flow velocity at vectors at 360 °CA ATDC(F) (left column) and 370 °CA ATDC(F) (right column).

Figure 81: CFD prediction of different bore to stroke ratios on in-cylinder flow velocity at vectors at 580 °CA ATDC(F) (left column) and 670 °CA ATDC(F) (right column).

Case4, 360 CA °ATDC(f)

Case4, 370 CA °ATDC(f)

Case5, 360 CA °ATDC(f)

Case5, 370 CA °ATDC(f)

Case6, 360 CA °ATDC(f)

Case6, 370 CA °ATDC(f)

Figure 82: CFD prediction of different bore to stroke ratios on in-cylinder flow velocity at vectors at 360 °CA ATDC(F) (left column) and 370 °CA ATDC(F) (right column).

Figure 83: CFD prediction of different bore to stroke ratios on in-cylinder flow velocity at vectors at 580 °CA ATDC(F) (left column) and at 670 °CA ATDC(F)(right column).

1300rev/min VVT Combustion Prediction

Burn Angles

Key Point	Speed [rev/min]	BMEP [bar]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
8	1300	6.5	26	329	599	136	405
9			26	349	619	116	375
10			24	339	609	146	415

Figure 84: Predicted and Experimental CA10 (graph A), CA50 (graph B) (graph C) and CA10-90 (graph D) for different valve timing. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red error bands.

Figure 85: Experimental spark and SRM input timing comparison for different valve timing.

Pressure Traces

Key Point	Speed [rev/min]	BMEP [bar]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
8	1300	6.5	26	329	599	136	405
9			26	349	619	116	375
10			24	339	609	146	415

Figure 86: Predicted pressure and experimental pressure traces for key point 8 (graph A), key point 9 (graph B), key point 10 (graph C) and key point 11 (graph D).

1300rev/min Charge Dilution Combustion Prediction

Burn Angles

Key Point	Speed [rev/min]	BMEP [bar]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
11	2000	7.5	26	349	619	146	415
12			23				
13			20				
14			17

Figure 87: Predicted and Experimental CA10 (graph A), CA50 (graph B) (graph C) and CA10-90 (graph D) for different charge dilution. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red error bands.

Figure 88: Experimental spark and SRM input timing comparison for different charge dilution

Pressure traces

Key Point	Speed [rev/min]	BMEP [bar]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
11	2000	7.5	26	349	619	146	415
12			23				
13			20				
14			17

Figure 89: Predicted pressure and experimental pressure traces for key point 12 (graph A), key point 13 (graph B) and key point 14 (graph C).

2000rev/min VVT Combustion Prediction

Burn Angles

Key Point	Speed [rev/min]	BMEP [bar]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
1	2000	7.5	21	334	604	121	390
2			18	344	614	111	400
3			16	354	624	141	410

Figure 90: Predicted and Experimental CA10 (graph A) and CA90 (graph B) for different valve timing. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red error bands.

Pressure Traces

Key Point	Speed [rev/min]	BMEP [bar]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
1	2000	7.5	21	334	604	121	390
2			18	344	614	111	400
3			16	354	624	141	410

Figure 91: Predicted pressure and experimental pressure traces for key point 1 (graph A), key point 2 (graph B) and key point 3 (graph C)

2000rev/min Charge Dilution Combustion Prediction

Burn Angles

Key Point	Speed [rev/min]	BMEP [bar]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
4	2000	7.5	29	334	604	121	390
5			17				
6			14				
7			12

Figure 92: Predicted and Experimental CA10 (graph A) CA50 (graph B) and CA90 (graph C) for different charge dilution. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red error bands.

Pressure Traces

Key Point	Speed [rev/min]	BMEP [bar]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
4	2000	7.5	29	334	604	121	390
5			17				
6			14				
7			12

Figure 93: Predicted pressure and experimental pressure traces for key point 4 (graph A), key point 5 (graph B), key point 6 (graph C) and key point 7 (graph D).

3500rev/min VVT Combustion Prediction

Burn Angles

Key Point	Speed [rev/min]	BMEP [bar]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
15	3500	8	8	359	629	136	405
16			17	349	619	146	415
17			18	349	619	126	395

Figure 94: Predicted and Experimental CA10 (graph A), CA50 (graph B) (graph C) and CA10-90 (graph D) for different valve timing. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red error bands

Figure 95: Experimental spark and SRM input timing comparison for different valve timing

Pressure Traces

Key Point	Speed [rev/min]	BMEP [bar]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
15	3500	8	8	359	629	136	405
16			17	349	619	146	415
17			18	349	619	126	395

Figure 96: Predicted pressure and experimental pressure traces for key point 15 (graph A), key point 16 (graph B) and key point 17 (graph C)

3500rev/min Charge Dilution Combustion Prediction

Burn Angles

Key Point	Speed [rev/min]	BMEP [bar]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
18	3500	8	18	349	619	126	395
19			14				
20			10

Figure 97: Predicted and Experimental CA10 (graph A), CA50 (graph B) (graph C) and CA10-90 (graph D) for different charge dilution. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red bands.

Figure 98: Experimental spark and SRM input timing comparison for different charge dilution

Pressure Traces

Key Point	Speed [rev/min]	BMEP [bar]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
18	3500	8	18	349	619	126	395
19			14				
20			10

Figure 99: Predicted pressure and experimental pressure traces for key point 18 (graph A), key point 19 (graph B) and key point 20 (graph C).

5500rev/min VVT Combustion Prediction

Burn Angles

Key Point	Speed [rev/min]	BMEP [bar]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
21	5500	11	3	354	624	116	385
22				344	614	116	385
23				344	614	136	405
24				334	604	126	395

Figure 100: Predicted and Experimental CA10 (graph A), CA50 (graph B) (graph C) and CA10-90 (graph D) for different valve timing. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red error bands.

Figure 101: Experimental spark and SRM input timing comparison for different valve timing.

Pressure Traces

Key Point	Speed [rev/min]	BMEP [bar]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
21	5500	11	3	354	624	116	385
22				344	614	116	385
23				344	614	136	405
24				334	604	126	395

Figure 102: Predicted pressure and experimental pressure traces for key point 21 (graph A), key point 22 (graph B), key point 23 (graph C) and key point 24 (graph D).

ENGINE B

In-cylinder Turbulence analysis

Figure 103: CFD prediction of different engine variants effect on the in-cylinder turbulent kinetic energy, k (graph A), the in-cylinder dissipation rate, ε (graph B)

Figure 104: CFD prediction of different engine speeds on the turbulent mixing time, τ_t .

Figure 105: Polynomial coefficients' value of the 4th grade polynomial curves fitted to the turbulent mixing time from different engine speeds. Error bands correspond to the standard coefficients' error calculated with a 95% confidence interval.

Figure 106: Comparison between CFD derived τ_t and mixing time values derived using a single 4th grade polynomial curve, fitted to τ_t at 2000rpm. Y-intercept coefficients' values changed for each speed.

2000rev/min Combustion Prediction

Burn Angles

Key Point	Speed [rev/min]	Brake Torque [Nm]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
1	2000	30	45	330	612	117	417
2		40	30	314	595	122	422
3		50	10	307	588	115	415

Figure 107: Predicted and Experimental CA10 (graph A), CA90 (graph B) and CA10-90 (graph C) for different operating points. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red bands.

Pressure Traces

Key Point	Speed [rev/min]	Brake Torque [Nm]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
1	2000	30	45	330	612	117	417
2		40	30	314	595	122	422
3		50	10	307	588	115	415

Figure 108: Predicted pressure and experimental pressure traces for key point 1 (graph A), key point 2 (graph B) and key point 3 (graph C).

3000rev/min Combustion Prediction

Burn Angles

Key Point	Speed [rev/min]	Brake Torque [Nm]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
4	3000	30	37	335	617	102	402
5		40	27	320	601	102	402
6		55	5	306	588	103	403

Figure 109: Predicted and Experimental CA10 (graph A), CA90 (graph B) and CA10-90 (graph C) for different operating points. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red bands.

Pressure Trace

Key Point	Speed [rev/min]	Brake Torque [Nm]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
4	3000	30	37	335	617	102	402
5		40	27	320	601	102	402
6		55	5	306	588	103	403

Figure 110: Predicted pressure and experimental pressure traces for key point 4 (graph A), key point 5 (graph B) and key point 6 (graph C).

4000rev/min Combustion Prediction

Burn Angles

Key Point	Speed [rev/min]	Brake Torque [Nm]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
7	4000	55	10	324	605	98	398
8		40	5	320	601	102	402
9		30	8	325	606	102	402

Figure 111: Predicted and Experimental CA10 (graph A), CA90 (graph B) and CA10-90 (graph C) for different operating points. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red bands.

Pressure Traces

Key Point	Speed [rev/min]	Brake Torque [Nm]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
7	4000	55	10	324	605	98	398
8		40	5	320	601	102	402
9		30	8	325	606	102	402

Figure 112: Predicted pressure and experimental pressure traces for key point 7 (graph A), key point 8 (graph B) and key point 9 (graph C).

5000rev/min Combustion Prediction

Burn Angles

Key Point	Speed [rev/min]	Brake Torque [Nm]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
10	5000	20	10	315	596	97	397
11		40	8	325	606	99	400
12		55	6	325	606	102	402

Figure 113: Predicted and Experimental CA10 (graph A), CA90 (graph B) and CA10-90 (graph C) for different operating points. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red bands.

Pressure Traces

Key Point	Speed [rev/min]	Brake Torque [Nm]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
10	5000	20	10	315	596	97	397
11		40	8	325	606	99	400
12		55	6	325	606	102	402

Figure 114: Predicted pressure and experimental pressure traces for key point 10 (graph A), key point 11 (graph B) and key point 12 (graph C).

ENGINE C

In-cylinder Turbulence Analysis

Figure 115: CFD prediction of different engine speeds and loads on the turbulent mixing time, τ_t

Figure 116: Polynomial coefficients' value of the 4th grade polynomial curves fitted to the turbulent mixing time from different engine speeds. Error bands correspond to the standard coefficients' error calculated with a 95% confidence interval.

Figure 117: Comparison between CFD derived τ_t and mixing time values derived using a single 4th grade polynomial curve, fitted to τ_t at 2000rpm. Y-intercept coefficients' values changed for each speed.

Engine map combustion predictions

Figure 118: Engine C predicted and experimental burn duration at different operating points.

Figure 119: Experimental spark (circle symbols) and SRM input ignition input (triangle symbol) timing comparison for different engine speed and load

2000rev/min Combustion Prediction

Burn Angles

Key Point	Speed [rev/min]	Brake Torque [Nm]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
1	2000	40	16	280.9	569.1	124.8	380.8
2		60	0	340.9	629.1		
3		95	0	320.9	609.1

Figure 120: Predicted and Experimental CA10 (graph A), CA90 (graph B) and CA10-90 (graph C) for different operating points. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red bands.

Pressure Traces

Key Point	Speed [rev/min]	Brake Torque [Nm]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
1	2000	40	16	280.9	569.1	124.8	380.8
2		60	0	340.9	629.1		
3		95	0	320.9	609.1

Figure 121: Predicted pressure and experimental pressure traces for key point 1 (graph A), key point 2 (graph B) and key point 3 (graph C).

3000rev/min Combustion Prediction

Burn Angles

Key Point	Speed [rev/min]	Brake Torque [Nm]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
4	3000	40	15	290.9	579.1	124.8	380.8
5		60	8	303.9	591.1		
6		100	0	330.9	619.1

Figure 122: Predicted and Experimental CA10 (graph A), CA90 (graph B) and CA10-90 (graph C) for different operating points. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red bands.

Pressure Traces

Key Point	Speed [rev/min]	Brake Torque [Nm]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
4	3000	40	15	290.9	579.1	124.8	380.8
5		60	8	303.9	591.1		
6		100	0	330.9	619.1

Figure 123: Predicted pressure and experimental pressure traces for key point 4 (graph A), key point 5 (graph B) and key point 6 (graph C).

4000rev/min Combustion Prediction

Burn Angles

Key Point	Speed [rev/min]	Brake Torque [Nm]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
7	4000	40	0	304.9	593.1	124.8	380.8
8		60	3	325.9	614.1		
9		95	5	325.9	614.1

Figure 124: Predicted and Experimental CA10 (graph A), CA90 (graph B) and CA10-90 (graph C) for different operating points. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red bands.

Pressure Traces

Key Point	Speed [rev/min]	Brake Torque [Nm]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
7	4000	40	0	304.9	593.1	124.8	380.8
8		60	3	325.9	614.1		
9		95	5	325.9	614.1

Figure 125: Predicted pressure and experimental pressure traces for key point 7 (graph A), key point 8 (graph B) and key point 9 (graph C).

5000rev/min Combustion Prediction

Burn Angles

Key Point	Speed [rev/min]	Brake Torque [Nm]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
10	5000	90	0	320.9	609.1	124.8	380.8
11		60	3	329.9	617.1		
12		40	6	309.9	597.1

Figure 126: Predicted and Experimental CA10 (graph A), CA90 (graph B) and CA10-90 (graph C) for different operating points. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red bands.

Pressure Traces

Key Point	Speed [rev/min]	Brake Torque [Nm]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
10	5000	90	0	320.9	609.1	124.8	380.8
11		60	3	329.9	617.1		
12		40	6	309.9	597.1

Figure 127: Predicted pressure and experimental pressure traces for key point 10 (graph A), key point 11 (graph B) and key point 12 (graph C).

6000rev/min Combustion Prediction

Burn Angles

Key Point	Speed [rev/min]	Brake Torque [Nm]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
14	6000	75	0	340.9	629.1	124.8	380.8
15		60	0	333.9	621.1		
16		40	5	325.9	614.1

Figure 128: Predicted and Experimental CA10 (graph A), CA90 (graph B) and CA10-90 (graph C) for different operating points. Black error bands represent the experimental standard deviation. The ± 2 °CA confidence interval from experimental (averaged) values is shown by red bands.

Pressure Traces

Key Point	Speed [rev/min]	Brake Torque [Nm]	EGR (Int.+Ext.) [%]	IVO [°CA ATDC(F)]	IVC [°CA ATDC(F)]	EVO [°CA ATDC(F)]	EVC [°CA ATDC(F)]
14	6000	75	0	340.9	629.1	124.8	380.8
15		60	0	333.9	621.1		
16		40	5	325.9	614.1

Figure 129: Predicted pressure and experimental pressure traces for key point 13 (graph A), key point 14 (graph B) and key point 15 (graph C).

ENGINE D

In-cylinder Turbulence Analysis

Figure 130: Effect of different Start of Injection (SOI) timing on the in-cylinder turbulent kinetic energy production during the closed part of the engine cycle (graph A) and the turbulence dissipation (graph B).

Injector A combustion predictions at different engine loads

Figure 131: Engine D fitted with injector A predicted (red line) and measured (blue line) pressure and RoHR at 2000rpm_2barBMEP.

Injector B combustion predictions at different engine loads

Figure 132: Engine D fitted with injector B predicted (red line) and measured (blue line) pressure and RoHR at 2000rpm_8barBMEP (top graph) and 2000rpm_2barBMEP (bottom graph).

Injector A combustion prediction at different start of injection timing

Figure 133: Engine D fitted with injector A measured (blue) and predicted (red) pressure traces for different SOI