

The Significance of Research and Motor Octane Numbers to Anti-Knock Performance and Fuel Efficiency of Modern Spark-Ignition Engines

Ph.D. Thesis

Zhenbiao Zhou

Submitted in total fulfillment of the requirement of the degree of

Doctor of Philosophy

Supervised by

A/Prof. Yi Yang

Co-Supervised by

Dr. Joshua Lacey

The Department of Mechanical Engineering

The University of Melbourne

15th February 2020

Abstract

Improving fuel efficiency and reducing CO₂ emissions are the primary targets of Spark-Ignition (SI) engine development. Realizing these targets is limited by an abnormal combustion phenomenon known as engine knock which depends on both fuel's anti-knock properties and engine's thermodynamic conditions. Fuel's knock resistance is conventionally quantified by Research Octane Number (RON) and Motor Octane Number (MON) that are measured using the Cooperative Fuel Research (CFR) engine under standardized conditions. Whereas higher RON and MON generally means higher knock resistance, the relevance of two octane numbers to knock resistance in modern SI engines has changed, largely due to the different in-cylinder conditions than those in CFR engines. The Octane Index, $OI = (1-K) \cdot RON + K \cdot MON$, has been found to be a more suitable indicator of knock resistance in modern engines. The K factor in the OI model weights the relative contribution of RON and MON to fuel's actual knock resistance and is primarily dependent on engine design and operating conditions. Quantifying the K factor is of central importance to understanding the knock in modern SI engines.

This work therefore investigates the significance of RON and MON to modern engine combustion using the Octane Index model. It first evaluates the methods for determining OI and K reported in the literature and identifies that the method that matches the anti-knock performance of primary reference fuels (PRFs) with the interested fuel produces accurate results. This method does not require specially blended fuel sets or assume arbitrary correlations between OI and knock-limited performance. A novel fuel-blending system is developed in this work to implement this method, which is capable to supply PRF mixtures of varying octane (0 to 100) on the fly to the engine.

K values are then determined over the operation map of a 4-cylinder 2L Ford EcoBoost engine with a standard EPA certification gasoline (RON 91.6). The K values vary from low to high (-1 to 1.1) and is negative at most knock-limited conditions tested. The experiment data are further analyzed with GT-Power simulation to investigate the relation between in-cylinder end-gas states and K values. It reveals that the variation of K with engine operating conditions is primarily driven by the unburned gas temperature at the later stage of combustion just before the onset of autoignition.

The engine K-maps are then applied to determine the K-distributions in several standard drive cycles where the engine is adopted to a mid-sized passenger vehicle in conventional, full hybrid and plug-in hybrid powertrain configurations. For all drive cycles, there is a significant fraction of engine operating time and fuel consumption at conditions of positive K. However, with conventional powertrain, the knock-induced fuel efficiency losses primarily occur at conditions where K is near zero or negative. With deeper degree of electrification, hybridized powertrains are more knock-limited and the fuel efficiency losses due to knock mainly occur at conditions of more negative K. Further analysis is conducted to quantify the impact of RON and MON on the knock-limited fuel efficiency losses. For all drive cycles and powertrains studied, increasing RON has a strong effect on fuel efficiency improvement over a drive cycle, while increasing MON yields neutral or modestly negative effect on fuel efficiency improvement.

Declaration

This is to certify that:

- (i) the thesis comprises only original work towards my PhD study,
- (ii) due acknowledgement has been made in the text to all other material used,
- (iii) the thesis is fewer than 100,000 words in length, exclusive of tables, figures, bibliographies and appendices.

Acknowledgements

I would like to express my gratitude to the following people for their immense support and help throughout my study. This work would not have been successful without them.

❖ Yi Yang, Joshua Lacey and Michael Brear

Thanks for their insightful guidance and tremendous help to my study. Their wealth of knowledge, constructive advice and continuous encouragement have deeply inspired me. It was a great privilege and honor to work and study under their supervision.

❖ Tanmay Kar

Tanmay and I spent a lot of time together building and setting up the engine test facility. We shared the frustration and satisfaction throughout our PhD study. It was such a wonderful journey to work with him.

❖ Thomas Leone, James Anderson, Michael Shelby and Eric Curtis (Ford Motor Company)

Thanks for their expertise and interest in this project. They provided tremendous help in both conducting engine experiment and analysis of results. This project would have not been complete without assistance from them and financial support from Ford Motor Company.

❖ Daniel Jones and Al Knox

Daniel helped a lot in fixing the problems of engine. Al assisted me with building the fuel blending system. I am extremely grateful to all useful technical support from them.

❖ Monica Pater and Jan May

Thanks for Monica's assistance with purchasing of research equipment and Jan's help with administrative works.

❖ Jianbo Zhou and Rong Dang (my parents), Yintao Zhou (my brother) and Huiyin Zhou (my sister)

I would like to thank my parents for their love and support throughout my life and giving me strength to chase my dreams. My brother and sister deserve my wholehearted thanks as well.

❖ Yue Liu (my fiancée)

Finally, I would thank with love to my fiancée, Yue for her companion, love and understanding during my pursuit of PhD degree. The time with her through the difficulties and happiness has been the most invaluable part of my life.

Contents

1	Introduction	1
1.1	Application of Internal Combustion Engine in Transport and Its Future Challenges.	1
1.2	Motivation of Research	2
1.3	Thesis Layout	3
2	Literature Review	4
2.1	Engine Knock.....	4
2.1.1	Causes of Engine Knock and Impacts on Engine Durability	4
2.1.2	Knock Constraints on SI Engine Efficiency	5
2.1.3	Effect of Fuels on Efficiency Improvement for Knock-Limited Engines	7
2.2	Fuel Properties for Knock Resistance	8
2.2.1	Octane Numbers.....	9
2.2.2	Octane Sensitivity	10
2.2.3	Relevance of RON and MON to Modern Engine Knock	13
2.3	Octane Index and K Value	16
2.3.1	Introduction of Octane Index	16
2.3.2	Methods for Determining K.....	17
2.3.3	Effect of Engine Operating Conditions on K.....	18
2.3.4	Relation between K value and End-gas Condition	21
2.3.5	Fuel-Specific Issues of Octane Index and K.....	22
2.4	Hybridized Powertrains with Combustion Engine.....	24
2.4.1	Conventional Powertrain	25
2.4.2	Hybrid Electric Powertrains.....	25
2.4.3	Plug-in Hybrid Powertrains	33
2.5	Summary and Research Questions.....	34
3	Experimental and Numerical Methods	36

3.1	EcoBoost Engine Setup	36
3.1.1	Engine Test System.....	36
3.1.2	The Turbocharged DISI Engine	38
3.1.3	High-Speed Data Acquisition System for In-cylinder Pressure Measurement and Knock Detection	40
3.2	Determination of Trace Knock Condition.....	41
3.3	Development of the Online Octane Blending System	46
3.3.1	Design Targets	46
3.3.2	Control Logic	46
3.3.3	Configuration of the On-line Fuel Blending System	48
3.3.4	Validation of the Fuel Blending System.....	49
3.4	Experimental Fuels.....	52
3.5	Experimental Conditions.....	53
3.5.1	Operating Conditions	53
3.6	SI Engine Combustion Modelling.....	59
3.6.1	Modelling Method	59
3.6.2	GT-Power Modelling	67
3.7	Vehicle Modelling.....	68
4	Evaluation of Methods for Determining Octane Index and K value	71
4.1	Introduction of Literature Data	71
4.2	Numerical Methods	73
4.2.1	Regression Methods.....	73
4.2.2	PRF Methods	76
4.3	Results and Discussion.....	79
4.3.1	Comparing Different Methods for Determining K	79
4.3.2	Effects of Engine Operating Conditions on K	82
4.4	Summary	89

5	Octane Index and K values in a Modern Boosted DISI engine.....	90
5.1	Repeatability Test.....	90
5.2	Results of Normal Temperature Tests.....	91
5.2.1	Low-Speed Conditions: 1000-1500 RPM.....	91
5.2.2	Mid-Speed Conditions: 2000-3000 RPM	94
5.2.3	High-Speed Conditions: 4000-5000 RPM.....	98
5.2.4	Results of Normal Temperature K-Map	101
5.3	Results of High Temperature Tests.....	102
5.3.1	Mid-Speed Conditions: 2000-3000 RPM	102
5.3.2	High-Speed Conditions: 4000-5000 RPM.....	105
5.3.3	Results of High-Temperature K-Map	107
5.4	Effect of Engine Operating Conditions on K.....	108
5.4.1	Effect of Engine Speed	108
5.4.2	Effect of Increased Intake Air and Coolant Temperatures	112
5.5	End-Gas States and Their Correlation with K.....	113
5.5.1	Temperature-Pressure Trajectory in End-Gas	114
5.5.2	Relationship between End-Gas Temperature and K.....	118
5.5.3	Relationship between Cylinder Pressure and K.....	121
5.6	Summary	124
6	Significance of RON and MON for Different Powertrains on Various Driving Cycles	125
6.1	Driving Cycles.....	125
6.1.1	Standard Environmental Protection Agency (EPA) Drive Cycles	125
6.1.2	Davis Dam Towing Drive	127
6.2	Powertrain Configurations	128
6.2.1	Conventional Powertrain	128
6.2.2	Full Hybrid Electric Vehicle.....	134
6.2.3	Plug-in Hybrid Electric Vehicle.....	139

6.3	Distributions of K on Different Powertrains and Driving Cycles	143
6.3.1	Calculation Method.....	144
6.3.2	K-Distributions of Conventional Powertrain	148
6.3.3	K-Distributions of Hybrid Powertrain	155
6.3.4	K-Distributions of Plug-in Hybrid Powertrain	162
6.4	Discussion	167
6.5	Summary	169
7	Conclusions and Recommendations for Future Study	170
7.1	Conclusions	170
7.2	Recommendations	172
7.2.1	Effect of fuel composition on K.....	172
7.2.2	Octane Index Model and Detailed Chemical Kinetics.....	172
7.2.3	Relationship between Octane Index on Knock-Limited Engine Performance	173
7.2.4	Significance of RON and MON for High Compression Ratio Engines	173
A.	References.....	174
B.	Appendix.....	180
B.1.	Interpolation Methods	180
B.2.	Determination of Knock-Limited Fuel Efficiency Loss	182
C.	Abbreviations	185

List of Figures

Figure 1-1 The distributions of (a) energy consumption by fuel type from 2000 to 2040 in transport sector and (b) new passenger cars production by fuel type from 2000 to 2040 [1].	1
Figure 2-1 The damaged piston caused by knocking combustion [14].	5
Figure 2-2 Combustion phasing and BTE vs engine load at 1000 RPM [20]. Dashed lines are for higher compression ratio and lines of same color and mark are for the same fuel.	7
Figure 2-3 Effect of octane sensitivity on the (a) knock limit and (b) engine efficiency at 1800 RPM and CR=11.5:1 condition. Adapted from [26].	11
Figure 2-4 Heat release rates from chemical kinetic modelling of PRF80 and a sensitive fuel (3-hexene) at RON rating condition and MON rating condition. Two fuels share the same MON value of 80 but 3-hexene has high octane sensitivity. Figure from [29]	12
Figure 2-5 RON values of ethanol/gasoline blends from standard RON test and modified RON test. Adapted from [30]	13
Figure 2-6 The average specific power of the LDVs from 1975 to 2017 in US market. Adapted from [17].	14
Figure 2-7 Effects of (a) MON and (b) RON on the knock-limited spark advance for a downsized DISI engine at 2000 RPM. Data from [34].	15
Figure 2-8 Effects of (a) MON and (b) RON on the 25-80 mph acceleration at fixed 5 th gear. Data from [35].	16
Figure 2-9 (a) KLSA vs OI with the same data in Figure 2-7 and (b) acceleration time vs OI with the same data in Figure 2-8. Adapted from [34, 35].	17
Figure 2-10 The demonstration of K for characterizing the significance of RON and MON to improving knock resistance and the relationship between OI and ONs.	19
Figure 2-11 Effect of intake pressure (engine load) on K at two different engine speeds [41].	20
Figure 2-12 K factor vs engine speed from literatures. The numbers in legend are SAE paper number.	20
Figure 2-13 Correlation of T_{comp15} with K values. Replotted with data from [41].	21
Figure 2-14 Pressure-temperature evolutions of four fuels at two operating conditions. Noted that these profiles end at the spark timing and all fuels have the similar CA50 of 37-39 ° aTDC. Figure from [53].	23

Figure 2-15 Temperature-pressure evolutions of unburned gas leading to the autoignition point for three fuels at two engine operating conditions. Figure from [55].	24
Figure 2-16 Fuel consumption data of conventional vehicles and hybrid vehicles (light-duty segment) sold in US market from 2000 to 2017. Fuel consumption is based on US EPA 2-cycle test. Figure from [17].	26
Figure 2-17 Power demand of a midsize sedan on US06 driving cycle. The vehicle power demand is decomposed into average power and dynamic power. (Data from [64]).	28
Figure 2-18 The flow of power for a series powertrain.	30
Figure 2-19 Torque and power curves of an AC induction motor [68]. Electric motor can operate at a constant peak power over a wide range of speed, making transmission unnecessary for a series hybrid.	30
Figure 2-20 The power flow of a parallel hybrid powertrain (P2 configuration where motor is installed before multi-gear transmission). ICE and motor/generator are connected through a torque coupler with a constant speed ratio and speeds of them are proportional to transmission inlet speed.	31
Figure 2-21 Planetary gear set of the power-split device for a series-parallel hybrid powertrain. Sun gear connects to electric machine 1, carrier connects to ICE and ring gear connects to generator electric machine 2 and differential. Figure from [60].	32
Figure 2-22 Power flow of a power-split hybrid powertrain. It can operate at series mode, parallel mode or a blended mode of these two.	33
Figure 3-1 Experimental setup of intake temperature control for the GTDI engine.	38
Figure 3-2 Pressure transducers mounting on the cylinder head for in-cylinder pressure measurement.	40
Figure 3-3 PSD analysis or raw in-cylinder pressures at 1000RPM, 1500RPM, 6 bar BMEP and 8 bar BMEP under normal combustion (left figures) and trace knocking (right figures) conditions.	44
Figure 3-4 Example of filtered pressure traces for a normal and a trace knocking conditions at 1500 RPM 8 bar BMEP.	45
Figure 3-5 Maximum peak-to-peak pressures of the filtered pressure traces with 3-10 kHz bandpass.	45
Figure 3-6 Knocking percentage of cycles whose maximum peak-to-peak values of the filtered pressure traces were above the threshold.	45
Figure 3-7 Control logics of online octane blending system	48
Figure 3-8 Simplified drawing of the configuration for blending system.	49

Figure 3-9 Comparison of densities of toluene/iso-octane blends from calculation and measurement.	50
Figure 3-10 PRF numbers at 3000 RPM 6 bar BMEP condition.	51
Figure 3-11 Flow rates of iso-octane and n-heptane at 3000RPM 6bar BMEP condition.	51
Figure 3-12 Total flow rate and fuel pressure from the blending system at 3000 RPM 6 bar BMEP condition.	52
Figure 3-13 Engine operating conditions of a mid-sized SUV (Ford Edge MY19) equipped with 2.0L 4-cylinder EcoBoost engine over different EPA drive cycles.	54
Figure 3-14 Experimental design of engine operating conditions at normal temperature.....	54
Figure 3-15 Measured temperatures of coolant, intake manifold and oil from vehicle test of Ford Edge MY19 with 2L EcoBoost during UDDS cycle.	55
Figure 3-16 Engine operating points of mid-sized Ford SUV equipped with 2L EcoBoost engine in tow rating tests.	56
Figure 3-17 Design of engine operating conditions at high temperature.....	56
Figure 3-18 Measured temperatures in the intake manifold, water jacket and oil passage on Davis Dam vehicle tests (SAE J2807 tow rating).	56
Figure 3-19 Flow chart of engine combustion modelling using GT-Power.	61
Figure 3-20 Simulated cylinder pressure for 3000RPM, 12bar BMEP, normal temperature condition using different h_{port}	65
Figure 3-21 Measured cylinder pressure vs. simulated cylinder pressure from reverse run model for 3000 RPM, 12 bar BMEP, normal temperature condition.....	66
Figure 3-22 Simulated cylinder pressure for 3000 RPM, 12 bar BMEP, normal temperature condition using different h_{comb}	67
Figure 3-23 Hierarchy tree for vehicle modelling. The targets for fuel consumption reductions are based on [62].....	70
Figure 4-1 The RON and S of all test fuels in the engine experiment from [90].	73
Figure 4-2 K determination using the linear regression method with data from two operating conditions. The fuels used here are subsets of those in Figure 4-1.	75
Figure 4-3 Variation of K with intake pressure at DI 1500 RPM and CR=10:1 condition using the linear regression method with dataset including iso-octane and excluding iso-octane.	75
Figure 4-4 K determination using the quadratic regression method with the same data sets in Figure 4-2.....	76

Figure 4-5 K determination using PRF direct comparison method with data at DI 1500RPM CR=10:1 and intake pressure sweep conditions.	78
Figure 4-6 K determination using the PRF interpolation method. The polynomial curve of iso-octane intersects with that of a gasoline B97E20. The error bars show the error of the polynomial fitting relative to the experimental data.	79
Figure 4-7 Comparison of results from linear regression and non-linear regression methods with data from (a) DI 1500 RPM CR=10:1 and (b) PFI 1500 RPM CR=10:1.	80
Figure 4-8 Nonlinear regression at PFI 1500 RPM CR=10:1 and P_{in} =68 kPa.	80
Figure 4-9 Variation of K with intake pressure for (a) DI, (b) PFI and (c) UFI at 1500 RPM and CR=10:1 conditions using PRF interpolation method, linear regression method and PRF direct comparison method.	82
Figure 4-10 K values determined from the matching points on the CA50-NMEP curves(solid circles) and on the KLSA- P_{in} curves (open circles) with data from DI 1500 RPM CR=10:1 condition.	83
Figure 4-11 The effect of engine fueling on K at (a)1500 RPM CR=10:1 and (b) 2500 RPM CR=10:1 conditions. The dashed line indicates the MBT limit with knock-limited combustion on the right and over-advanced combustion on the left.	85
Figure 4-12 Production share of engine fuel delivery technologies on light-duty vehicles in US market from MY 2008 to MY 2017 [17].	86
Figure 4-13 The effect of engine speed on K for (a) DI, (b) PFI and (c) UFI CR=10:1 conditions. The dashed line indicates the MBT limit for iso-octane with knock-limited combustion on the right side and over-advanced combustion on the left side.	87
Figure 4-14 The effect of compression ratio on K for (a) PFI 1500 RPM and (b) UFI 2500 RPM conditions. The dashed line indicates the MBT limit for iso-octane with knock-limited combustion on the right side and over-advanced combustion on the left side.	89
Figure 5-1 CA50 of the certification gasoline and PRFs at trace knock condition from repeatability tests conducted at different stages of project.	91
Figure 5-2 Measured K values from repeatability tests. Repeatability tests show 0.025 variation in K.	91
Figure 5-3 Intake manifold pressure of certification gasoline from load sweep at 1000 RPM, 1250 RPM and 1500 RPM. Solid points are for knock-limited conditions while hollow points are for over-advanced conditions and this convention lasts in all figures in this section.	93

Figure 5-4 Combustion phasing of gasoline at trace knock condition from load sweep at 1000 RPM, 1250 RPM and 1500 RPM.	93
Figure 5-5 Exhaust lambda from load sweep at 1000 RPM, 1250 RPM and 1500 RPM.	93
Figure 5-6 Measured octane index of gasoline from load sweep at 1000 RPM, 1250 RPM and 1500 RPM.	94
Figure 5-7 K values from load sweep at 1000 RPM, 1250 RPM and 1500 RPM.	94
Figure 5-8 Intake manifold pressure of certification gasoline from load sweep at 2000 RPM, 2500 RPM and 3000 RPM. Solid points are for knock-limited conditions while hollow points are for over-advanced conditions.	95
Figure 5-9 Valve overlap from load sweep at 2000 RPM, 2500 RPM and 3000 RPM.	95
Figure 5-10 Combustion phasing at trace knock from load sweep at 2000 RPM, 2500 RPM and 3000 RPM.	96
Figure 5-11 Exhaust lambda from load sweeps at 2000 RPM, 2500 RPM and 3000 RPM.	97
Figure 5-12 Exhaust gas temperature measured before turbine from load sweep at 2000 RPM, 2500 RPM and 3000 RPM.	97
Figure 5-13 Measured OI from load sweeps at 2000 RPM, 2500 RPM and 3000 RPM.	98
Figure 5-14 Measured K values from load sweeps at 2000 RPM, 2500 RPM and 3000 RPM.	98
Figure 5-15 Manifold pressure from load sweep at 4000 RPM and 5000 RPM.	99
Figure 5-16 Exhaust lambda from load sweep at 4000 RPM and 5000 RPM.	99
Figure 5-17 Exhaust temperature from load sweep at 4000 RPM and 5000 RPM.	99
Figure 5-18 Combustion phasing at trace knock from load sweep at 4000 RPM and 5000 RPM.	100
Figure 5-19 Measured OI from load sweep at 4000 RPM and 5000 RPM.	101
Figure 5-20 K values from load sweep at 4000 RPM and 5000 RPM.	101
Figure 5-21 Final matrix of engine operating conditions for normal temperature tests. Solid points are for knock-limited conditions while hollow points are over-advanced from MBT.	102
Figure 5-22 Normal operating temperature K map. Conditions above the red line are knock-limited conditions.	102
Figure 5-23 Manifold pressure from load sweep at 2000 RPM and 3000 RPM high temperature conditions. Solid points are for knock-limited conditions and open markers are for over-advanced conditions.	103

Figure 5-24 Combustion phasing at trace knock from load sweep at 2000 RPM and 3000 RPM high temperature conditions.	103
Figure 5-25 Exhaust lambda from load sweep at 2000 RPM and 3000 RPM high temperature conditions.....	103
Figure 5-26 Exhaust temperature from load sweep at 2000 RPM and 3000 RPM high temperature conditions.....	104
Figure 5-27 Octane index from load sweep at 2000 RPM and 3000 RPM high temperature conditions.....	104
Figure 5-28 K values from load sweep at 2000 RPM and 3000 RPM high temperature conditions.....	105
Figure 5-29 Manifold pressure from load sweep at 4000 RPM and 5000 RPM high temperature conditions.....	105
Figure 5-30 CA50 from load sweep at 4000 RPM and 5000 RPM high temperature conditions.	105
Figure 5-31 Exhaust lambda from load sweep at 4000 RPM and 5000 RPM high temperature conditions.....	106
Figure 5-32 Exhaust temperature from load sweep at 2000RPM and 3000RPM high temperature conditions.....	106
Figure 5-33 Octane index from load sweep at 4000RPM and 5000RPM high temperature conditions.....	107
Figure 5-34 K values from load sweep at 4000 RPM and 5000 RPM high temperature conditions.....	107
Figure 5-35 High-temperature K map. Conditions above red line are knock-limited conditions.	107
Figure 5-36 CA50 at trace knock from speed sweeps at part- and high-load, normal temperature conditions.....	109
Figure 5-37 Exhaust lambda from speed sweeps at part- and high-load, normal temperature conditions.....	109
Figure 5-38 (a) unburned gas temperature and (b)cylinder pressure from 3000 RPM to 5000 RPM at 12 bar BMEP, normal temperature condition.	109
Figure 5-39 K values from speed sweeps at part- and high-load, normal temperature conditions.	110
Figure 5-40 GIMEP corresponding to 10 bar and 16 bar BMEP at different engine speeds.	111

Figure 5-41 Simulated unburned gas temperature as a function of the mass fraction burned (MFB) at 2000 – 5000 RPM, 12 bar BMEP and normal operation temperature.....	111
Figure 5-42 Results of (a) intake pressure, (b) CA50, (c) exhaust lambda and (d) K value from load sweeps at normal temperature and high temperature, 2000 RPM conditions.	112
Figure 5-43 Unburned gas temperatures from GT-Power modelling for conditions at 2000 RPM.	113
Figure 5-44 Conceptual diagram of the relationship between K and the different responses of fuels to engine operating conditions in knock resistance.	114
Figure 5-45 Temperature-pressure trajectories for load sweep at 2000 RPM normal T condition.	115
Figure 5-46 Temperature-pressure trajectories for different temperatures and loads at 2000 RPM.	115
Figure 5-47 Temperature-pressure trajectories for speed sweep at 10 bar BMEP normal T condition.	116
Figure 5-48 T_{comp15} for various conditions on EcoBoost engine tests as well as CFR engine test. The shapes of the markers represent for different engine speeds and colors stand for engine loads.	117
Figure 5-49 Linear fitting of K vs. unburned gas temperature at IVC.	119
Figure 5-50 R2 of the linear fitting of K and end-gas temperatures at different position during the combustion process.....	119
Figure 5-51 Linear fitting of K vs. unburned gas temperature at spark ignition.	120
Figure 5-52 End-gas temperatures at different loads at 3000 RPM normal temperature condition.	120
Figure 5-53 Linear correlation of K and unburned gas temperatures at CA70.	121
Figure 5-54 Linear fitting of K vs. pressure at IVC.....	122
Figure 5-55 R2 for linear fitting of K and cylinder pressures during the combustion process.	122
Figure 5-56 Linear fitting of K vs. pressure at spark ignition.	123
Figure 5-57 Linear fitting of K vs. pressure at 70% fuel burned.	124
Figure 6-1 EPA Urban Dynamometer Driving Schedule (UDDS) cycle	126
Figure 6-2 EPA Highway Fuel Economy Test (HWFET) cycle.	126
Figure 6-3 EPA US06 cycle.....	127
Figure 6-4 Vehicle speed of Ford SUV towing a 1591 kg (3500 lbs.) trailer in the highway gradeability tests on Davis Dam Grade (part of the SAE J2807 tow rating test). ...	128

Figure 6-5 The simplified power flow of a conventional vehicle.....	130
Figure 6-6 Comparison of engine powers from vehicle test and Autonomie modelling.....	130
Figure 6-7 Engine power from vehicle test and Autonomie modelling for UDDS cycle.....	132
Figure 6-8 Engine speed from vehicle test and Autonomie modelling before adjusting gear shifting strategy for UDDS cycle.	132
Figure 6-9 Gear shifting events from vehicle test and Autonomie modelling before adjusting gear shifting strategy for UDDS cycle.....	132
Figure 6-10 Gear shifting events from vehicle test and Autonomie modelling using the calibrated gear shifting strategy for UDDS cycle.....	133
Figure 6-11 Engine speed from vehicle test and Autonomie modelling using calibrated gear shifting strategy for UDDS cycle.	133
Figure 6-12 Engine torque from vehicle test and Autonomie modelling using calibrated gear shifting strategy for UDDS cycle.	133
Figure 6-13 Effect of motor power on vehicle 0-96 kph (0-60 mph) acceleration performance for the P2 hybrid.	135
Figure 6-14 Power on wheels for HEV on UDDS cycle. Positive power means propulsion and negative power means braking.	136
Figure 6-15 Battery SOC of the HEV over 5 consecutive UDDS cycles.....	138
Figure 6-16 The engine power, motor power and wheels power of the HEV during the UDDS drive cycle.....	138
Figure 6-17 The demanded motor power for a PHEV running in pure electric mode on the UDDS cycle and HWFET cycle.	140
Figure 6-18 All electric ranges along UDDS cycle with different battery capacities.	141
Figure 6-19 The battery SOC and engine power of PHEV64 over 10 consecutive UDDS cycles. Results are from the Autonomie simulation of the developed vehicle model.....	142
Figure 6-20 The correlation curve between CA50 retard from MBT and relative fuel efficiency from [18]. The correlation was validated with spark sweep tests in the present study (solid points).	145
Figure 6-21 Simulated exhaust temperatures at high-speed, stoichiometric, MBT CA50 conditions.....	146
Figure 6-22 Lambda requirement (λ_{req}) map at MBT CA50 to ensure exhaust temperature below 900 °C. (a) is for normal-temperature conditions and (b) is for high-temperature conditions.....	147
Figure 6-23 The correlation of ΔOI and $\Delta CA50$ based on literature data.	148

Figure 6-24 The engine operating conditions in UDDS and HWFET cycles spread over the normal-T K-map.	149
Figure 6-25 The distributions of knock-limited K based on KLFEL in the UDDS and HWFET drive cycles.	149
Figure 6-26 The engine operating conditions in US06 cycle spread over the normal-T K-map.	150
Figure 6-27 The distributions of knock-limited K based on (a) percent of entire drive cycle time, (b) fuel consumption and (c) KLFEL in US06 cycle.	151
Figure 6-28 The effect of (a) RON and (b) MON the KLFEL-based distributions of K for US06 cycle.	151
Figure 6-29 The effect of RON and MON on the overall KLFEL for US06 cycle.	151
Figure 6-30 The distributions of K based on fuel consumption at the knock-limited conditions in the highway gradeability tests on Davis Dam Grade at 72 kph (45 mph) and 104 kph (65 mph).	152
Figure 6-31 The engine operating conditions in the highway gradeability tests on Davis Dam Grade at 72 kph (45 mph) and 104 kph (65 mph). Note: the negative BMEP is due to the fuel cut-off during vehicle deceleration.	153
Figure 6-32 The distributions of K based on KLFEL in the highway gradeability tests on Davis Dam Grade at 72 kph (45 mph) and 104 kph (65 mph).	153
Figure 6-33 The engine speed and engine power in US06 cycle and Davis Dam tow rating.	154
Figure 6-34 The effect of RON and MON on the overall KLFEL in the highway gradeability tests on Davis Dam Grade at (a) 72 kph and (b) 104 kph.	155
Figure 6-35 The comparison of engine operating conditions of the HEV and conventional vehicle in (a) UDDS cycle and (b) HWFET cycle.	156
Figure 6-36 The distribution of knock-limited K based on fuel consumption of HEV vs. conventional powertrain in (a) UDDS cycle and (b) HWFET cycle.	157
Figure 6-37 The KLFEL-based distributions of K of HEV vs. conventional powertrain in (a) the UDDS cycle and (b) in the HWFET cycle.	158
Figure 6-38 The effect of RON and MON on the overall KLFEL for HEV in (a) the UDDS cycle and (b) the HWFET cycle.	159
Figure 6-39 The comparison of engine operating conditions of the HEV and conventional vehicle through the US06 cycle.	160

Figure 6-40 The distributions of knock-limited K of HEV vs. conventional powertrain based on (a) percent of drive cycle time, (b) fuel consumption and (c) KLFEL for the HEV through the US06 cycle.	161
Figure 6-41 The effect of RON and MON on the overall KLFEL for the HEV through the US06 cycle.	162
Figure 6-42 The distributions of knock-limited K based on fuel consumption for the PHEV64 vs. the other two powertrains in CS mode through the (a) the UDDS and (b) HWFET cycle.	164
Figure 6-43 The KLFEL-based distributions of K for the PHEV64 vs. the other two powertrains in CS mode through the (a) the UDDS and (b) HWFET cycle.	164
Figure 6-44 The (a) motor power, (b) engine power and (c) battery SOC in CS mode of PHEV64 vs. HEV in HWFET cycle.	165
Figure 6-45 The effect of RON and MON on the overall KLFEL of PHEV64 in CS mode over (a) the UDDS cycle and (b) the HWFET cycle.	166
Figure 6-46 The distributions of K based on (a) fuel consumption and (b) KLFEL for the PHEV64 vs the other two powertrains in the US06 cycle.	167
Figure 6-47 The effects of RON and MON the total KLFEL of the PHEV64 through the US06 cycle in the CS mode.	167
Figure 6-48 The fuel energy distributions of (a) HEV and (b) PHEV64 in the CS mode over the UDDS cycle (the energy density cloud was calculated with grids of 100 RPM and 1 bar BMEP).	168
Figure 7-1 The effect of interpolation method on the distribution of K including both over-advanced and knock-limited conditions.	181
Figure 7-2 The effect of interpolation method on the distribution of K including only knock-limited conditions.	181
Figure 7-3 The comparison of interpolation methods at several different conditions.	182
Figure 7-4 The simulated fuel consumption for lambda sweep at constant CA50=MBT and constant load.	183

List of Tables

Table 2-1 Composition of a European premium gasoline with RON 98. Only compounds accounting for more than 1 weight % are shown.	8
Table 2-2 The specifications of RON and MON rating conditions as prescribed by ASTM.	9
Table 2-3 Properties of fuels used in [53].	22
Table 2-4 Classification of hybrid and electric vehicles [62]	27
Table 2-5 Terminologies of different parallel HEV configurations	31
Table 3-1 The specifications of dynamometer of test system.	37
Table 3-2 Specifications of 2L Ford EcoBoost GTDI engine	39
Table 3-3 Comparison of the designed octane numbers vs. measured octane numbers by CFR engine.	50
Table 3-4 Fuel properties of n-heptane, iso-octane and EPA certification gasoline.	52
Table 3-5 Summary of engine conditions for normal and high temperature tests.	57
Table 3-6 Results from simulations for 3000RPM, 12bar BMEP, normal temperature condition using different h_{port}	65
Table 3-7 Results of NRMSE from final full engine simulation using different h_{comb}	67
Table 4-1 Summary of engine and test condition	72
Table 5-1 Octane numbers of TRF91-45 and EPA Tier 3 certification gasoline (cert fuel).	117
Table 5-2 The composition of TRF91-45 used as a gasoline surrogate for CFR engine test.	117
Table 6-1 General information of EPA Certification Cycles.	126
Table 6-2 General specifications of Ford Edge (MY19).	129
Table 6-3 Summary of parameters characterizing aerodynamic loss and rolling resistance.	131
Table 6-4 Vehicle performance and fuel consumption of the conventional vehicle. Results were modelled using vehicle modelling.	134
Table 6-5 Data sources of mass calculation for the HEV.	136
Table 6-6 The size of the electric drive system and the resulted vehicle mass of the HEV.	137
Table 6-7 Fuel consumption and vehicle performance of the full hybrid vehicle.	139
Table 6-8 The size of the electric drive system and the resulted vehicle mass of the PHEV64.	141
Table 6-9 HEV and PHEVs in production.	141
Table 6-10 Fuel consumption and vehicle performance of the PHEV64.	143

Table 6-11 Electricity and fuel usage of PHEV64 in the CD mode and CS mode on three drive cycles.	162
Table 6-12 Summary of KLFEL and K_w of different powertrains.....	169

1 Introduction

1.1 Application of Internal Combustion Engine in Transport and Its Future Challenges

The primary energy consumption has been growing from 5 billion toe (ton of oil equivalent, approx. 11,630 kWh/toe) in 1970 to 14 billion toe nowadays and is projected to increase to 18 billion toe in 2040 [1]. The transport sector accounts for 20% of the total, primary energy consumption. Despite increasing penetration of alternative energy sources for propulsion such as natural gas and electricity, petroleum still dominates the transport energy consumption as shown by Figure 1-1(a). There are few doubts that the electric cars will keep increasing in population, however, when comparing the number of battery electric vehicles (BEV) with that of vehicles with internal combustion engines (including conventional, hybrid and plug-in hybrid), the transport sector is still mostly powered by internal combustion engines (ICEs) as shown by Figure 1-1(b).

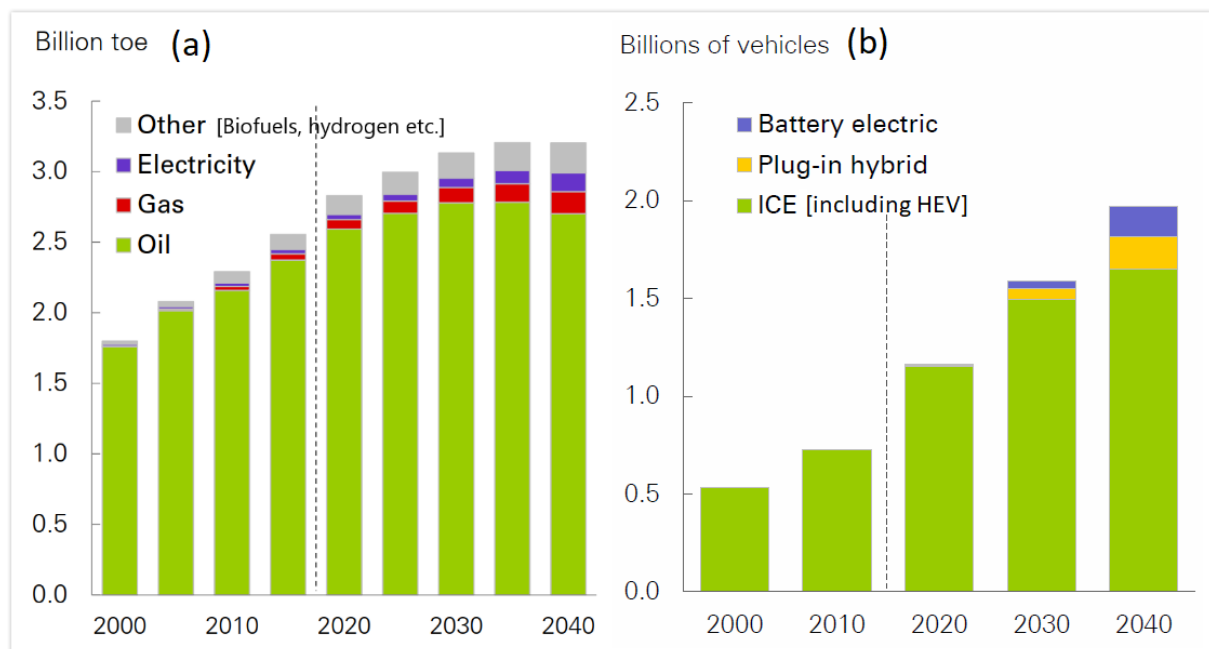


Figure 1-1 The distributions of (a) energy consumption by fuel type from 2000 to 2040 in transport sector and (b) new passenger cars production by fuel type from 2000 to 2040 [1].

Comparing Figure 1-1(a) and (b), the energy consumption by oil is expected to increase gradually and decrease after 2030, but the number of ICE powered vehicles is predicted to increase substantially. This apparent contradiction is due to the improved fuel efficiency driven

by tightening regulations across major markets. For example, the European Commission is targeting 60% or higher reduction of fleet-average CO₂ emission over 1990 levels by 2050, and the US is aiming to achieve 36% CO₂ reduction over 2016 levels by 2025 [2].

In response to these regulations, a wide range of powertrain technologies have been developed, among which advanced engine combustion technologies keep improving the efficiency of conventional powertrain in the near term, while electrification/hybridization has increasing significance in the future. Regardless of the approaches, improving the efficiency of ICE is still a key strategy for emissions reduction before large-scale adoption of BEVs and fuel cell vehicles (FCVs) [3]. The technologies for efficiency improvement of gasoline engines, includes but is not limited to engine downsizing with turbocharging, engine downspeeding with an advanced transmission, variable compression ratio and lean combustion. However, efficiency improvement of gasoline engines will be inevitably limited by engine knock [4].

The engine knock is not caused just by fuel oxidation or engine operating conditions, but by the interactions between the fuel and engine. A good example is the use of refinery stream fuel blends with ethanol in direct-injection spark-ignition (DISI) engines, where engine knock is mitigated by ethanol's strong anti-knock chemistry as well as the charge cooling effect from direct fuel injection [5]. Future fuel standards will therefore be an integral part of the strategies to improve SI engine efficiency and design advanced powertrains.

1.2 Motivation of Research

Research Octane Number (RON) and Motor Octane Number (MON) are primary properties to characterize a fuel's resistance to knock. Historically, it has been found that fuels of higher RON and MON are more knock-resistant. As introduced in the previous section, the anti-knock performance is not a singular function of fuel properties or engine conditions but an overall outcome of interactions of fuel and engine. With the application of advanced combustion technologies, the engine design and engine operating conditions have changed vastly from those of the standard Cooperative Fuel Research (CFR) engine where RON and MON are rated. The relevance of RON and MON to knock resistance is therefore shifted in modern SI engines. Understanding how this relevance changes in modern SI engines, and what impacts it has on fuel efficiency of vehicles is the motivation of the present study.

1.3 Thesis Layout

Following this introduction, Chapter 2 reviews the published research works related to this study and proposes research questions. In Chapter 3, both experimental and numerical methods used in the present study are introduced. The experimental methods include the engine setup and the design of a novel fuel blending system, while the numerical methods include thermodynamic simulation of engine combustion and vehicle simulation of conventional, hybrid and plug-in hybrid powertrains. Chapter 4, 5, and 6 are results chapters. Chapter 4 evaluates the methods for determining Octane Index (OI) and K with experimental data from the literature. Chapter 5 adopts the recommended measurement methodology from Chapter 4 and reports the measured K values over the operating map of a production gasoline turbocharged direct-injection (GTDI) engine, from which the correlations between K values and end gas conditions are proposed. Chapter 6 finally uses the measured K-maps to investigate the significance of RON and MON on the overall fuel efficiency when the engine is used in different powertrains over various driving conditions. Chapter 7 summaries the contributions of the thesis and enumerates the major findings, together with recommendations for future studies on this topic.

2 Literature Review

2.1 Engine Knock

2.1.1 *Causes of Engine Knock and Impacts on Engine Durability*

In SI engine combustion, a flame kernel around the spark plug is formed after spark discharge, and a turbulent flame starts propagating from the kernel, dividing the combustion chamber into two main zones. One zone inside the flame front is termed as the ‘burned zone’, and the region out of flame is called ‘unburned zone’ where unburned air-fuel mixture (end gas) is located. For the ignition that occurs before the top dead center (TDC), the end gas is compressed by the upward motion of the piston and the propagating flame front, both of which serve to increase end gas temperature and pressure. Due to the strong turbulence of the flame, the compressing effect of the flame front is so dominant that the end gas continues being compressed when the piston is moving away from TDC. For the normal combustion in spark-ignition (SI) engines, the flame propagates steadily towards cylinder wall and then combustion extinguishes. Abnormal combustion will emerge when end gas experiences temperature and pressure that are high enough to trigger autoignition, leading to spontaneous heat release [6].

Engine knock manifests as audible noise from the engine. Engine knock was attributed to the detonation when it was first studied and then with the photographic study it was believed that knock was caused by the combined effect of detonation and autoignition in end gas [7]. However, it is now identified that engine knock is caused solely by the end gas autoignition without the influence of flame acceleration or detonation. The runaway exothermic reactions in end gas led by autoignition always result in sharp pressure increase and fluctuation of pressure which normally hits metal cylinder walls and produces pinging noises [8].

As inferred from its name, autoignition is a combustion mode that does not require an external ignition source: instead it is triggered when the temperature starts increasing exponentially with the heat released from chain branching reactions[9]. Compared with the premixed flame propagation, autoignition features spontaneous heat release in the end gas that causes the pressure and temperature of the system to increase sharply[10]. Autoignition is fundamentally controlled by the chemical kinetics of end gas. At different temperature conditions, the chain-branching reactions responsible for the autoignition respond differently. In a review on the hydrocarbon autoignition by Westbrook, it was concluded that autoignition is a simple process

that is controlled by several elementary reactions but it can be affected by different conditions [11].

The strong pressure waves and spontaneous temperature increase from engine knock can cause severe engine damages. The pressure waves generated by knock can impinge on the piston and piston rings and it can cause piston land cracking and breakage of the piston rings after a period of knocking as shown in Figure 2-1 [12]. Furthermore, piston blow-by associated with damage to piston rings will cause engine oil to burn, resulting in significant increases in the emissions of volatile organic compounds. Blow-by will also negatively impact the expansion in the power stroke, reducing engine efficiency. Worse yet, the induced high pressure from autoignition results in localized high temperature regions near the center of autoigniting end gas zone, which will prompt erosion to the cylinder head, piston crown and top land. In the most extreme cases, it can even melt the piston [13].



Figure 2-1 The damaged piston caused by knocking combustion [14].

2.1.2 Knock Constraints on SI Engine Efficiency

The simplest method to improve thermal efficiency is to use higher compression ratio [6]. As given by Eq. 2-1, the thermal efficiency of an ideal constant-volume cycle (an approximation of the SI engine's Otto cycle), increases with higher compression ratio (CR). An example for this is ref. [15], in which a SI engine fueled with ethanol-gasoline blends at three compression ratios showed that engine performance and efficiency can be improved with higher compression ratio throughout engine speeds.

$$\eta_{\text{thermo}} = 1 - \frac{1}{CR^{\gamma-1}} \quad \text{Eq. 2-1}$$

Engine downsizing with turbocharging is widely employed to increase vehicle efficiency. The peak power of a SI engine in light-duty vehicles (LDVs) is designed to provide adequate propulsion for aggressive transient driving, but the engine typically operates at a small fraction of this peak power. The engine efficiency is degraded at light-load conditions where parasitic losses such as pumping and friction loss consume a relatively larger fraction of the total produced work [6]. Turbocharged engines typically have lower compression ratio than naturally aspirated engines as a compromise to knock at high load, resulting in a lower peak thermal efficiency than aspirated engines. However, for a given vehicle, when an engine is downsized with turbocharging, the engine operation shifts to the higher-load region in most driving conditions, while the specific peak power demand can still be produced with intake boosting. This strategy improves the average efficiency of a vehicle as compared to using a larger naturally aspirated engine. An analysis of a turbocharged, downsized gasoline engine showed that the fuel consumption could be reduced by ~20% compared with a larger displacement, naturally aspirated engine for a given vehicle weight [16].

Another common method for improving engine efficiency is downspeeding of an engine. Similar to engine downsizing, by using engine downspeeding, the engine operation shifts to higher torque and lower speed for a given power demand of vehicle, resulting in lower pumping and friction losses. This is achieved by the application of advanced transmissions that have more gears. A report from US Environmental protection agency (EPA) shows that over 80% of new vehicles produced in 1999 had a 4-speed transmission, while 60% of new vehicles produced in 2013 were equipped with a 6-speed transmission. The share of vehicles with more than 6 gears is still increasing [17].

In practice, SI engine efficiency does not improve monotonically with higher compression ratio and higher load operation. At high load or when using a high compression ratio, the engine's in-cylinder pressure and temperature are increased which makes engine knock more likely to happen. To avoid engine knock, spark timing must be retarded from the maximum brake torque (MBT) timing and a significant degradation in efficiency and torque output is resulted [18]. Moreover, spark timing retard increases combustion instability and exhaust temperature. Fuel enrichment is usually used to control the combustion phasing or mitigate the thermal load of the turbomachinery, as the compressed temperature are lower with a lower specific heat ratio

and exhaust temperature is reduced with a higher heat capacity. However, this measure results in an additional penalty in efficiency. The overall efficiency of SI engines is diminished in these circumstances because efficiency loss due to retarded combustion phasing or fuel enrichment cannot be compensated by the efficiency gain from the operation at higher load or higher compression ratio [19].

2.1.3 Effect of Fuels on Efficiency Improvement for Knock-Limited Engines

Results from ref. [20] for knock-limited engine tests under two different compression ratios and various loads at 1000 RPM (revolution per minute) are shown in Figure 2-2. In Figure 2-2(a), combustion phasing is more retarded at higher compression ratio than at lower compression ratio for a given fuel. Consequently, as given in Figure 2-2(b), the brake thermal efficiency (BTE) is increased for the higher compression ratio case at light-load, but BTE decreases with increasing load due to the retarded CA50 (crank angle at 50% of the total heat release). At sufficiently high Brake Mean Effective Pressure (BMEP), the BTE at higher compression ratio is less than that at a lower compression ratio, indicating higher compression ratio does not necessarily improve engine efficiency when knock is present.

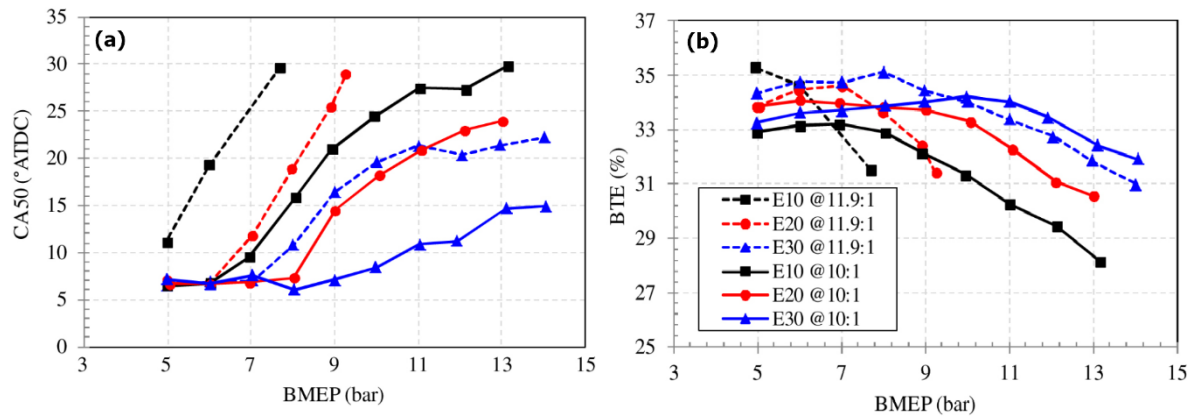


Figure 2-2 Combustion phasing and BTE vs engine load at 1000 RPM [20]. Dashed lines are for higher compression ratio and lines of same color and mark are for the same fuel.

Comparing different fuels in Figure 2-2(a) where E30 has the highest octane number and E10 has the lowest octane number, the CA50 (Crank angle at 50% of the total heat release) of E30 is less retarded than that of E10 and E20 when compression ratio is increased. The load range of higher BTE by higher CR is extended when using fuels of higher octane number as shown in Figure 2-2(b).

By reviewing these results, it can be concluded that knock limits engine efficiency and higher CR produces higher engine efficiency at light-load condition, but engine efficiency at higher CR can be lower than that at lower compression ratio when engine operates in knock-limited regions of the operating map. This knock-limited efficiency can be relaxed by using fuels of higher knock resistance, suggesting fuel properties play a significant role in enabling higher engine efficiency.

2.2 Fuel Properties for Knock Resistance

Many fuel properties can affect engine combustion, and for knock resistance in particular, the Octane Numbers (ONs) of fuels are most important ones. The autoignition of a fuel is fundamentally dependent on its chemistry so the ultimate metric for evaluating the resistance to knock is to investigate its chemistry at engine-like conditions [21]. However, the composition of gasoline is extremely complex. For example, a typical European Premium gasoline has over 20 major components (Table 2-1), and apart from these compounds, the remaining 30% is made up by over hundreds of other species [22]. The intricate chemistry of all the species and their chemical interactions make it unrealistic to use the fundamental chemistry to evaluate and understand the knock resistance of practical fuels at present. Therefore, a fit-for-purpose metric, octane number, for evaluating fuels' knock resistance was developed and has been accepted as a worldwide standard test for fuels used for SI engines.

Table 2-1 Composition of a European premium gasoline with RON 98. Only compounds accounting for more than 1 weight % are shown.

Species	Weight %	Species	Weight %
toluene	11.7	n-pentane	2.02
isopentane	11.43	isobutane	1.87
m-xylene	6.93	trans-pent-2-ene	1.7
n-butane	5.41	m-ethyltoluene	1.65
iso-octane	4.34	2-methyl-1-ene	1.39
o-xylene	4.04	2-methylbut-1-ene	1.39
ethylbenzene	3.04	3-methylpentane	1.31
1,2,4-trimethylbenzene	2.69	2,3,4-trimethylpentane	1.3
p-xylene	2.58	2-methylhexane	1.24
2-methylbut-2-ene	2.3	benzene	1

2-methylpentane	2.07		
-----------------	------	--	--

2.2.1 Octane Numbers

Two octane numbers, RON and MON, are assigned to a fuel. Both are determined in the CFR engine at two standardized conditions as listed in Table 2-2 [23, 24]. The RON is measured at a lower engine speed and a lower intake temperature than the MON. Both the RON and MON are assigned to a test fuel by referencing the knocking performance to the octane scale that is defined by the volumetric blending of iso-octane and n-heptane, of which the binary mixture is called Primary Reference Fuel (PRF). The 0 point on the octane scale is defined by pure n-heptane that is a straight-chain alkane of high autoignition reactivity. The 100 point on the octane scale is defined by pure iso-octane that is highly branched alkane and is difficult to auto-ignite. The octane number higher than 100 is defined by mixtures of iso-octane and tetraethyllead (TEL). In the standardized octane tests, the ON of the fuel is determined by matching the test fuel with a PRF that has the same knocking intensity at the same compression ratio. Depending on the operating conditions, the ON determined at Research condition is assigned to be Research Octane Number (RON) and ON determined at Motor condition is named Motor Octane Number (MON).

Table 2-2 The specifications of RON and MON rating conditions as prescribed by ASTM.

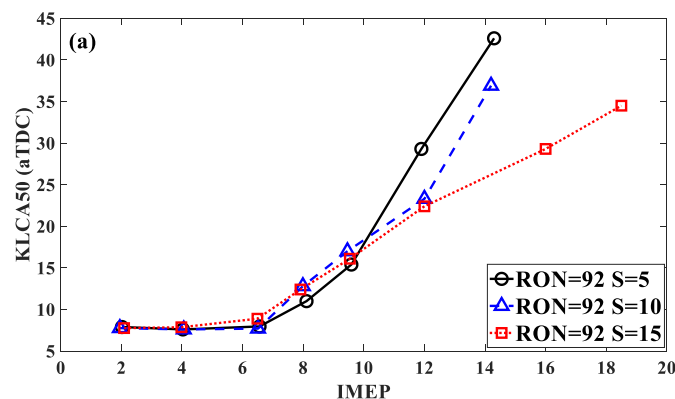
Condition	Research	Motor
Engine Speed (RPM)	600	900
Intake Temperature (°C)	52 (Intake air)	149 (Intake air-fuel mixture)
Spark Timing (CAD bTDC)	13	14-26
Compression Ratio	Variable	
Fuel supply	Carburetor	
Lambda	Adjusted to maximum knock intensity	
Intake pressure	Unthrottled	

2.2.2 Octane Sensitivity

The octane sensitivity (S) of a fuel is defined as the difference between RON and MON, as given by Eq. 2-2 [23, 24]. Fuels of zero octane sensitivities are generally called ‘non-sensitive fuels’ while fuels of non-zero octane sensitivities are grouped as ‘sensitive fuels’. The octane sensitivity is generally positive since RON in most cases is higher than MON for sensitive fuels. Paraffins generally have low octane sensitivities because iso-octane and n-heptane have zero octane sensitivity by definition and other paraffins chemically behave similarly to them. Other fuels such as olefins, aromatics, alcohols, diolefins, are sensitive fuels [25]. The commercial gasolines have different compositions in different markets, but all have aromatics and olefins as major components, for instance the gasoline shown in Table 2-1. As a result, most gasolines have octane sensitivity in the range of 7-12 [22].

$$S = RON - MON \quad \text{Eq. 2-2}$$

The octane sensitivity has drawn much interest because of its significance for improving the knock limit and thus engine efficiency at some engine operating conditions. The results from a study by Prakash et al. [26] are adapted for better presentation in Figure 2-3a where the fuel of higher S shows less CA50 retard from MBT than another fuel of lower S from mid-load i.e. 10 bar indicated mean effective pressure (IMEP) to high-load at 1800 RPM. With less retarded combustion phasing from MBT timing, engine efficiency is higher with the high sensitivity fuel at the tested conditions (Figure 2-3b).



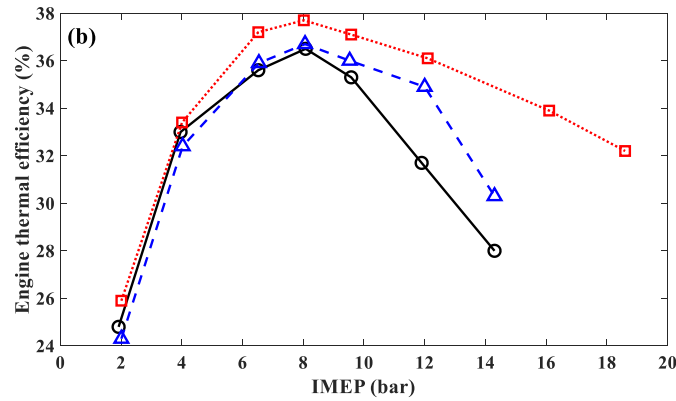


Figure 2-3 Effect of octane sensitivity on the (a) knock limit and (b) engine efficiency at 1800 RPM and CR=11.5:1 condition. Adapted from [26].

To reveal the reasons behind the superiority of using sensitive fuels at some conditions, the chemical and physical origins of octane sensitivity were investigated. The first study on the chemical origin was done by Leppard in 1990 who concluded that the alkanes have a two-stage ignition mechanism where low-temperature heat release is followed by a negative temperature coefficient (NTC) behavior that the reaction rates are inverse to temperature increase. After the NTC region, a hot-ignition process featuring high-temperature heat release will happen. Octane sensitivity is therefore correlated with the presence of strong NTC behavior of PRFs at MON condition which makes the autoignition less promoted by the higher temperature at MON condition when compared with sensitive fuels that do not have two-stage ignition mechanism and do not show noticeable NTC behavior [27]. A later study by Mehl et al. confirmed this finding using the chemical kinetics modelling which demonstrated that the pressure-temperature evolutions of PRFs go through the NTC region at MON condition while it is not the case for sensitive fuels that do not exhibit the strong NTC behavior [28]. A recent study by Westbrook et al. on the chemical kinetics of octane sensitivity showed the low-temperature reactivity of PRFs is much stronger at RON-like condition than at MON-like condition, while sensitive fuels, on the other hand, have less or no low-temperature reactivity at both RON and MON conditions [29]. The plots in Figure 2-4 show the heat release profiles of a non-sensitive fuel (PRF80) and a sensitive fuel (3-hexene, RON=94, MON=80) having the same MON value. At MON condition, PRF80 exhibits small intermediate temperature heat release (ITHR) before the hot-ignition with a plateau related to NTC behavior in between. Although 3-hexene (sensitive fuel) shows no ITHR, it autoignites at the same timing as PRF80, indicating they have similar anti-knock performance at MON condition. At RON condition, the low-temperature heat release (LTHR) of PRF80 emerges, producing active species and temperature increase that accelerate the hot-ignition process, making PRF less knock-resistant compared

with 3-hexene that has no LTHR at RON condition. Therefore, the RON of 3-hexene is higher than 80 i.e. it has positive octane sensitivity.

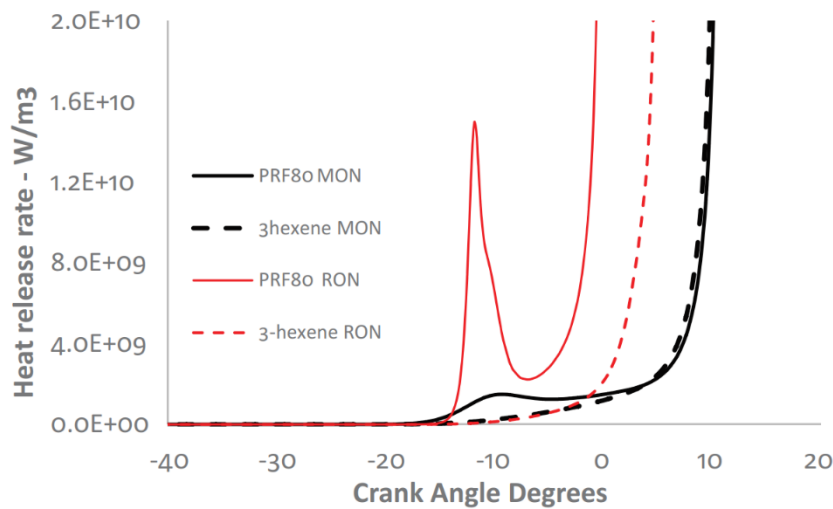


Figure 2-4 Heat release rates from chemical kinetic modelling of PRF80 and a sensitive fuel (3-hexene) at RON rating condition and MON rating condition. Two fuels share the same MON value of 80 but 3-hexene has high octane sensitivity. Figure from [29]

In the perspective of physical origin, it has been found that the heat of vaporization (HoV) of fuels contributes to the octane sensitivity [25, 30, 31]. Comparing the RON and MON conditions listed in Table 2-2, one of the main differences is the intake temperatures. At MON condition, the air-fuel mixture temperature downstream of carburetor is controlled at 152°C in which case no charge cooling effect presents. By contrast, at RON condition, the intake air temperature (IAT) upstream of carburetor is controlled at 52°C where the vaporization of fuel will happen downstream of carburetor and hence the charge temperature is lowered by the charge cooling effect. The autoignition is therefore inhibited by the lower temperature caused by the charge cooling effect at RON condition, and this interaction contributes to the RON, especially for ethanol contained fuels. To quantify the effect of charge cooling on RON (or S), Foong et al. developed a so-called ‘modified RON’ test in which the intake air temperature was adjusted to separate the effects of charge cooling and autoignition chemistry [30]. The results are re-plotted in Figure 2-5 and it shows when ethanol content is high i.e. HoV is high, charge cooling effect contributes significantly to the high RON.

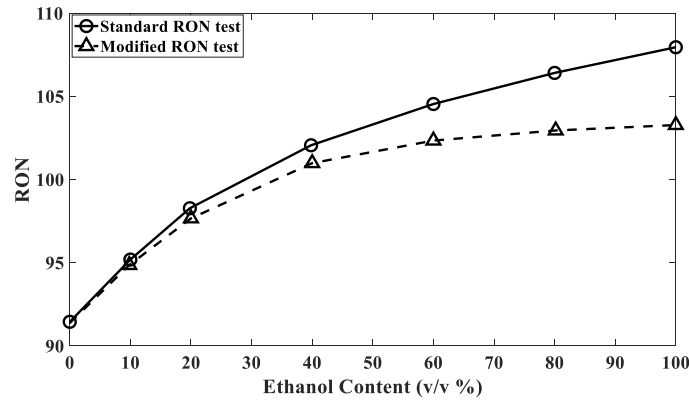


Figure 2-5 RON values of ethanol/gasoline blends from standard RON test and modified RON test. Adapted from [30]

2.2.3 Relevance of RON and MON to Modern Engine Knock

As introduced in 2.2.1, MON condition features higher charge temperature than RON condition, resulting a higher gas temperature at MON condition than that at RON condition for a given pressure. Historically, these two conditions were designed to bracket operating conditions in typical engines in 1930s [32]. However, compared with the CFR engine for ON rating, the efficiency and performance of modern SI engines have been improved considerably through the iterations of engine technology, and correspondingly, the operational regimes have been extended beyond those in the CFR engine [33]. For example, nearly all engines had carburetors and only two valves per cylinder with fixed timing before 1975. Nowadays, more than half of new vehicles are equipped with direct injection (DI) and almost all have variable valve timing (VVT) [17]. Advanced engine technologies have significantly improved the specific output of engine (Figure 2-6) which produce much higher in-cylinder pressure i.e. engine operating conditions in modern engines have changed notably. Given these differences, a question drawn here is how fuel's RON and MON that are rated with CFR engine are relevant to the actual knock limit in modern SI engines.

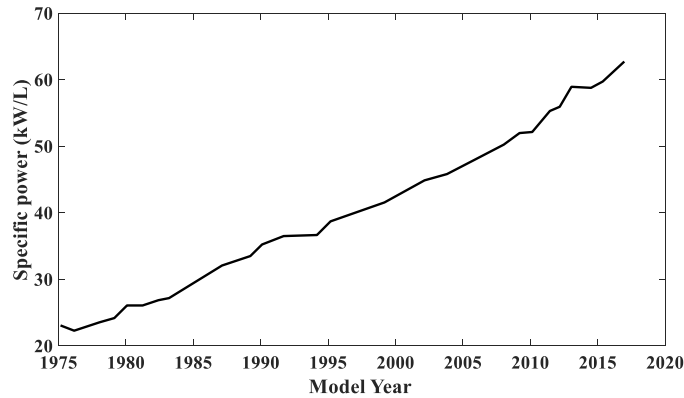
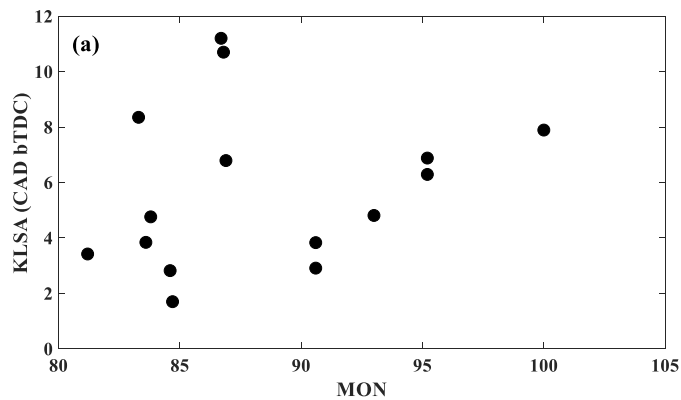


Figure 2-6 The average specific power of the LDVs from 1975 to 2017 in US market. Adapted from [17].

In response to this question, the effect of RON and MON on the knock limit in a modern DISI engine was investigated in ref.[34]. Figure 2-7 shows some results of the knock-limited spark advance (KLSA) for fuels of various RON and MON on a boosted downsized DISI engine. From Figure 2-7(a), MON is not well correlated with KLSA while RON is overall better correlated with KLSA compared with MON as shown by Figure 2-7(b). It should also be noted that for MON in range of 80-90 and RON in range of 95-100, increasing MON or RON did not necessarily improve the knock limit.



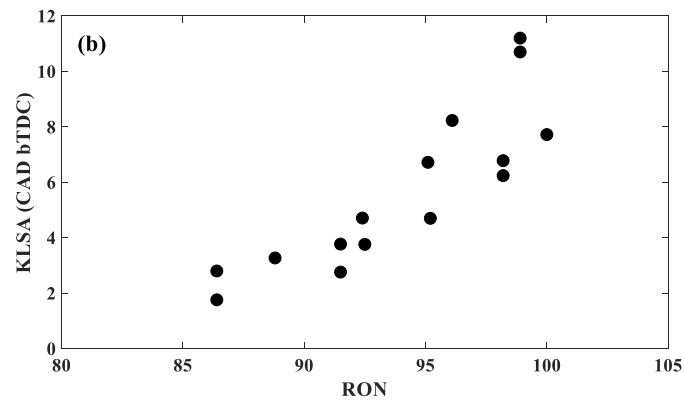


Figure 2-7 Effects of (a) MON and (b) RON on the knock-limited spark advance for a downsized DISI engine at 2000 RPM. Data from [34].

Apart from engine tests, vehicle tests were also conducted to investigate the relevance of ONs to vehicle performance in ref.[35]. Figure 2-8 shows results from vehicle tests in which vehicle equipped with 2L turbocharged DISI engine accelerated from 25-80 mph at the fixed 5th gear and tests were repeated for fuels of different octane numbers. Comparing (a) and (b) in Figure 2-8, RON better correlates to the vehicle acceleration performance than MON does. However, no strong correlation can be observed. For example, for MON of 82-88 and RON of 90-98, the vehicle performance does not improve accordingly with either higher MON or higher RON.

From above reviews, it can be summarized that RON can correlate better to the knock limit in modern SI engines than MON, but it might not be appropriate way to directly use RON or MON solely to characterize fuels anti-knock quality.

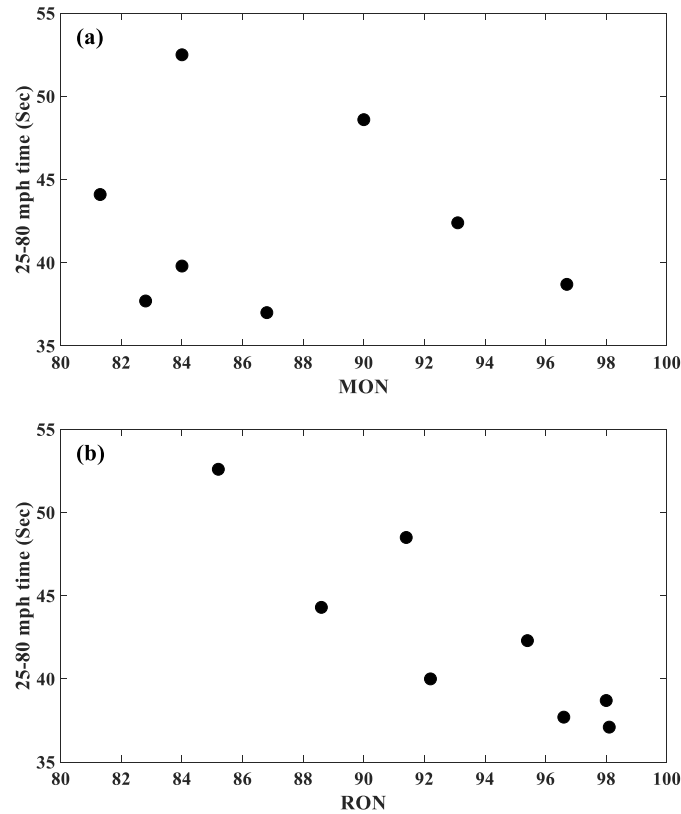


Figure 2-8 Effects of (a) MON and (b) RON on the 25-80 mph acceleration at fixed 5th gear. Data from [35].

2.3 Octane Index and K Value

2.3.1 Introduction of Octane Index

Due to the decreased relevance of RON and MON to the knock limit of modern SI engine, a more appropriate indicator, octane index (OI), for defining fuel's actual anti-knock quality was proposed by Kalghatgi in 2001 [36, 37]. As given by Eq. 2-3, OI is a linear function of RON and MON of a fuel and K is a factor that is primarily dependent on engine design and engine operating condition. Equivalent to Eq. 2-3, a more commonly used formula of OI is expressed by Eq. 2-4 where S is octane sensitivity as given by Eq. 2-2. As shown by Eq. 2-3, K factor weights the relative contribution of RON and MON to OI. This concept is essentially same as Road Octane Number that is defined by ASTM [23, 24] as given by Eq. 2-5 where K_1 , K_2 and K_3 vary with vehicles. For example, anti-knock index (AKI) of a fuel approximates the Road ON by setting K_1 , K_2 and K_3 at 0.5, 0.5 and 0 respectively and is commonly labelled on all service stations in US, Canada and some other countries. The OI is not an arbitrary definition but instead it is based on the octane scale prescribed by PRFs. Since any PRF has zero sensitivity ($S=0$), the OI of a PRF is always equal to its RON or MON, which means the OI

concept can be regarded as a variant octane rating method with K interpolating or extrapolating the standardized RON and MON conditions to any actual engine operating condition.

$$OI = (1 - K) \cdot RON + K \cdot MON \quad \text{Eq. 2-3}$$

$$OI = RON - K \cdot S \quad \text{Eq. 2-4}$$

$$\text{Road ON} = K_1 \cdot RON + K_2 \cdot MON + K_3 \quad \text{Eq. 2-5}$$

There are many studies showing that OI is a more proper indicator for characterizing fuel's anti-knock ability than either RON or MON only [26, 34, 36-46]. Taking the same data in Figure 2-7 and Figure 2-8 as an example, the actual knock-limited performances such as KLSA and acceleration time were better correlated with OI than with either MON or RON as shown in Figure 2-9 when compared with Figure 2-7 and Figure 2-8.

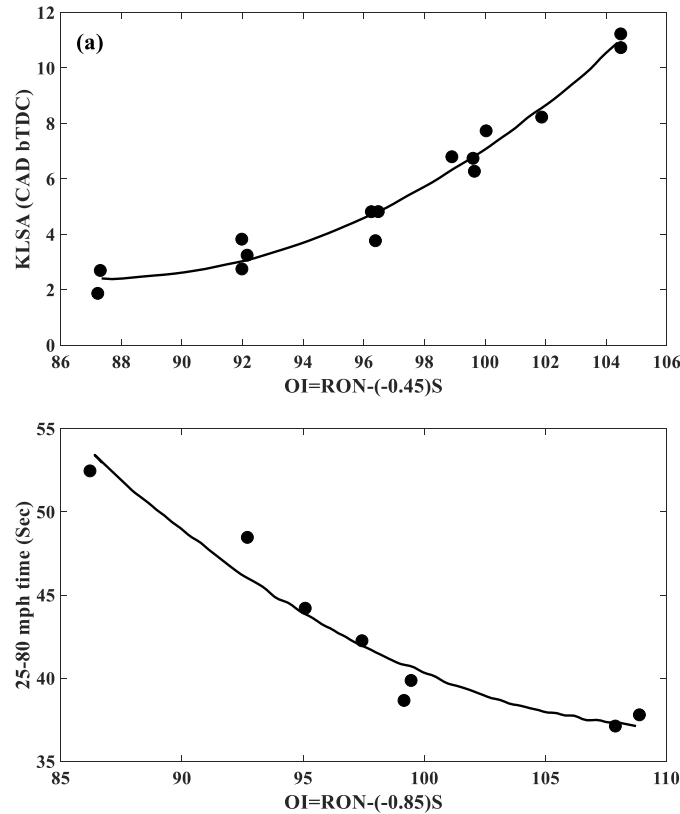


Figure 2-9 (a) KLSA vs OI with the same data in Figure 2-7 and (b) acceleration time vs OI with the same data in Figure 2-8. Adapted from [34, 35]

2.3.2 Methods for Determining K

Several methods were used in literature to determine the K value, which can be categorized as regression methods and PRF methods.

When the OI concept was proposed by Kalghatgi [37], a linear regression method was used, in which a linear relationship between KLSA and OI was assumed and K was determined by finding the K value producing the best linear fitting of KLSA and OI. In a later study by Davies et al. [34], a 2nd order polynomial relationship between KLSA and OI was used. In regression methods, several fuels of uncorrelated RON and MON were used at the same engine operating condition, and regression was used to find the best fitting of the experimental data.

In a study by Mittal et al. [40], the PRF method was adopted. This method used a more rigorous definition that the OI of a PRF is equal to its RON and MON (S=0). In this method, a range of PRFs were tested at knock-limited conditions, from which the calibration curve of OI was established. Then, the knock limits of a sensitive fuel were tested, and OI was determined by comparing the sensitive fuel's knock limit to that of PRFs. Once OI of a sensitive fuel is known, the K can be calculated with Eq. 2-6.

$$K = \frac{RON - OI}{S} \quad \text{Eq. 2-6}$$

Davies et al.[47] also used the PRF method to determine the K value. Different from the studies introduced above, the K value in [47] was obtained using simulation. The trajectory of pressure and unburned gas temperature for a certain engine operating condition was calculated. Then the ignition delay times of PRFs along the trajectory were determined using detailed chemical kinetics and the Livengood-Wu autoignition integral (Eq. 2-7) [48], which provided the autoignition timings (τ_e) of PRFs. The same calculation was done for a Toluene Reference Fuel (TRF, toluene/n-heptane mixture) that has the similar RON and MON of gasoline. The OI was determined by referencing the autoignition timing of TRF to that of PRFs, from which the K value was determined with Eq. 2-6.

$$\int_{t=0}^{t=\tau_e} \frac{1}{\tau} dt = 1 \quad \text{Eq. 2-7}$$

Where: τ_e is the autoignition timing,
 τ is the ignition delay time of the condition at a time instance dt

2.3.3 Effect of Engine Operating Conditions on K

The K value gives the information of the relative significance of MON and RON to actual anti-knock performance under a certain engine operating condition. Knowing the K values for

different engine conditions helps interpret the effects of fuel properties (RON and MON) on knock suppression and design fuels for better efficiency improvement [43]. Figure 2-10 demonstrates how to design the RON and MON of a fuel to improve knock resistance using this concept. For example, when K is negative, the OI of a sensitive fuel is higher than its RON and using a fuel of higher RON or lower MON can improve the knock resistance. There are several studies that experimentally determined K values and provided some observations of variation of K with engine related factors, as summarized in the following.

Higher RON Lower MON	Higher MON Higher RON	Higher MON Lower RON
OI>RON	$RON \geq OI \geq MON$	OI>MON
0	0.5	1
K factor		

Figure 2-10 The demonstration of K for characterizing the significance of RON and MON to improving knock resistance and the relationship between OI and ONs.

Amongst the engine parameters affecting K value, engine load or intake pressure has the most dominant effect over others. A decreasing trend of K with increasing engine load or intake pressure has been observed in many studies (Figure 2-11) [34, 37, 39-41, 49].

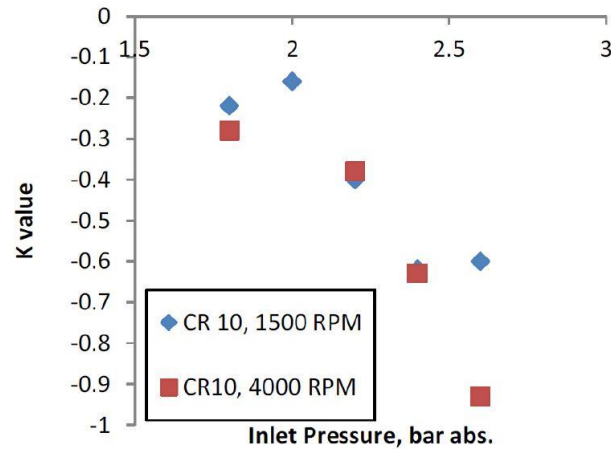


Figure 2-11 Effect of intake pressure (engine load) on K at two different engine speeds [41].

In some studies, K factors have been found to increase with engine speed regardless of compression ratio, engine load or other engine operating conditions [37, 39, 40, 47, 49, 50]. Examining Figure 2-12, though K factors are different depending on the data sources, they generally show that K increases with increasing engine speed. But this trend is not strictly monotonic and the change in K is not so sensitive to engine speed, with the slope approximately ranging from 0.15/1000RPM to 0.3/1000RPM.

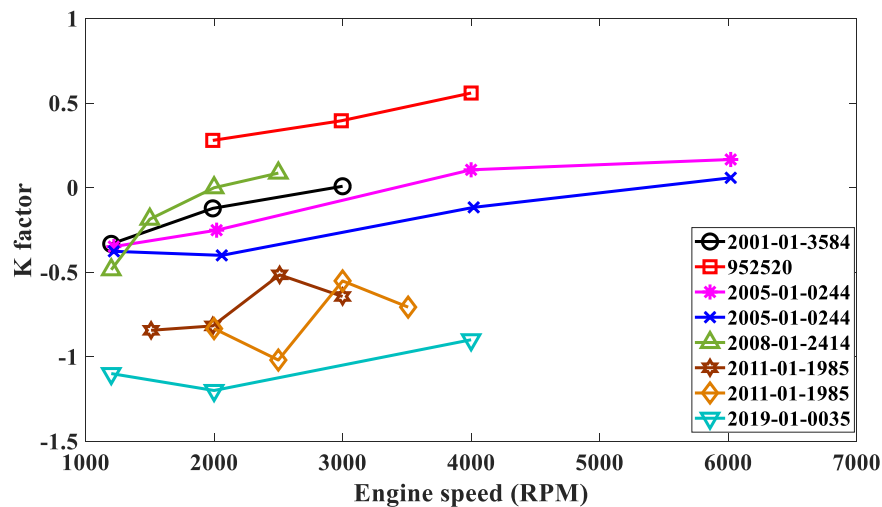


Figure 2-12 K factor vs engine speed from literatures. The numbers in legend are SAE paper number.

Compression ratio effect is controversial, some studies showed K is insensitive to compression ratio change [40, 49] but experiment from Kalghatgi showed K slightly decreases with higher compression ratio [39]. Mittal et al. explained that the change in compression ratio resulted in approximately the same change in knock-limited combustion phasing for a PRF as for other test fuels. As a result, K showed almost no change with compression ratio [40].

Effect of air-fuel mixture strength (λ) has not been investigated much as SI engine combustion is mainly or entirely at stoichiometric condition. Engine experiments from Gerty et al.[51] and Mittal et al. [40] revealed that K decreases when combustion becomes either leaner or richer from stoichiometric condition.

2.3.4 Relation between K value and End-gas Condition

There are only a few studies on the fundamental cause of K in the prospective of end-gas conditions. Kalghatgi et al. first investigated the end-gas conditions at conditions of different K in the HCCI engine and used a single parameter, T_{comp15} that is the temperature of unburned gas at pressure of 15 bar, to characterize the pressure-temperature trajectory of the unburned gas [52]. Kalghatgi found there was a strong correlation between K and T_{comp15} and summarized that at higher pressures or lower temperatures i.e. T_{comp15} was lower, K was lower. Kalghatgi then applied the same idea to SI engine combustion and proposed T_{comp15} could also be used in SI engine to characterize the variation of K with engine operating conditions.

A later study by Amer et al. calculated T_{comp15} for SI engine tests and found there was indeed an obvious increasing trend of K vs T_{comp15} as illustrated by Figure 2-13. However, it should be noted that this correlation is not very strong. Scattered points from 550 to 600K can be observed and R^2 of the linear fitting is only 0.77. Recently, a research work by Szybist et al. found the proposed correlation of K and T_{comp15} was not universally applicable [53].

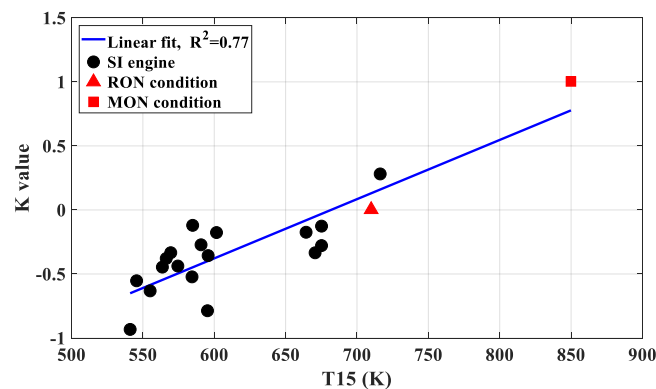


Figure 2-13 Correlation of T_{comp15} with K values. Replotted with data from [41].

2.3.5 Fuel-Specific Issues of Octane Index and K

Autoignition in SI engine is such a complicated process that is fundamentally relied on fuel's autoignition chemistry. It is therefore critical to identify whether the OI model is capable to fully characterize different fuel's practical anti-knock ability in SI engine combustion.

Szybist et al. investigated several fuels in a DISI engine under boosting conditions [53]. The fuels' properties are listed in Table 2-3 in which Alkylate, Aromatic and E30 have the similar RON=98 but different S. Alkylate has the smallest S while Aromatic and E30 have similar S=11. Also noted is E30 has the lowest LHV but the highest HoV. The combustion analysis showed some fuel-specific differences in pressure-temperature history at certain engine operating conditions as illustrated by Figure 2-14. At the first condition (left figure), all fuels exhibit a cooling hook around TDC due to the heat loss. Alkylate, Aromatic and Tier III share the identical history while temperature of E30 is 10-15 K lower. This difference is caused by high HoV and low LHV of E30. Under the second condition of higher intake pressure and intake temperature (right figure), Alkylate, Aromatic and Tier III show the diminished cooling hook near TDC. Although not depicted in the figure, this change is due to the net heating effect caused by pre-spark heat release [54]. Comparing the pressure-temperature trajectories of E30 and Aromatic, the separation is obvious despite they have almost same RON and MON. The results shown in Figure 2-14 indeed demonstrate the pressure-temperature trajectory at a given engine operating condition is affected by the fuel-specific properties other than RON and MON. As OI model assumes that RON and MON are the only properties describing the fuel chemistry and K is the only property describing engine thermochemical conditions, the fuel impact on pressure/temperature trajectories inside the cylinder reveals some limitations of applying the OI model.

Table 2-3 Properties of fuels used in [53].

	Alkylate	Aromatic	E30	Tier III E10
<i>RON</i>	98.0	98.1	97.9	91.8
<i>MON</i>	96.7	87.6	87.1	84.2
<i>S</i>	1.3	10.5	10.8	7.6
<i>LHV (MJ/kg)</i>	44.52	42.95	38.17	41.69
<i>HoV (kJ/kg)</i>	308	361	532	416

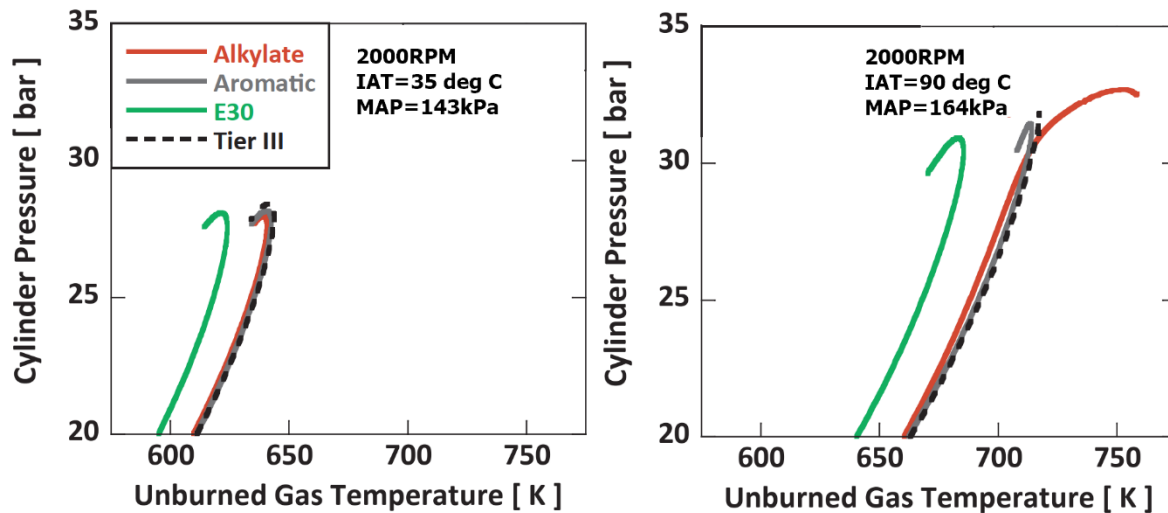


Figure 2-14 Pressure-temperature evolutions of four fuels at two operating conditions. Noted that these profiles end at the spark timing and all fuels have the similar CA50 of 37-39 ° aTDC. Figure from [53].

Another study using the above four fuels shows similar results regarding the pressure-temperature trajectories[55]. However, different from [53], the pressure-temperature evolution of the unburnt gas is extended from the spark timing to the point just before autoignition. The plots in Figure 2-15 are for the fuels in Table 2-3 tested under two engine operating conditions. At lower intake pressure condition, Aromatic and Alkylate share the end-gas condition in the early portion of the profile but then diverge after spark timing with Alkylate experiencing higher temperature than Aromatic. The higher temperature of Alkylate is due to the LTHR after TDC. By contrast, E30 experiences lower temperature throughout the cycle, mainly due to its high HoV. Of interest is that E30 autoignites at the lowest temperature among the test fuels and Alkylate autoignites at the highest temperature, indicating E30 is the least resistant to high temperature while Alkylate is the most resistant to high temperature. At 110 kPa intake pressure, E30 still experiences the lowest temperature over the cycle and the divergence between Aromatic and Alkylate after TDC is more obvious. The temperatures of Alkylate and Aromatic are lifted by the LTHR and Alkylate still reaches the highest temperature. In summary, although E30 is sensitive to high temperature but it has greater HoV and no LTHR which causes lower temperature compared with the other two fuels at the same engine condition; on the other side, Alkylate has great resistance to high temperature but the temperature of it is higher due to the presence of strong LTHR and absence of high HoV. As a result, these fuels have similar overall practical knock resistance i.e. similar CA50 as predicted by the similar OI of these fuels.

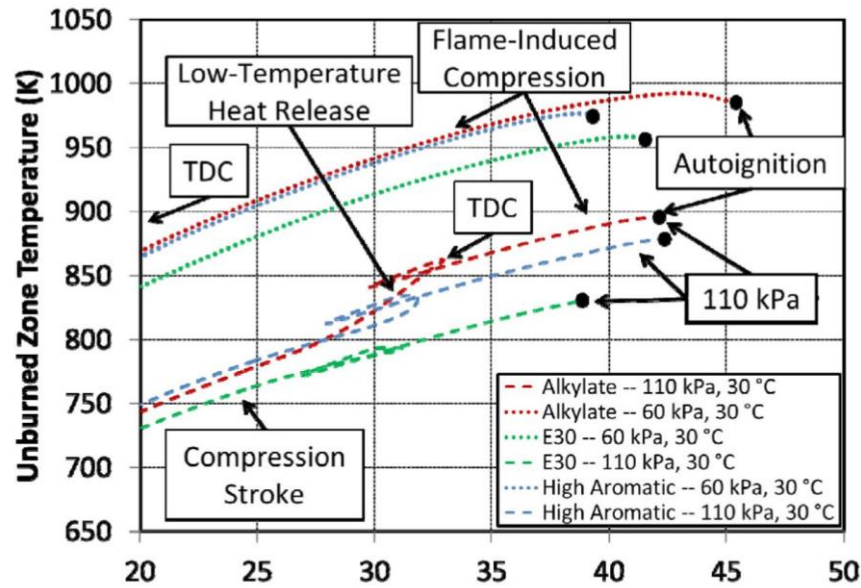


Figure 2-15 Temperature-pressure evolutions of unburned gas leading to the autoignition point for three fuels at two engine operating conditions. Figure from [55].

A follow-up study by Vuilleumier et al. assessed the uncertainty of OI framework for predicting knock limits of several gasoline blends of the same RON and MON [56]. Results showed that fuels of similar RON and S (RON=98, S=10) yielded very similar knock limits across the entire engine operating conditions investigated. Uncertainty analysis indicates approximately 84% of the fuel's behavior is captured by OI, while the remaining 16% may be caused by molecule-specific effects of fuel formation.

To sum up, despite of fuel-specific deviations, OI is able to characterize the majority of knock-limited behavior of fuels and is a better predictor of anti-knock performance than either RON or MON only.

2.4 Hybridized Powertrains with Combustion Engine

Driven by the regulations of emissions and customers' expectations for fuel saving, advanced powertrain technologies have been adopted. One of the most effective approaches is powertrain hybridization that combines ICE with electric motor for propulsion which significantly alters engine operation relative to a conventional powertrain. In this section, different powertrain configurations are reviewed and engine operations on those powertrains are introduced.

2.4.1 Conventional Powertrain

The conventional powertrain mainly consists of an internal combustion engine, transmission and transaxle without any electrical-assistant drive. The efficiency of it can be increased by improving engine efficiency or optimizing transmission or the combination of these two. A long-term trend in engine efficiency improvement is attributable to the exclusive application of advanced engine technologies [17], as discussed in Sections 2.1.2 and 2.1.3 of this thesis.

In addition to using advanced engine technologies, the development of transmission evolves applications of dual clutch transmission (DCT), continuously variable transmission (CVT) and automatic transmission of more gears [57, 58]. Lemazurier et al. investigated the impact of transmission gear ratios on engine operation by simulating the vehicles of different transmissions but with the same engine over the UDDS cycle (typical city driving) [58]. The results show engine predominantly operates between 1200 and 1700 RPM for a vehicle with 6-speed automatic transmission. The engine operation range is narrower, and speed is lower by 200 RPM when an 8-speed automatic transmission is used. The engine speed range for 8-speed DCT is even slightly narrower than that of 8-speed automatic and centralizes to 1300 RPM. Since the power for vehicle propulsion is same, the engine operation shifts to higher BMEP when engine speed moves to the lower range.

To sum up, the technical approaches for improving fuel efficiency of conventional powertrain normally transfer the engine operation to lower RPM and higher load range where efficiency is higher, but knock is more likely to happen at these conditions. Furthermore, the change in engine operation range affects the thermodynamic conditions of combustion and thus may alter the requirement for fuel properties [59].

2.4.2 Hybrid Electric Powertrains

2.4.2.1 Degree of Electrification of Hybrid Vehicles

The hybrid electric powertrain uses electric motor(s) and an ICE to provide power to the vehicle. The most distinct benefit of powertrain hybridization is fuel saving. As shown in Figure 2-16, although the fuel consumption of conventional vehicles has been decreasing remarkably over the years thanks to the advanced engine technologies, the hybrid vehicles still have overwhelming advantage than conventional vehicles in terms of fuel economy.

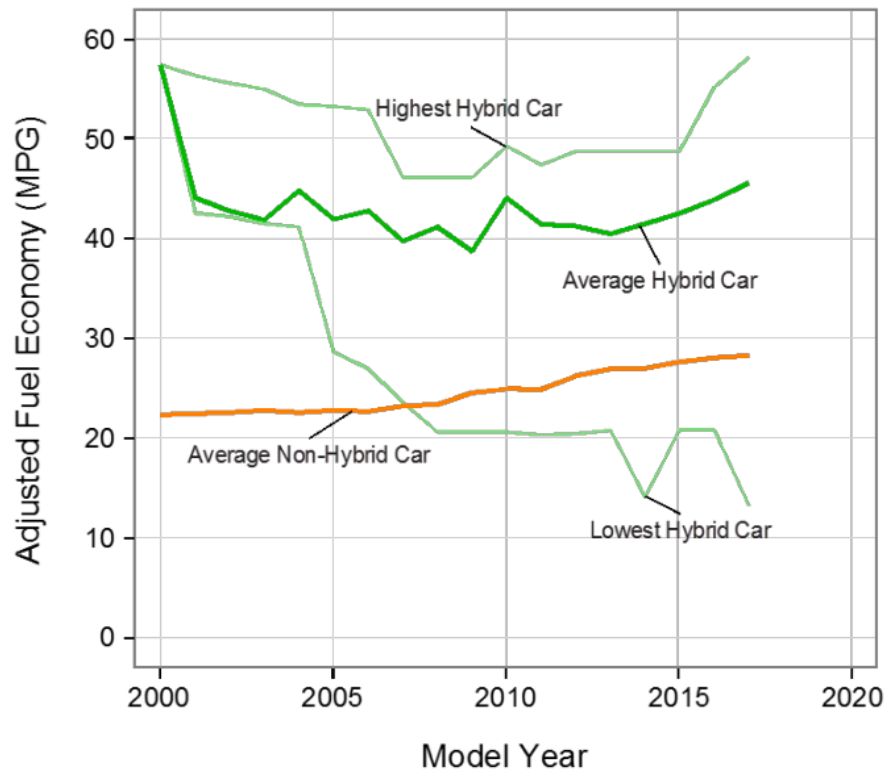


Figure 2-16 Fuel consumption data of conventional vehicles and hybrid vehicles (light-duty segment) sold in US market from 2000 to 2017. Fuel consumption is based on US EPA 2-cycle test. Figure from [17].

Depending on the degree of electrification, there are different types of hybrid powertrains, as listed in Table 2-4 [60]. The lowest class is called micro hybrid which is basically a conventional powertrain with engine stop-start function and in some cases, this type of powertrain is classified as conventional powertrain. It uses the 12V battery available to shut down ICE during vehicle stop and restart engine immediately when brake paddle is released. Micro hybrid vehicles have no or very limited brake energy regeneration and cannot provide any electric propulsion, so fuel saving is achieved by avoiding the fuel consumption at engine idling. The next class of higher degree of electrification is the mild hybrid which has limited regenerative braking capacity and limited power from motor to assist engine. Traction motor on a mild hybrid typically has 5-20 kW of power which requires battery pack of more energy and higher voltage than a micro hybrid, for example, most mild-hybrid systems use 48V electric power supply [61]. Higher than micro hybrid fuel saving is attributed to regenerative braking and optimized engine operation with motor assistance in addition to the stop-start function.

Table 2-4 Classification of hybrid and electric vehicles [62]

Types	Degree of electrification	Functions	Source of energy	Fuel saving relative to conventional
Micro hybrid	Low	Stop-start, no or limited regenerative braking	Fuel	2% - 5%
Mild hybrid	Medium	Stop-start, regenerative braking, assisting engine	Fuel	8% - 16%
Full hybrid	High	Stop-start, regenerative braking, assisting engine, limited all electric range (AER)	Fuel	20% - 50%
Plug-in hybrid	Very high	Stop-start, regenerative braking, assisting engine, 10-50 miles AER	Fuel and electricity	40% - 80%
Battery electric vehicle	Full	Stop-start, regenerative braking, over 100 AER	Electricity	100%

Both micro hybrid and mild hybrid cannot drive the vehicle solely with electric motor and ICE is still the only power or main power supply for vehicle. The full hybrid electric vehicle (HEV), on the other hand, has enough electric power and energy to drive vehicle solely in certain circumstances. HEVs have more powerful motor/generator (up to 80kW) to capture over 90% kinetic energy during deceleration and store over 70% of that energy back to battery. The all electric range (AER) of a full hybrid is limited by the capacity of energy storage system (ESS) which does not require external charging.

The next level is plug-in hybrid electric vehicle (PHEV) which features bigger battery pack than a full hybrid and can take external electrical energy to recharge ESS. The ICE of a PHEV is not the main power supply for the vehicle but a range extender, and thus fuel consumption can be significantly reduced.

2.4.2.2 Micro and Mild Hybrid Powertrains

Various powertrain configurations for hybrid vehicles have been adopted by different manufactures. For micro hybrid, the configuration is essentially same as the conventional powertrain where the start-stop function can be achieved using conventional alternator and starter. While mild hybrid is commonly configured by replacing alternator with an electric motor/generator (EGM) which can be integrated to ICE either through a crank (Crank integrated starter generator, CISG) or a belt (belt integrated starter generator, BISG). The EGM

is typically connected to the engine in a parallel way and it can recapture part of kinetic energy from braking or coasting down and add on torque to engine during transient vehicle operation, improving vehicle performance and fuel economy [60].

Engine operation changes slightly. Engine idling is avoided at vehicle stop for both micro and mild hybrid vehicles. Some low-load operation during transient can also be replaced by the electric drive in a mild hybrid, but this effect is limited due to the limitations of power and energy capacity of the mild hybrid.

2.4.2.3 Architectures of Full Hybrid Powertrains

The load on a vehicle for vehicle movement composes rolling resistance, aerodynamic drag, grading resistance and vehicle dynamic load (acceleration) and sum of these loads can be resolved into two parts: one representing averaged power that is a constant and one representing dynamic power that is of zero average. The principle behind hybrid powertrains is using one power source that favors steady-state operation, i.e. ICE, to provide average power, while another power source that has both positive and negative powers, such as electric motor, to supply dynamic power. The dynamic power source (electric motor) ideally has zero energy output and only functions as an energy damper [63]. The steady-state operation of ICE allows for narrower engine operation range where efficiency is high. On the other hand, electric machine(s) can work as motor (positive power output) and generator (negative power output) making it an ideal power source for dynamic load.

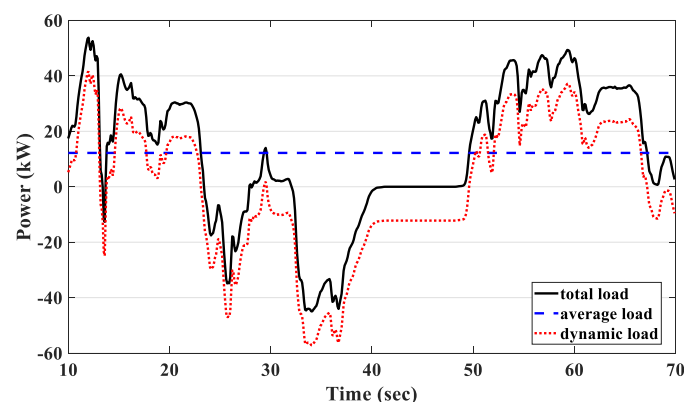


Figure 2-17 Power demand of a midsize sedan on US06 driving cycle. The vehicle power demand is decomposed into average power and dynamic power. (Data from [64])

Sharing the same principle of fuel saving, hybrid powertrains can be configured in various ways and each of them has different characteristics and pros/cons. Depending on the coupling

configurations of ICE and electric drive system, HEVs can be classified into three configurations, series hybrid, parallel hybrid and power-split hybrid (or termed series/parallel hybrid). These three configurations are introduced below.

Series hybrid powertrain uses an ICE to drive a generator and the output of generator charges battery that powers traction motor. As illustrated by Figure 2-18, only the electric motor is connected to the drivetrain and drives the wheels, using the energy from either generator or battery or in the combination of two. Electric motor is the only torque source to propel the vehicle which simplifies the vehicle speed control. Because electric motor can spin at a constant power over a wide range of speed, as shown in Figure 2-19, making it unnecessary to use a sophisticated transmission as conventional powertrain does [65]. ICE does not directly provide power to vehicle and is decoupled from vehicle speed, so ICE oftentimes operates at the best efficiency region. This mechanically decoupled operation of ICE from drivetrain permits significant advantage in transient city driving situation where conventional vehicles have significant efficiency losses from dissipated kinetic energy during vehicle deceleration and inefficient engine operation at low-load conditions[66].

However, fuel efficiency gain degrades on highway driving when vehicle speed is relatively constant and less regenerative braking energy is available. Serial powertrains have multiple energy conversion processes, from fuel to electricity and from electricity to mechanical work, and each conversion process involves inevitable inefficiencies, resulting in lower overall efficiency compared with other configurations.

Packing is another disadvantage. Serial hybrid requires two electric machines (one generator and one motor) and one combustion engine. Traction motor is typically in large size in order to be powerful enough to propel the vehicle under various driving conditions. Due to its inherent advantages and disadvantages, for most of its use, series configuration is used for heavy vehicles, buses and light-duty plug-in vehicles that have large battery onboard and need external charge. In this case, vehicle acts as a BEV for the most of time, while a small ICE is only used to extend the range and fuel is no longer a primary energy source. The Chevrolet Volt, for example, is powered by a 16 kWh Li-ion battery and a 55 kW ICE. The Chevrolet Volt uses battery pack for the first 20-50 miles and engine starts to extend additional 300 miles range once battery is depleted to a pre-set lower limit of state-of-charge (SOC) [67].

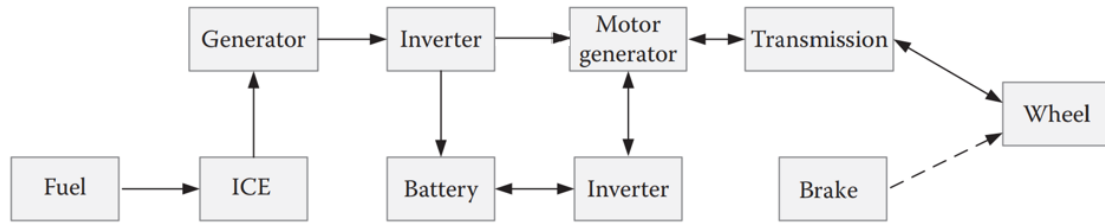


Figure 2-18 The flow of power for a series powertrain.

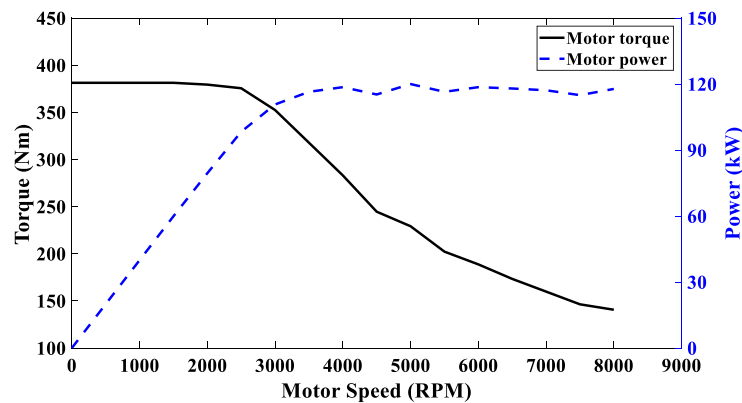


Figure 2-19 Torque and power curves of an AC induction motor [68]. Electric motor can operate at a constant peak power over a wide range of speed, making transmission unnecessary for a series hybrid.

Parallel hybrid powertrain also consists of an ICE and an ESS but different from series HEV, it needs only one traction motor that can work as both motor and generator (EGM). The ICE and EGM can either individually or parallelly drive the vehicle. In a parallel HEV, depending on the position of electric motor, there are four different configurations of parallel hybrid as enumerated by Table 2-5 [69]. The most common parallel hybrid architecture is P2 where an EGM is placed between ICE and transmission with one or multiple clutches. The P2 configuration is widely adopted by Volkswagen, Hyundai, Mercedes etc., whose power flow is illustrated in Figure 2-20. In city driving, the EGM propels vehicle and works as a generator to recapture kinetic energy from braking or decelerating. When the vehicle power demand is high, ICE and electric motor will supply the power in parallel. In contrast with series HEV, engine power and motor power are mechanically coupled through a torque coupler in a parallel hybrid, so both ICE and motor directly provide torques to drivetrain without multiple energy conversions. This leads to higher efficiency in highway driving than a series hybrid. Since only one electric machine is used, the overall packing is more compact. Furthermore, the peak power of vehicle is supplied by the combined power of ICE and motor, a smaller motor can be used. However, since vehicle speed and engine speed are coupled by the mechanical connection between ICE and drivetrain through transmission, the range of engine speed is broadened,

limiting the freedom of optimization of engine operation [65]. Despite that, engine efficiency can still be improved by adjusting the torque of engine at a given speed because the torque coupling between ICE and motor allows the torques of ICE and motor to be adjusted independently. For example, when vehicle power demand is low and ESS has enough energy, EGM can supply power independently, avoiding low-load engine operation. When SOC of ESS is low, ICE works at higher load producing power higher than demanded by vehicle propulsion, so excessive power can be used to charge battery. As a result, the inefficient, low-load engine conditions are avoided [63, 70].

Table 2-5 Terminologies of different parallel HEV configurations

Terminology	Configuration
P1	Motor mounted on engine cranks shaft before the clutch and gearbox
P2	Motor mounted at the input of gearbox after the clutch
P3	Motor mounted at the output of gearbox before the transaxle
P4	Motor(s) mounted on the transaxle

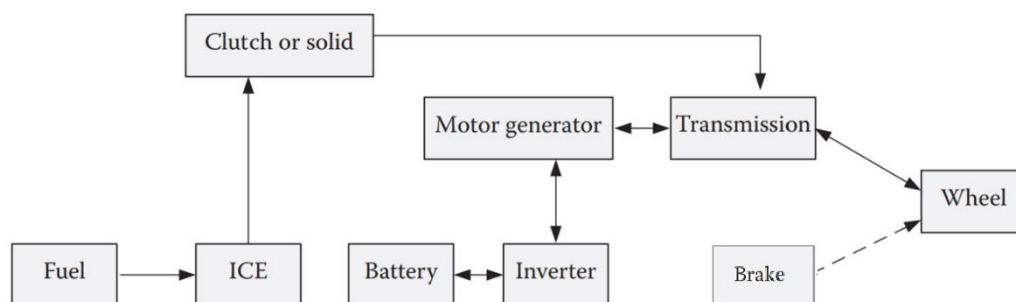


Figure 2-20 The power flow of a parallel hybrid powertrain (P2 configuration where motor is installed before multi-gear transmission). ICE and motor/generator are connected through a torque coupler with a constant speed ratio and speeds of them are proportional to transmission inlet speed.

Power-split (or series-parallel) hybrid powertrain is a combination of series mode and parallel mode. It has the largest market share in hybrid segment at present and is mainly adopted by Toyota and Ford [71]. It incorporates one ICE and two electric machines (both can work as motor and generator) and these three machines are connected with a power-split device (or called E-CVT) that is essentially a planetary gear set as illustrated by Figure 2-21. The power-split device gives much flexibility in propulsive powers. Series mode is achieved when engine power is transferring to generator (electric machine 1, EM1), and generator power is transferring to battery and EM2. Parallel mode is achieved when EM2 is assisting engine power

and EM1 stalls. In power-split mode, EM2 propels vehicle, while ICE power can be divided into two routes: one goes to drivetrain and the other one goes to generator (electric machine 1, EM1). Thanks to the characteristics of planetary gear set, at a given vehicle speed, engine speed can be adjusted by changing the speed of EM1, allowing more freedom to optimize engine operation for high efficiency. Regenerative braking is achieved when EM2 works as a generator and stores energy into battery [72]. Being controlled by the vehicle-level controller, different modes are selected at different driving conditions and the combination of series and parallel hybrids makes it have good fuel economy in both city and highway driving conditions. However, this configuration needs two electric machines and complex planetary gear unit. The hybrid control is also more complicated than series and parallel hybrids. The pure parallel mode is generally not possible and multiple energy conversions still involves when vehicle speed or power demand is high [73].

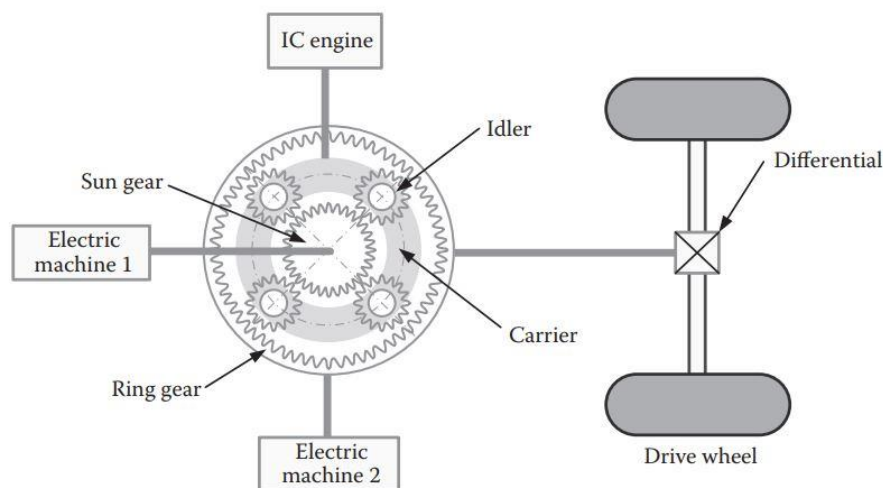


Figure 2-21 Planetary gear set of the power-split device for a series-parallel hybrid powertrain. Sun gear connects to electric machine 1, courier connects to ICE and ring gear connects to generator electric machine 2 and differential. Figure from [60].

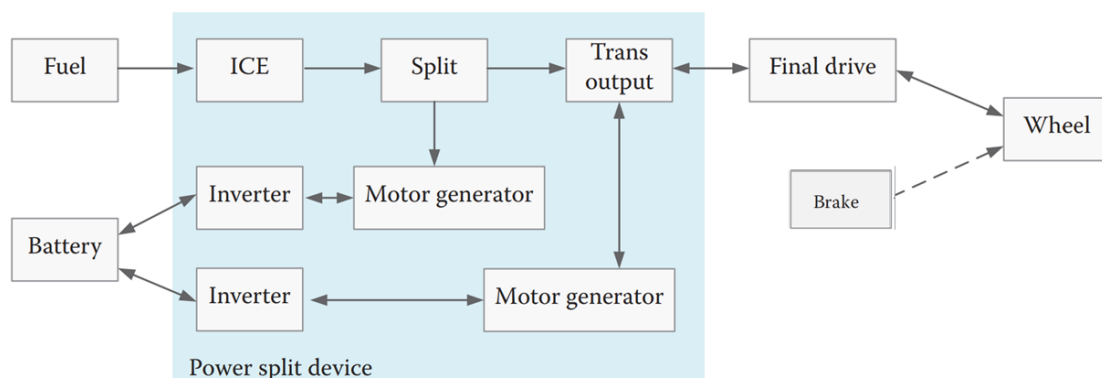


Figure 2-22 Power flow of a power-split hybrid powertrain. It can operate at series mode, parallel mode or a blended mode of these two.

2.4.2.4 Hybrid Powertrain Control Strategies

Because of dual power sources involvement, hybrid powertrains need more complicated control in addition to engine control and electric control. The highest control level is vehicle control which coordinates both ICE and electric propulsion system. Depending on the vehicle power demand, vehicle speed, and SOC of the battery, vehicle level controller assigns power demand to ICE controller and electric motor controller coordinately. ICE controller and electric system controller then operate their subsystems correspondingly.

Different strategies can be used for vehicle level control. A typical strategy is to maintain a constant level of battery SOC while optimizing engine efficiency for high fuel efficiency [66]. The engine control involves adjusting engine operation to achieve the as high efficiency as possible while satisfying power demand. The main target of electric control is to maintain the of the battery SOC at a certain level, for most cases at 60%-80% on a full hybrid powertrain[74].

2.4.3 Plug-in Hybrid Powertrains

The configurations of a plug-in hybrid electric vehicle (PHEV) are very similar to the full hybrid and a PHEV can also be configured to be series, parallel or power-split. The main differences between PHEV and HEV are AER and external charging capability. Compared with HEV, a PHEV has a more substantial electric driving system of higher power and more energy. Higher power of electric drive system is able to propel the vehicle under more aggressive driving conditions in electric-only mode in which case zero-emission vehicle is possible. Battery of more capacity allows longer AER (typically 20 – 40 miles) and it can be charged from a wall outlet. The combination of higher power and more energy extends the usage of electricity and displaces fuel consumption.

The higher degree of hybridization adds more complexity to the control system because there are more possible combinations of motor operation and engine operation. Generally, there are two different modes: charge-depleting (CD) mode and charge-sustaining (CS) mode [75]. When the SOC is higher than a certain level (typically 30%), a PHEV uses electricity as energy source for propulsion and ICE is shut down unless power demand for propelling vehicle is beyond motor capacity. SOC of the battery decreases continuously as ICE is not charging the

battery. This mode is ‘charge-depleting’ mode. When the SOC of the battery is lower than the preset value, a PHEV works as a full hybrid where ICE provides power and SOC of the battery is maintained at a constant level. This is called ‘charge sustaining’ (CS) mode [60, 66].

In terms of the engine operation, because electric system has more power and more energy, the operating time of engine can be further reduced. Engine only starts up when power demand is high, or vehicle is in CS mode and engine operation range can be narrower and closer to the highest-efficiency region [58].

2.5 Summary and Research Questions

Improving engine efficiency by increasing the compression ratio, turbocharging and downsizing makes autoignition of unburned air-fuel mixture more likely to happen and thus more knock prone. Furthermore, engines on hybrid powertrains tend to operate at knock-limited conditions for optimal thermal efficiency [72]. If knock is strong, severe engine damages can be resulted. Fuels of better anti-knock ability that is conventionally quantified by RON and MON are used to suppress knock propensity. As reviewed, autoignition in modern SI engine combustion is not a single function of fuel properties only but a result of fuel and engine interactions. The OI model that incorporates both fuel properties (RON and MON) and engine conditions parameter (K) has been found to be a better indicator for knock-resistance with a K factor weighting the relative contributions of RON and MON to OI. Knowing K values provides information of the significance of RON and MON to anti-knock performance which is important for industry to design fuels and develop high-efficiency SI engines.

This study therefore aims to investigate the significance of RON and MON on a modern SI engine and assess the requirement of fuel properties for high efficiency for both conventional and hybrid vehicles. Accordingly, following research questions are proposed.

1. What is the best experimental method for determining K?

Several methods for determining OI and K have been used by different researchers, but an important question remain is whether results from different methods are comparable. Furthermore, those methods have different pros and cons, choosing a proper method from those options for next-step engine tests is essential.

2. What are K values of a modern production GTDI engine over the operation map?

Previous studies have deemphasized the importance of the MON standard using results from low-speed and high-load conditions where K is negative. Because there are many engine operating conditions involved in vehicle driving, the knowledge of K values over the entire engine operation map is necessary for a more comprehensive evaluation of the significance of RON and MON. But this information is blank in literature.

3. What is the relation between end-gas condition and K factor?

The relation between K and end-gas condition has not been well understood in literature. The pressure-temperature trajectory can only qualitatively explain the variation of K with some engine operating conditions. T_{comp15} correlates well with K in HCCI engine but the correlation becomes relatively weak in SI engine. More investigation is therefore necessary for fundamentally understanding the cause of variation of K with engine operating conditions.

4. What is the significance of RON and MON in improving fuel efficiency for conventional vehicle, hybrid vehicle and plug-in hybrid vehicle?

K values span a wide range from negative to positive in vehicle driving, therefore the conclusions yielded from a single condition will be opposite. To answer the question that how the fuel properties need to be tailored for the application of high-efficiency powertrains, OI and K framework should be evaluated with vehicle-level analysis. Furthermore, with the increasing penetration of hybrid vehicles, many studies have been published with emphasis on vehicle control optimization, cost reduction etc. But the engine combustion on those advanced powertrains has not drawn enough attention. Particularly, engine operates at more knock-limited region and understanding the significance of RON and MON to engines on hybrid vehicles becomes an emerging necessity.

3 Experimental and Numerical Methods

To understand the significance of RON and MON in modern engine combustion, K values were experimentally determined over a wide range of conditions on a production 4-cylinder GTDI engine using factory calibration setting. A PRF method was used for the measurement of K. The PRF method relies on Eq. 3-1 to calculate the K, provided that the RON and S of a test fuel and the knock-limited OI of a test condition are known. RON and S of the test fuel, an EPA Tier 3 Certification gasoline, was measured by the supplier and is reported in Section 3.4 of this thesis. The OI of the tested fuel was measured experimentally with the aid of a PRF blending system developed in this study (Section 3.3).

$$K = \frac{RON - OI}{S} \quad \text{Eq. 3-1}$$

In addition to the engine experiments, engine modelling and vehicle modelling were performed using experimental data. End-gas conditions were calculated with an engine modelling software of GT-Power [76] to investigate the cause of K variations with changing engine operating conditions and to develop the relationship between K and end-gas thermodynamic states in SI engines. Vehicle modelling with Autonomie software [77] was performed to determine the significance of RON and MON on the engine's fuel efficiency over several common, regulatory driving cycles when the engine is used in vehicles featuring conventional and hybrid powertrain configurations.

3.1 EcoBoost Engine Setup

The experimental setup consisted of a GTDI engine, a dynamometer, conditioning subsystems for the coolant and intake air and a fuel mixing system. The engine speed was regulated by a transient dynamometer. The engine coolant temperature was controlled by a coolant conditioning system. The intake air temperature was controlled by a water-to-air intercooler connected to the process water in the test cell.

3.1.1 Engine Test System

The *Horiba Automotive Test System (Titan T460)* was used for the engine test. The test stand includes several sub-systems for both engine control and performance measurement. The engine and dynamometer were mounted on an air suspension bed to reduce the vibrations

caused by the engine and dynamometer spinning. The dynamometer and engine were connected with a flexible shaft that was specially designed for this 2L engine to avoid torsional vibrations [78]. The dynamometer had the capability to absorb the maximum engine power and torque and its specifications are listed in Table 3-1.

Table 3-1 The specifications of dynamometer of test system

Maximum torque (Nm)	1000
Maximum power (kW)	460
Maximum speed (RPM)	6500
Moment of inertia (kgm²)	>0.3

Two fluid conditioning systems were incorporated into the test system. One was for engine coolant, which circulated coolant through the engine while sustaining a constant coolant inlet temperature. The other conditioning system was for intake air temperature control by adjusting the temperature of water flowing through a liquid-to-air intercooler as shown in Figure 3-1. The water temperature for the intercooler could vary from 15 °C to 100 °C, enabling the intercooler to either cool or heat the intake air. Depending on the engine load, the heating function was used when the compressor of the turbocharger was not compressing the intake air, and the cooling function was used at boosted conditions.

Two fuel systems were used in the test engine, with one for the certification gasoline, and the other for PRFs. The gasoline supply system was composed of a 25 L fuel tank and a low-pressure fuel pump with internal fuel return. The low-pressure fuel pump supplied a constant fuel pressure of 6 bar upstream of the high-pressure direct-injection (DI) pump. In between the low-pressure fuel pump and high-pressure DI pump, a Coriolis flow meter was installed to measure the fuel flow rate.

The PRF blending system was also connected to the DI pump to supply PRF mixtures to the engine when the gasoline supply system was switched off. The PRF blending system also pressurized the PRF mixture to 6 bar upstream of DI pump, regardless of fuel flow rates and PRF compositions. The details of the PRF blending system is given in Section 3.3.

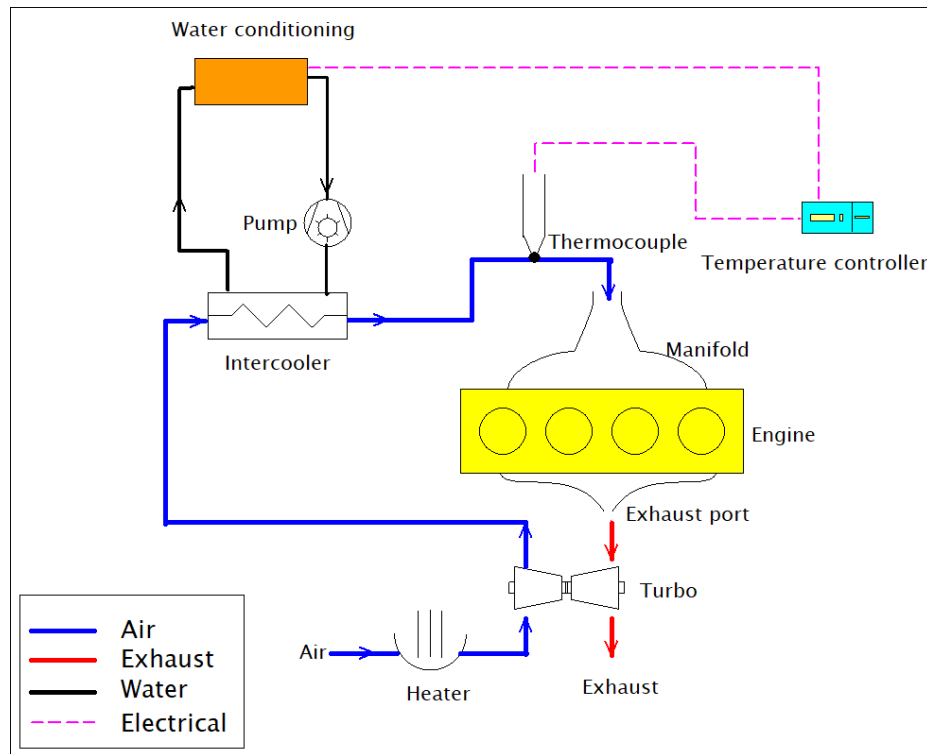


Figure 3-1 Experimental setup of intake temperature control for the GTDI engine.

3.1.2 The Turbocharged DISI Engine

A 2L 4-cylinder, GTDI engine was used. The engine was developed by Ford Motor Company and was one version of EcoBoost family that begun production from 2009 and was recognized as a Ford's near-term engine technology for fuel economy improvement and CO₂ emission reductions [79]. The engine is representative of modern downsized gasoline engines with advanced technologies, such as twin independent variable cam timing (Ti-VCT), high-pressure direct fuel injection and turbocharging. In order to maintain the production configuration of the engine, no cylinders were deactivated, and all stock engine systems were preserved (i.e. fueling system, turbomachinery, etc.).

3.1.2.1 Engine Specifications

The engine specifications are shown in Table 3-2. The Ti-VCT of the engine allows independent control of the intake valves and exhaust valves with 50 degrees adjustment relative to base valve timings. The base timings of intake valve opening (IVO) and closing (IVC) are 11° after top dead center (aTDC) and 67° after bottom dead center (aBDC) respectively while that of exhaust valve opening (EVO) and closing (EVC) are 36° before bottom dead center (bBDC) and 8° aTDC respectively. The intake cam timing can be advanced by up to 50 degrees from the base timing while the exhaust cam can be retarded by up to 50 degrees relative to base

timing. The turbocharger provides for a torque peak of 340 Nm from 1750 RPM to 4000 RPM at maximum of 1.1 bar boost pressure (relative pressure). Depending on the octane of gasoline, the engine can deliver up to 159 kW with 91 RON gasoline and 177 kW with 98 RON premium gasoline. The DI fuel system is comprised of side-mounted, 7-holes injectors and a high-pressure fuel pump that can supply up to 15 MPa fuel pressure to the injectors.

Table 3-2 Specifications of 2L Ford EcoBoost GTDI engine

Engine type	GTDI, inline 4-cylinder, with Ti-VCT
Instrumentation	Four top-mounted Kistler piezoelectric pressure transducers (6125C)
Displacement volume	1999 cc
Bore × stroke	87.5 mm × 83.1
Connecting rod	156 mm
Peak power	159 kW (91 RON) and 177 kW (98 RON)
Peak torque	340 Nm @ 1750 – 4000 RPM
Compression ratio	9.3: 1
Maximum speed	6500 RPM
Maximum boost	1.1 bar (gage) 2.1 bar (absolute)
IVO base timing	11° aTDC
IVC base timing	67° aBDC
Intake cam adjustment	0-50° advance
EVO base timing	36° bBDC
EVC base timing	8° aTDC
Exhaust cam adjustment	0-50° retard
Fuel injector	Bosch 7-hole gasoline injector
Fuel pump	15 MPa max.

3.1.2.2 Engine Control

The engine was controlled and monitored by a *Motec M142 ECU* with fully open, developmental access. A custom firmware was developed to allow for full authority over all the engine's production systems such as ignition, fuel injection, boost pressure control, camshaft phasers and the throttle body. The engine calibration data provided by Ford was implemented in the ECU software to allow for engine operation with OEM settings.

Although engine could run with OEM tuning, manual adjustment to the spark timing and closed loop lambda target were required during the experiments. The spark timing was advanced manually from base knock-free timing to achieve trace knock. The throttle position was adjusted to reach the required load with the engine speed controlled by the dynamometer. Fuel injection strategy and valve timings were not changed during the engine experiment, and the OEM-optimized calibration of those controls was preserved.

3.1.3 High-Speed Data Acquisition System for In-cylinder Pressure Measurement and Knock Detection

To record the in-cylinder pressure data for combustions analysis and knock detection, the high-speed data acquisition system running on LabVIEW was developed. Four Kistler piezoelectric pressure transducers (6125C) were mounted between intake valves and exhaust valves on the cylinder head as shown in Figure 3-2. Many previous studies used a single cylinder configuration by deactivating other cylinders to simplify the pressure measurement. In this study pressures of all four cylinders were measured so that trace knock could be detected if it happened in any cylinder.

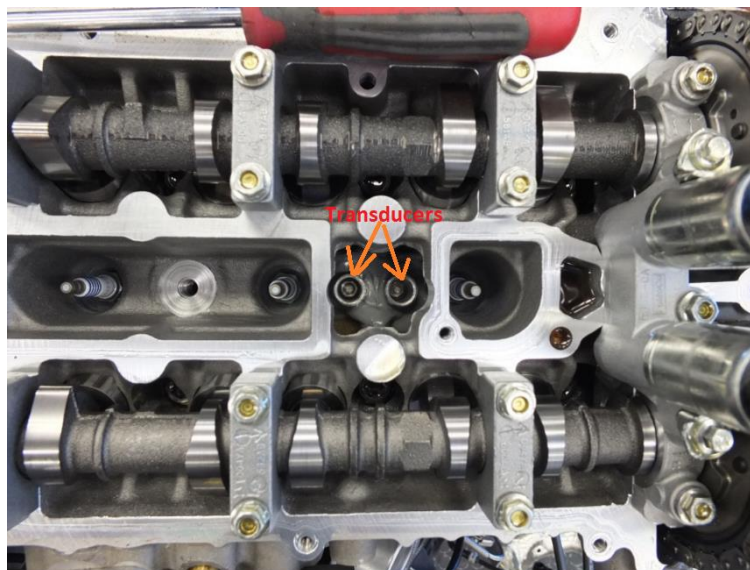


Figure 3-2 Pressure transducers mounting on the cylinder head for in-cylinder pressure measurement.

The National Instruments cDAQ devices were used for data acquisition. The data system sampled the in-cylinder pressure data at 0.1° crank angle (CA) resolution and provided real-time display of in-cylinder pressures. Combustion analysis was incorporated into the data system to give operators information such as IMEP, mass fraction burnt (MFB), cycle-to-cycle variation (CoV) etc. With the real-time MFB calculation in the data system, operator was able

to know combustion phasing by observing the CA50 and determine if a condition was knock-limited or over-advanced. The knock-limited condition in this study is defined as when CA50 at trace knock is retarded from the MBT timing for a test condition, while the over-advanced condition is defined as when CA50 at trace knock is earlier than the MBT timing. The MBT timing in CA50 for this engine was determined using an empirical equation (Eq. 3-2) where MBT timing in CA50 is independent of load but slightly dependent on engine speed which is consistent with other study's finding [45]. This MBT timing is independent of the fuel, however, changes to ignition timing are typically required to achieve this MBT timing as fuels and operating conditions vary.

$$CA50_{MBT} = -0.0007RPM + 8.809 \quad Eq. 3-2$$

Another important feature of the high-speed data system is the knock detection function. The knock detection method in the data system is based on the filtered in-cylinder pressure data, which is a common practice for knock detection in SI engines [80]. This is discussed with more details in Section 3.2.

3.2 Determination of Trace Knock Condition

Trace knock, or conventionally called 'borderline knock', is a transition condition between normal combustion and continuous knocking. During trace knock condition, knocking is normally intermittent which can be determined by both human hearing and a pressure filtering algorithm. A microphone was placed close to the original knock sensor on the cylinder block to help the operator pick up the pinging sound at trace knock condition. Audio detection of trace knock, however, relied on operators' technical experience. In addition, the pressure filtering was applied to raw in-cylinder pressure data with the Butterworth bandpass filter. Using both methods in combination demonstrated consistent results.

The cut-off frequencies of the filter were determined through Power-spectral-density (PSD) analysis of raw pressure data. The PSD for different engine speeds and loads is given in Figure 3-3 where left figures show the PSD of pressures from knock-free combustion with base spark timing and right figures show the PSD of pressures from trace knock combustion where the spark timings were advanced relative to base timing. The spikes can be observed at trace knock condition around 6.4 kHz in the frequency domain. Regardless of the engine speed and engine load, the frequency of interest for detecting knock is around 6.4 kHz which is close to the

calculated first mode of the cylinder (6.7 kHz) using the acoustic pressure wave formula proposed by Draper [81] (Eq. 3-3). The lowest mode constant $f_{m,n}=1.84$ was chosen as this mode typically has highest power [82]. Speed of sound, c_s , was estimated to be 1000 m/s from ref.[80] and cylinder bore is 0.0875 m.

$$f_{m,n} = \frac{\alpha_{m,n} \cdot c_s}{\pi \cdot B} \quad \text{Eq. 3-3}$$

where:

$f_{m,n}$ is the resonant frequency [Hz];

m, n is the mode constant. m and n are radial and circumferential pressure nodes.

c_s is the speed of sound in the combustion chamber [m/s];

B is the cylinder bore [m].

It was argued that the frequency from Eq. 3-3 is for acoustic modes of a combustion chamber and it is a characteristic of the chamber itself [82], but the pressure oscillations caused by engine knock principally corresponds to the lowest mode ($m=1, n=0$) where pressure waves propagate back and forth in the bore direction [83]. Therefore, pressure fluctuations at this frequency are markers for knocking combustion. Based on this, the cut-off frequencies of the Butterworth filter were set to 3 kHz and 10 kHz to capture the dominant spectral components associated with knocking. The lower cut-off of 3 kHz was determined to avoid unnecessary attenuation of pressure fluctuations at 6.4 kHz, while the upper cut-off of 10 kHz was determined due to negligible contribution of high-frequency modes. An example of filtered pressures for knock-free and trace knocking conditions at the same RPM and BMEP is shown in Figure 3-4 where the increased amplitude of knock-induced pressure fluctuations is observed.

After setting the cut-off frequencies of the filter, the maximum peak-peak pressures of the filtered pressure traces for 300 cycles were examined. As shown by Figure 3-5, the peak-to-peak pressures are higher at advanced sparking timing than at the base timing where peak-to-peak pressures are almost zero. The higher peak-to-peak values at advanced spark timing condition indicates the pressure oscillations related to knocking combustion were well captured by the filter. With the peak-to-peak value, a cycle was deemed to be knocking cycle if the peak-to-peak was over the threshold value which was set at 0.5 bar at 1000 – 3000 RPM and then

linearly increased to 1 bar at 5000 RPM due to stronger background noise at high engine speed [84].

As shown by Figure 3-5 the knock did not necessarily happen at every cycle (trace knock is intermittent) which was not straightforward for the operator to judge whether it was trace knock condition. So, the final criteria of the trace knock condition used the percentage of knocking cycles over every 30 cycles. An operating condition was considered to be trace knock when the knocking percentage was over 5% [84]. The knocking percentage was calculated with the moving average of maximum peak-to-peak values along the cycles. The results of the knocking percentages for a normal combustion and a combustion with advanced spark timing are shown in Figure 3-6. The knocking percentage for the combustion at base spark timing was zero whereas the knocking percentage increased to over 5% when the spark timing was advanced by 5 deg relative to base timing and audio pinging noise was detected by the operator. By doing so, both the audio monitoring method and pressure filtering method produced consistent results and the operator could easily identify the trace knock condition by hearing the engine sound and observing the filtered pressure.

Experimental and Numerical Methods

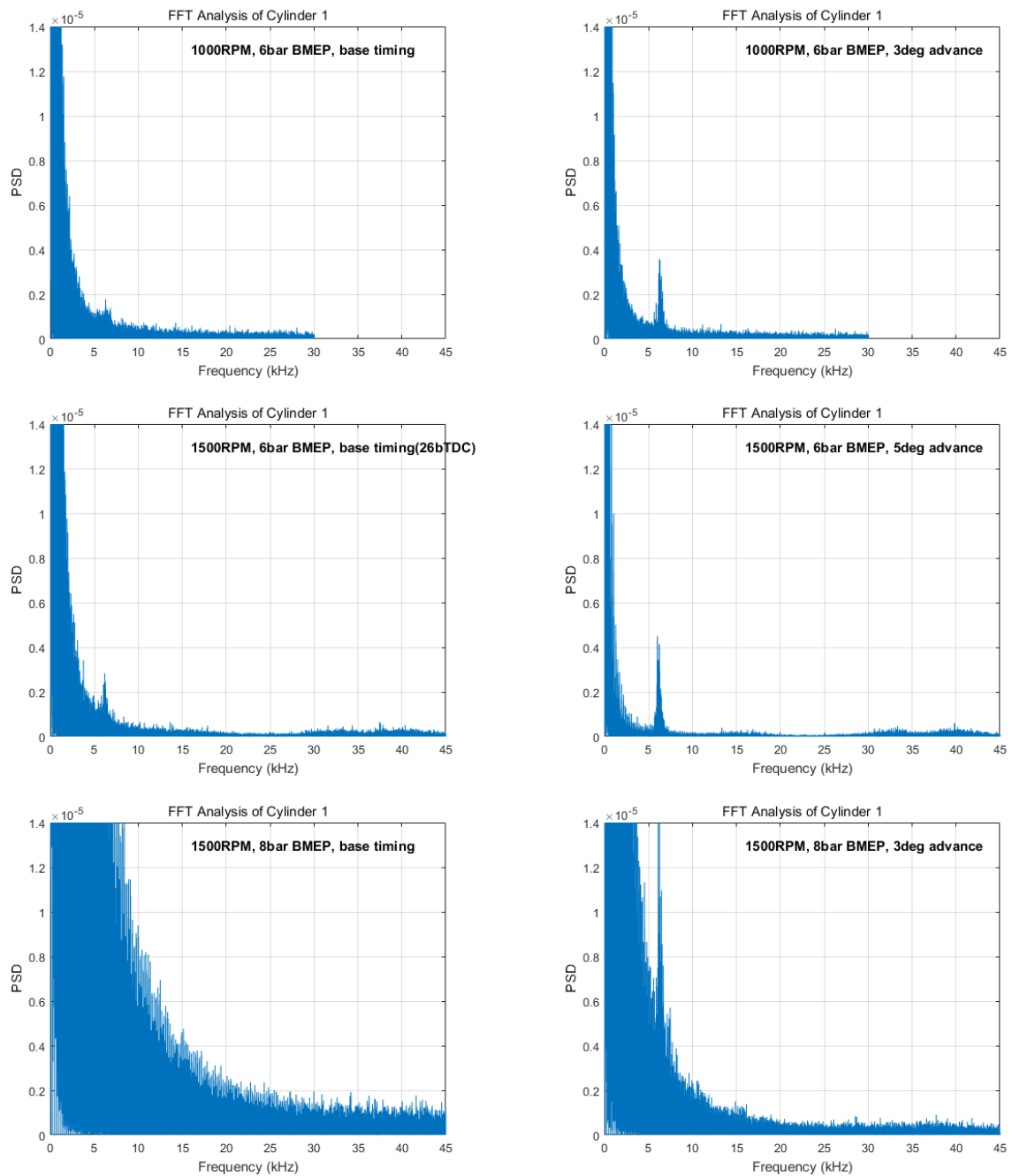


Figure 3-3 PSD analysis of raw in-cylinder pressures at 1000RPM, 1500RPM, 6 bar BMEP and 8 bar BMEP under normal combustion (left figures) and trace knocking (right figures) conditions.

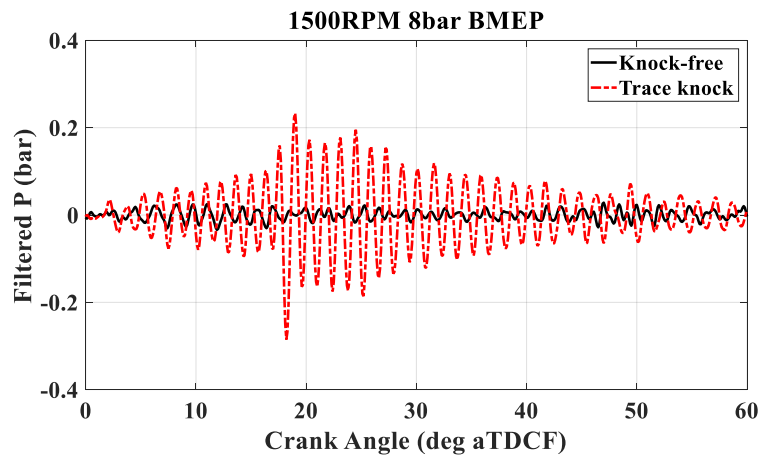


Figure 3-4 Example of filtered pressure traces for a normal and a trace knocking conditions at 1500 RPM 8 bar BMEP.

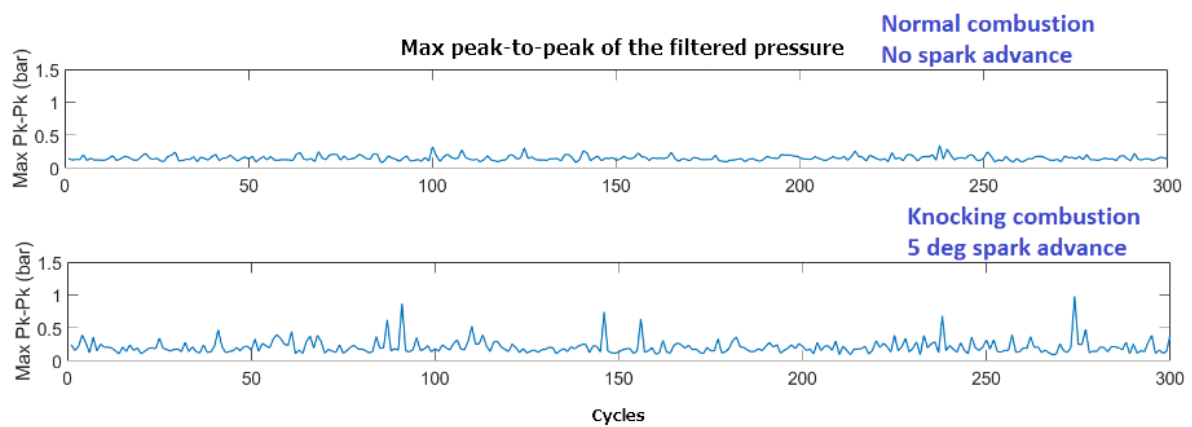


Figure 3-5 Maximum peak-to-peak pressures of the filtered pressure traces with 3-10 kHz bandpass.

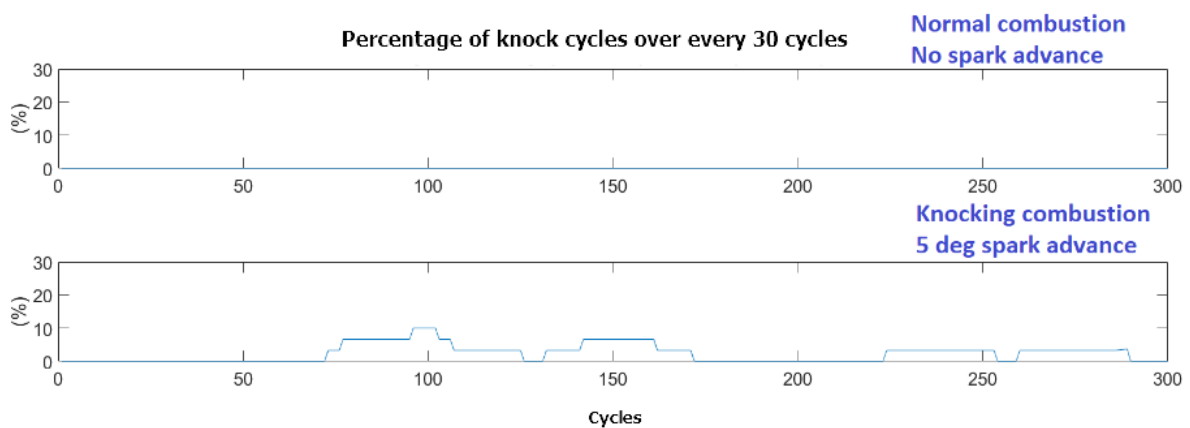


Figure 3-6 Knocking percentage of cycles whose maximum peak-to-peak values of the filtered pressure traces were above the threshold.

3.3 Development of the Online Octane Blending System

When determining K values at a given engine operating condition, the knock-limited OI needs to be known so that the K value can be calculated with Eq. 3-1. The octane index of the test fuel is defined as the octane number of the PRF matching the knock resistance of the test fuel at the same operating condition. The combustion phasing at trace knock, commonly quantified by CA50, was used as the indicator of the knock resistance. Therefore, to quantify the knock-limited OI at a certain condition, different PRFs were tested until a PRF whose CA50 matching that of the test fuel was found. The online PRF blending system was used to mix iso-octane and n-heptane to the desired octane number and then supplied the PRF mixture to the engine. This section introduces how the PRF blending system was designed and validated.

3.3.1 Design Targets

The target of the system was to supply the PRF mixtures of the designed octane number to the engine and maintain the required mass flow rate.

The original engine fuel system consists of a low-pressure pump, a high-pressure DI pump, a fuel rail and fuel injectors. The DI pump is to supply the fuel at high pressures to the fuel rail with no return. The DI pump is demand-controlled by adjusting the start of the delivery stroke with an internal fuel supply control valve. For example, if the control valve is open as the internal plunger is moving up, excess fuel in the DI pump will be returned to low-pressure circuit at the admission pressure (typically 5 – 6 bar). The low-pressure pump must maintain a constant fuel pressure upstream of the DI pump so the excess fuel can be released into the fuel tank if the fuel pressure on the low-side pressure is too high during fuel return, while more fuel can be drawn into the fuel line if low-side pressure is lower than the setting pressure [85].

3.3.2 Control Logic

The control logic of the blending system is setting the total flow rate according to the engine operating condition and dividing the total flow rate into the flow rates of iso-octane and n-heptane per the desired PRF number or octane index (which are the same for PRFs). Because the fuel flow rate demanded by the engine is a function of manifold air pressure (MAP) and engine speed, the MAP and engine speed were measured by a MAP sensor and an encoder

mounted on the engine crank respectively. The total flow rate is then determined with a look-up table (LUT) with respect to MAP and RPM.

Once the total flow rate was known, two Coriolis mass flow controllers (MFCs) were commanded to control the mass flow rates of iso-octane and n-heptane separately. As the PRF number is defined as the volumetric concentration of iso-octane in a PRF mixture, the mass flow rates of iso-octane and n-heptane were adjusted dynamically to achieve the required volumetric concentration of iso-octane. The calculation for the mass flow rates of n-heptane and iso-octane are expressed by Eq. 3-4 and Eq. 3-5 respectively.

$$\dot{m}_{nc7} = \frac{\dot{m}_{total}}{\frac{OI}{OI - 100} \cdot \frac{\rho_{ic8}}{\rho_{nc7}} + 1} \quad \text{Eq. 3-4}$$

$$\dot{m}_{ic8} = \dot{m}_{total} - \dot{m}_{nc7} \quad \text{Eq. 3-5}$$

Where:

$\dot{m}_{total}$ is the total mass flow rate;

OI is the octane index that is equal to PRF number by definition;

$\dot{m}_{nc7}$ are $\dot{m}_{ic8}$ the flow rates of n-heptane and iso-octane respectively;

ρ_{nc7} are ρ_{ic8} is the densities of n-heptane and iso-octane respectively;

The overall control logics of the blending system are shown by Figure 3-7.

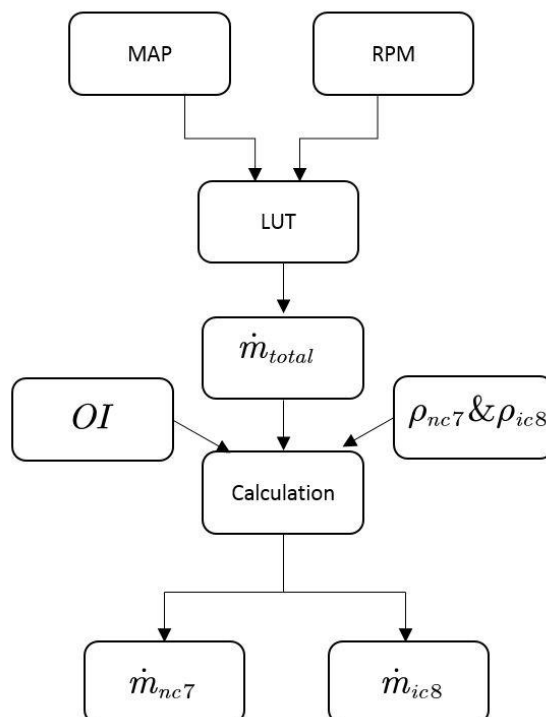


Figure 3-7 Control logics of online octane blending system

3.3.3 Configuration of the On-line Fuel Blending System

A simplified drawing of the blending system is given by Figure 3-8 where the bottom shows the conventional gasoline supply line and the upper part shows the PRF line. All fuels were stored in the fuel tanks that were connected to the low-pressure fuel pumps. The stable operation of MFCs required constant upstream and downstream pressures and this requirement was fulfilled by using backpressure (BP) regulators. The combination of low-pressure fuel pump and back-pressure regulator upstream of the MFC created a stable inlet fuel pressure at 2 bar. Excess fuel upstream of MFC was returned to the fuel tank. Two MFCs shared a common BP regulator at the downstream, creating a constant downstream pressure of 5.7 bar when BP regulator was cracked. During the operation, the total flow rate from two MFCs was set slightly higher than the engine-demanded flow rate to crack the BP regulator at the downstream otherwise the downstream pressure of two MFCs and flow rates would fluctuate. The iso-octane and n-heptane were well mixed by a static mixer before entering the DI pump. The entire fuel system was controlled by a programmable controller via serial communication protocol to LabVIEW.

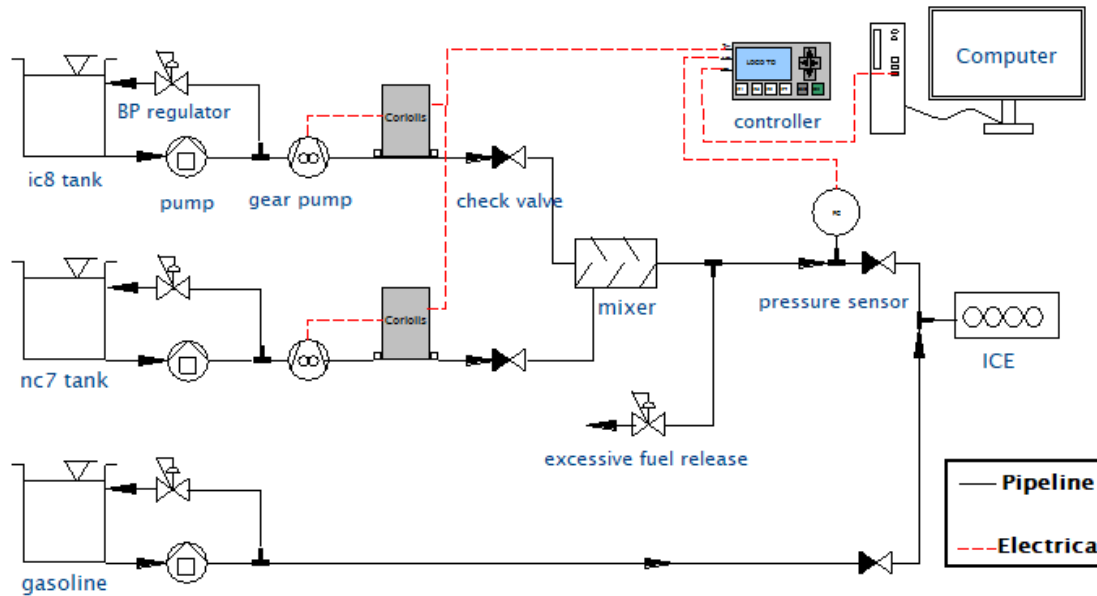


Figure 3-8 Simplified drawing of the configuration for blending system.

3.3.4 Validation of the Fuel Blending System

To check the accuracy of the blending system and applicability to engine experiments, both offline test and online engine test were performed.

3.3.4.1 Offline Tests

The offline test was done with standalone setup i.e. the system being disconnected from engine fuel pump, to check if the PRF compositions produced by the blending system were accurate. Different PRF mixtures were prepared and then the tested for the density and octane number of the mixtures. The density measurement is based the idea that the density of a binary mixture is determined by the linear blending of the two components, assuming ideal mixing. However, the densities of iso-octane and n-heptane are very similar (688.02 kg/m^3 of iso-octane vs 679.72 kg/m^3 of n-heptane at 25°C and 1 atm) resulting in very minor difference in density among PRFs. Therefore, to better distinguish the density differences, n-heptane was replaced with toluene that has density of 862.37 kg/m^3 at 25°C and 1 atm . The blending system was commanded to produce toluene/iso-octane mixtures of different volumetric concentrations of toluene. The densities of mixtures were then measured using volumetric flask and weight scale. The results are shown in Figure 3-9 where the measured densities of mixtures aligned with the densities produced by blending system. The relative errors in density shown by the redline were less than 0.1% which was equivalent to 0.1 octane number if iso-octane/n-heptane mixtures were prepared. This uncertainty was lower than the smallest tolerance of ASTM octane rating (0.2 octane number for repeatability at 90-100 ON) [23, 24].

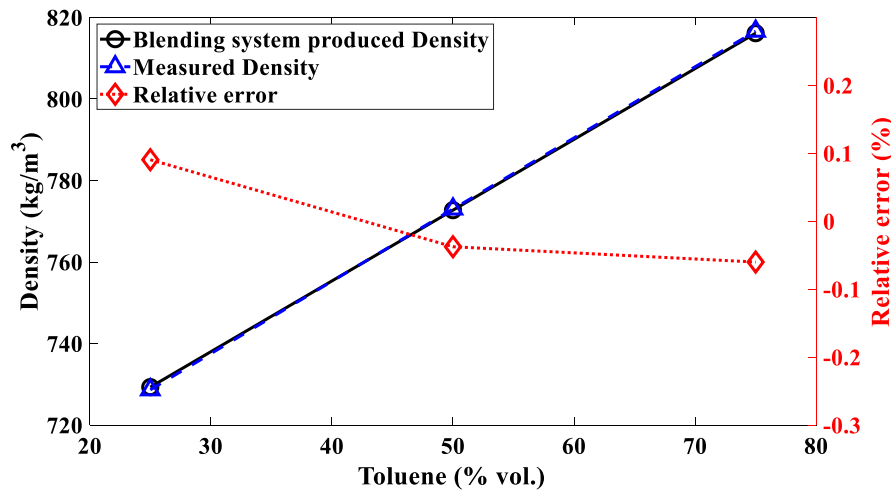


Figure 3-9 Comparison of densities of toluene/iso-octane blends from calculation and measurement.

The other offline test was done by measuring the octane numbers of the prepared PRFs. The blending system was commanded to supply PRFs of different octane numbers (87, 89 and 91), and samples were then collected for octane rating. The RONs for the samples were measured on the CFR engine following ASTM D2699 procedures. The results are shown in Table 3-3. The difference in octane number is no more than 0.2. This difference is greater than that from the density test because the octane rating test on CFR engine inevitably had some uncertainty and the differences in Table 3-3 actually included the errors of PRF preparation by the fuel blending system and errors of octane rating by the CFR engine. For the purpose of K determination, 0.2 different in ON will only result 0.024 difference in K value assuming the RON91 certification gasoline ($S=8.2$) is used. Therefore, despite of minor differences, the overall errors are deemed to be acceptable.

Table 3-3 Comparison of the designed octane numbers vs. measured octane numbers by CFR engine.

Commanded PRF number	87	89	91
Octane number measured by CFR engine	87.1	89.2	91.2

3.3.4.2 Online Engine Tests

To test the readiness of the fuel blending system for engine experiments, an online engine test was also conducted. In the online engine test, the blending system directly supplied PRF mixtures to the DI pump of the engine. The operator commanded the blending system to supply a PRF mixture of a desired PRF number and the system adjusted itself automatically to produce that required composition while maintain a constant total flow rate. The PRF number was

changed from 98 to 85 at a total flow rate of 15 kg/hr, which was approximately the flow rate required by the engine at a speed of 3000 RPM and a load of 6 bar BMEP. As shown by Figure 3-10 and Figure 3-11, the flow rates of iso-octane and n-heptane responded promptly to the command of change, leading to stable transitions between PRF numbers. The PRF numbers and flow rates of iso-octane and n-heptane reached the set points within ~ 20 seconds. The total flow rate and fuel pressure downstream of the blending system are shown in Figure 3-12 where fuel flow rate was stabilized at 15 kg/hr except for the transition points. During the transition, the total flow rate increased by 0.2 kg/hr, but this change in total flow rate was damped by the back-pressure regulator and attenuation of the DI pump, and as a result, the fuel pressure upstream of DI pump was not affected, nor was the engine performance. This online engine test confirmed the compatibility of the PRF blending system with the DI fuel system of the engine while providing a controllable PRF mixture in real time.

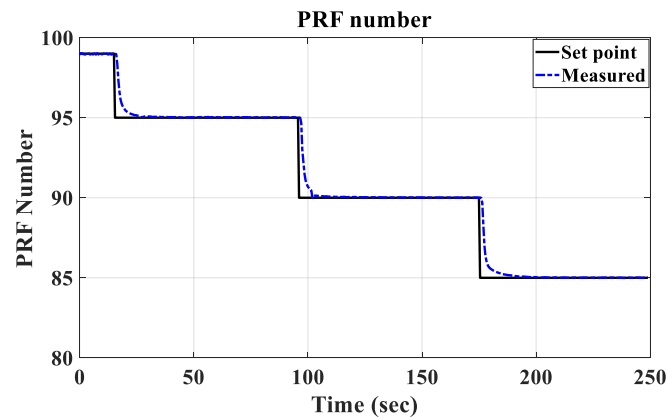


Figure 3-10 PRF numbers at 3000 RPM 6 bar BMEP condition.

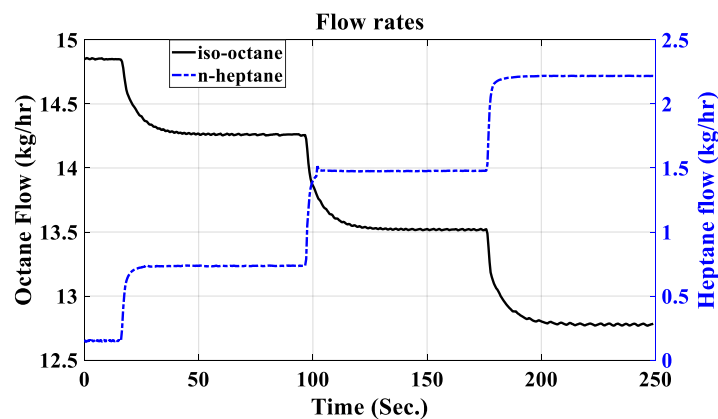


Figure 3-11 Flow rates of iso-octane and n-heptane at 3000RPM 6bar BMEP condition.

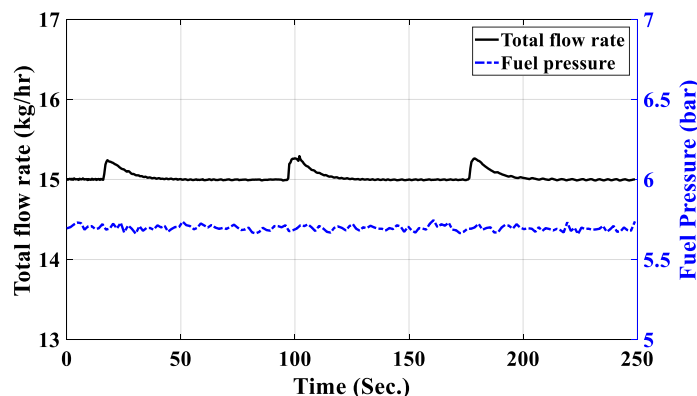


Figure 3-12 Total flow rate and fuel pressure from the blending system at 3000 RPM 6 bar BMEP condition.

3.4 Experimental Fuels

The test fuels used for engine experiments in this study were PRFs and a regular grade US EPA Tier 3 Certification Fuel whose properties are summarized in Table 3-4. With the aid of the online octane blending system, the PRFs of adjustable octane numbers from 0 to 100 could be mixed online with engine running. The n-heptane and iso-octane have the similar net heating values (NHV) and HoV so the PRFs of different octane numbers differentiate primarily in the chemical resistance to autoignition. The certification gasoline contains 10% ethanol by volume and thus it has lower NHV but higher HoV than PRFs. However, the higher HoV of the certification gasoline than PRFs is manifested by its high octane sensitivity [30, 31] which means the difference between the certification gasoline and PRFs in terms of anti-knock ability is predominantly due to the difference in octane numbers and octane sensitivity.

Table 3-4 Fuel properties of n-heptane, iso-octane and EPA certification gasoline.

	n-Heptane	Iso-Octane	Certification Gasoline
RON	0	100	91.6
MON	0	100	83.4
S	0	0	8.2
H/C (mole/mole)	2.286	2.250	2.026
O/C (mole/mole)	0	0	0.033
Ethanol (vol. %)	0	0	9.85
NHV (MJ/kg fuel)	44.57	44.31	41.67

HoV (MJ/kg fuel @25 °C)	0.31 ^[86]	0.37 ^[86]	0.41 ^[87]
Stoichiometric A/F	15.10	15.05	14.05

3.5 Experimental Conditions

3.5.1 Operating Conditions

Two sets of engine operating conditions were proposed in the present study. One set was for normal temperature condition where the intake temperature and coolant temperature were controlled to reproduce the thermal condition in the standard EPA drive cycles. The other set was for high temperature conditions where the intake temperature and coolant temperature were both elevated to reproduce the thermal condition in SAE J2807 Towing Test [88] that represents extreme driving conditions under hot ambient conditions. Experimental procedures for determining K values at both sets of engine operating conditions were same.

3.5.1.1 Matrix of Engine Operating Conditions

Previous studies on engine knock mostly focused on high-load and low-speed conditions where knock is most likely to happen[33, 34, 39, 40, 42-45, 89, 90]. The engine operations on a vehicle, however, cover a wide range of engine load and engine speed and during the most of time concentrate around part-load, low- and medium-speed conditions as shown by Figure 3-13. With regard to knock limit, downsized GTDI engines can be knock-limited from medium load condition (approx. 7-8 bar BMEP) with E10 and E20 (RON 91 and RON 96) at compression ratio of 10:1 [20]. So, in this study, the experimental conditions spanned from part- to high-load and low- to high-speed as shown by Figure 3-14. The load sweep was done with 2 bar BMEP increment until the highest achievable load at each speed. The engine speed sweep was performed with 500 RPM increment from 1000 to 3000 RPM and 1000 RPM increment from 3000 to 5000 RPM as most gasoline engines operate at below 3000 RPM on various driving cycles as shown by Figure 3-13 and ref. [91].

The temperatures measured in the intake manifold, water jacket and oil passage from Ford Edge vehicle test on one of EPA drive cycles are shown in Figure 3-15. To better mimic the thermal condition of engine in normal driving, manifold air temperature in experiment was controlled at 43 °C, and coolant temperature was maintained at 90 °C. Oil temperature was not

controlled other than using the factory oil cooler (approx. 80 °C). At all conditions, engine was fully warmed up before starting the test.

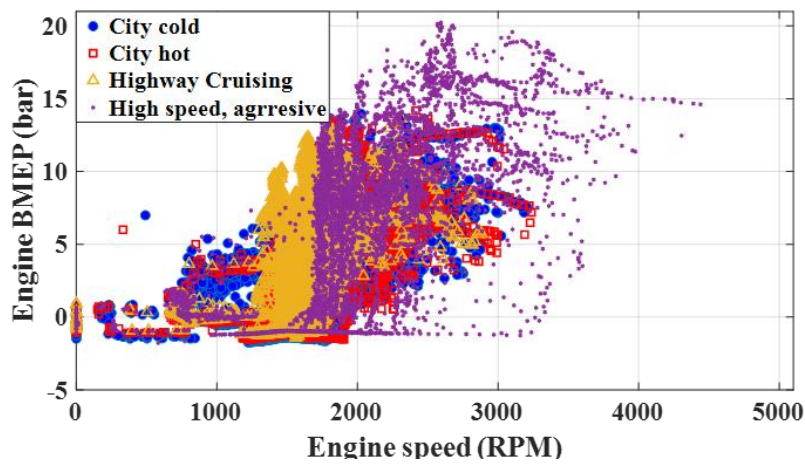


Figure 3-13 Engine operating conditions of a mid-sized SUV (Ford Edge MY19) equipped with 2.0L 4-cylinder EcoBoost engine over different EPA drive cycles.

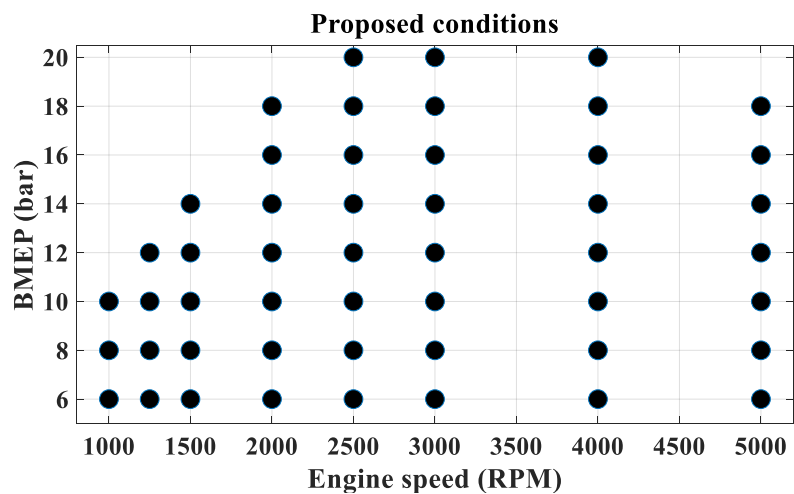


Figure 3-14 Experimental design of engine operating conditions at normal temperature.

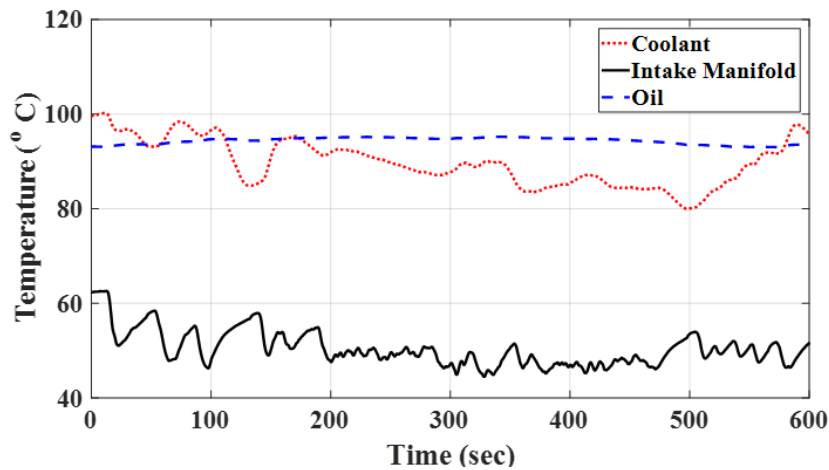


Figure 3-15 Measured temperatures of coolant, intake manifold and oil from vehicle test of Ford Edge MY19 with 2L EcoBoost during UDDS cycle.

High-temperature matrix was designed to mimic engine operation under a typically extreme driving condition – vehicle towing a trailer in hot ambient. The standard tow rating test, regulated by SAE J2807 standard, was used for reference. The SAE J2807 standard has been developed to determine the Gross Combination Weight Rating (GCWR) of a tow-vehicle [88] as towing capacity is becoming an appealing aspect in the market. In this test, a vehicle towing a trailer needs to launch on the Davis Dam Grade (4-7% grade) under at least 38 °C ambient temperature. Under this high-power demand and high-temperature driving condition, propensity to knocking increases, therefore investigating the significance of RON and MON on engine knock limit at this extreme condition is necessary as well.

Two highway gradeability tests on the Davis Dam Grade (part of the SAE J2807 test) of a mid-sized Ford SUV equipped with 2L EcoBoost engine were used as reference for designing high temperature test conditions. In Figure 3-16, engine operating conditions from vehicle tow rating tests of 0-45 mph (72 kph) and 0-65 mph (104 kph) with 3500 lbs (1588 kg) trailer are plotted. Based on this, matrix of engine operating conditions for extreme conditions was proposed (Figure 3-17). The temperatures of intake air, coolant and oil are shown in Figure 3-18, which are higher than those in Figure 3-15. To mimic this thermal condition, air temperature in the manifold was controlled at 70 °C and coolant temperature was maintained at 105 °C. The coolant temperature in the experiment was lower than that in vehicle tests, this was to protect the material sealing the interface between pressure transducer sleeves and coolant passage of cylinder head. Oil temperature was not controlled other than the factory oil cooler which cooled down oil temperature to approximately 95 °C in high temperature engine tests.

Experimental and Numerical Methods

A summary of engine conditions for normal temperature and high temperature tests are given by Table 3-5. It should be noted that not all proposed loads were achievable as there were some limits for engine operation. More details on this is given in following section 3.5.1.2.

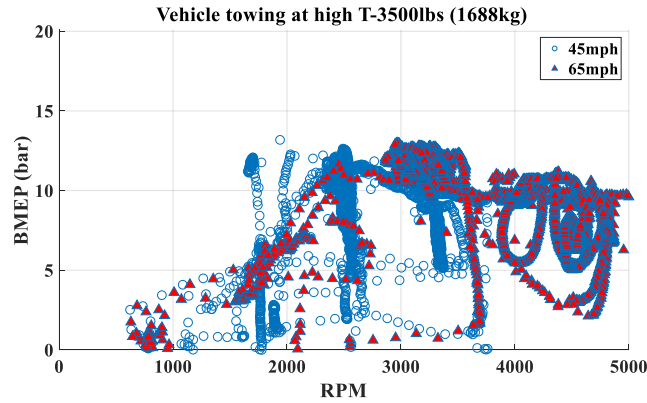


Figure 3-16 Engine operating points of mid-sized Ford SUV equipped with 2L EcoBoost engine in tow rating tests.

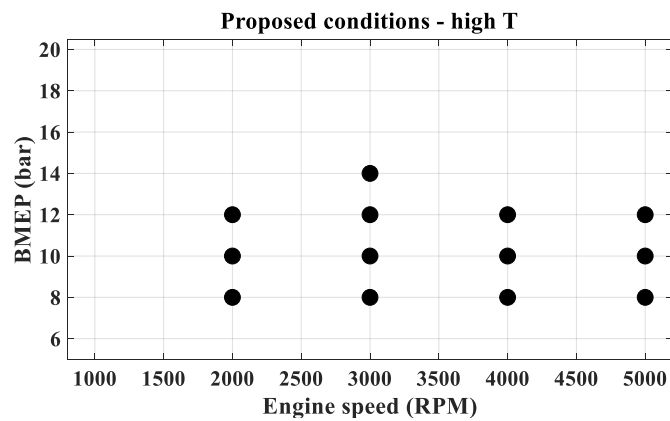


Figure 3-17 Design of engine operating conditions at high temperature.

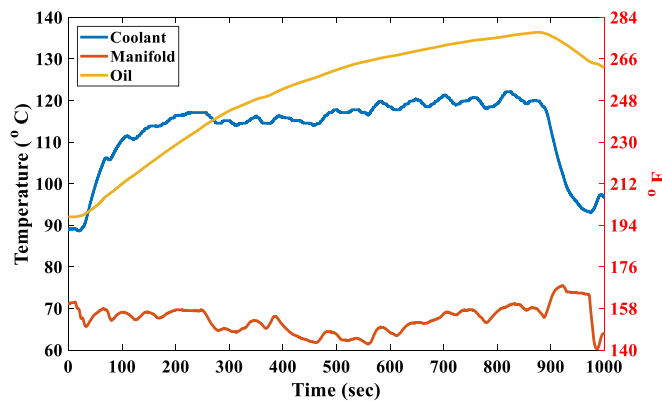


Figure 3-18 Measured temperatures in the intake manifold, water jacket and oil passage on Davis Dam vehicle tests (SAE J2807 tow rating).

Table 3-5 Summary of engine conditions for normal and high temperature tests.

	Normal T test	High T test
Engine speed (RPM)	1000 – 5000	2000 – 5000
Engine BMEP (bar)	6 – 18	6 – 14
Intake manifold temperature (°C)	43	70
Coolant temperature (°C)	90	105
Oil temperature (°C)	70 – 90 (with factory oil cooler)	80 – 100 (with factory oil cooler)
CA50 (° aTDC)	0 – 30	
Lambda	0.75 – 1	
Pre-turbo exhaust temperature (°C)	≤ 900 °C	

3.5.1.2 Experimental Procedures

At each engine speed and load in Figure 3-14 and Figure 3-16, the engine was operated to run at trace knock condition by advancing spark timing. As previously detailed, the spark timing for trace knock was determined by observing the maximum amplitude of pressure oscillations in the filtered pressure trace and through the use of a microphone mounted near the engine to listen for the characteristic pinging noise at the trace knock limit. At low-load conditions where the engine was not knock-limited, the spark timing was over-advanced from MBT timing in order to produce trace knock. If trace knock did not occur when CA50 was already advanced to TDC, engine BMEP would be increased while maintaining CA50 = 0° aTDC until the onset of trace knock. This load would be the lowest achievable load at which a K value could be measured. Therefore, not all low-load conditions in Figure 3-14 and Figure 3-16 are included in the experimental studies. At high-load conditions where spark timing had to be notably retarded, combustion could become unstable with unacceptable cycle-by-cycle based coefficient of variation (COV) when combustion phasing was retarded too much. Therefore, spark timing was not retarded further once CA50 reached 30° aTDC and fuel enrichment was then used when increasing engine BMEP.

The stoichiometric air-fuel mixture was used whenever possible and fuel enrichment was used only when combustion phasing was too retarded or pre-turbo exhaust temperature was too high. At high-load and high-speed condition, due to the high flow rate of exhaust gas and retarded combustion phasing, exhaust temperature increased significantly. To prevent turbine from

overheating (turbine inlet temperature ≤ 900 °C) fuel enrichment was applied to mitigate exhaust temperature. The limit of fuel enrichment was $\lambda \geq 0.75$, otherwise load would decrease [20, 40, 87]. Although the engine has a cylinder pressure limit of 100 bar, this limit was not encountered in the present study.

Because the K value was determined using the PRF method and the highest achievable PRF number using the blending system was 100, very high load conditions where the OI of certification gasoline was greater than 100 was not tested. Given these constraints, not all highest BMEP conditions in Figure 3-14 were achievable. The highest load at each engine speed was finalized when one of above constraints was reached.

The engine was running with the factory calibration for valve timing, fuel injection strategy and turbocharging to reproduce a production engine operation as much as possible. The valve timings were unchanged from factory calibration which was optimized for this engine. The factory injection pressure and injection timings were preserved as well, which were dependent on the engine speed and intake pressure (i.e. engine load). For example, higher fuel injection pressure was used at higher load and more advanced injection timing was applied at higher speed. Instead of using an external compressor, the original turbocharger fitted on the engine was used and a wastegate controller was developed to control boost pressure.

At each operating condition (a given combination of RPM and BMEP), subject to the engine operation constraints described above, the OI and K were determined following the procedures listed below:

1. The certification gasoline was first tested at stoichiometric condition, and the spark timing was adjusted until the trace knock condition emerging (CA50 at trace knock for gasoline is denoted as CA50_{gas});
2. Fuel enrichment was applied if exhaust temperature was close to 900 °C or CA50 = 30 ° aTDC.
3. Fuel system was switched to the PRF blending system and the gasoline supply was shut off;
4. When the engine being fueled by pure iso-octane, throttle position and lambda were adjusted until matching the same BMEP and lambda as gasoline.
5. Spark timing was adjusted to make CA50_{PRF} = CA50_{gas} while maintaining a constant BMEP and lambda.

6. The PRF number was reduced from 100 while keeping $CA50_{PRF} = CA50_{gas}$ until the trace knock was detected.
7. The final PRF number determined was considered as the OI at this condition, from which the K value was calculated with Eq. 3-1.

3.6 SI Engine Combustion Modelling

3.6.1 Modelling Method

The combustion modelling was performed with GT-Power, a computer software for engine modelling [76]. A full engine model with detailed engine geometry and a simplified model with cylinder and crankcase only were used. Some important experimental data were recorded from the engine tests and were used to calibrate the engine model, which are listed below:

- In-cylinder pressure data
- Air flow rate and fuel flow rate
- Temperature and pressure at the inlet and outlet of intercooler and in the manifold
- Engine RPM and BMEP
- Exhaust temperature and lambda
- Intake and exhaust valve timings
- Fuel injection pressure, timing and pulse width
- Spark timing

Once the engine model was able to reproduce all the measured parameters and in-cylinder pressure, it was deemed to be verified, and then used to produce data for further analysis. Significant effort was spent on calibrating the heat transfer through intake ports during the intake stroke, which affects volumetric efficiency, and the heat transfer inside cylinders during combustion, which affects the pressure rising rate during combustion. The flow chart of the modelling method is shown in Figure 3-19. The modelling method can be divided into four steps:

1. Use measured cylinder pressure to estimate the phasing, duration and Wiebe exponent of combustion.
2. Full engine model with a semi-predictive combustion model to calculate the initial conditions for reverse run.

Experimental and Numerical Methods

3. Reverse run model to accurately calculate the combustion burn rate.
4. Full engine model with the imposed burn rate to the non-predictive combustion model to simulate all data of a complete cycle.

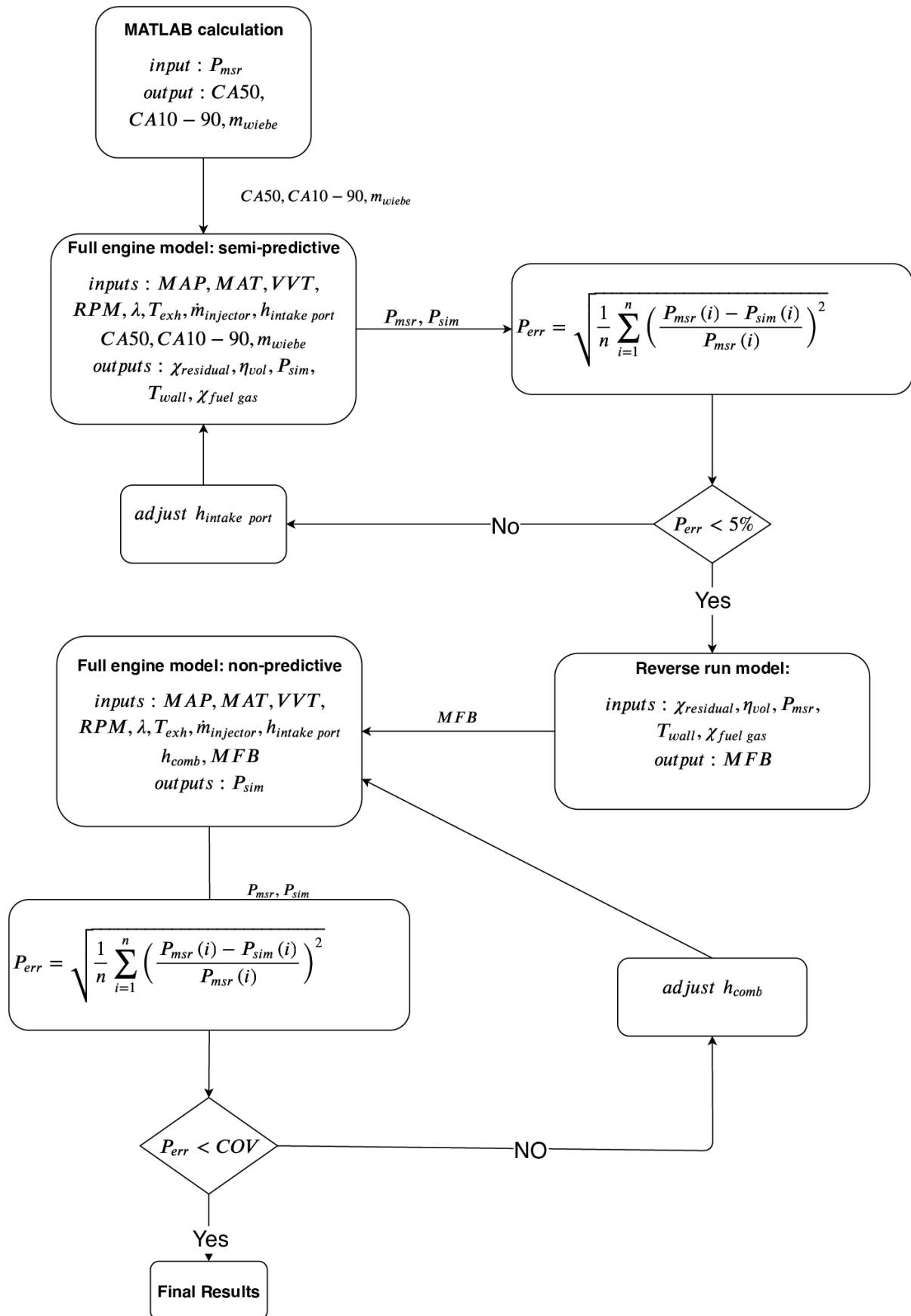


Figure 3-19 Flow chart of engine combustion modelling using GT-Power.

In Figure 3-19:

η_{vol} is the volumetric efficiency relative to air density at 25°C and 1 atm;

$\chi_{residual}$ is the residual gas mass fraction at IVC;

$\chi_{fuel\ gas}$ is the fuel mass fraction in gas phase from IVC to end of combustion;

$h_{intake\ port}$ is the heat transfer multiplier through intake ports;

h_{comb} is the heat transfer multiplier during combustion process.

P_{msr} and P_{sim} are the measured and simulated in-cylinder pressures respectively;

CA10 – 90 is the combustion duration defined from 10% to 90% of total fuel burned;

m_{wiebe} is the exponent for Wiebe function;

MFB is the profile for fuel mass fraction burned;

P_{err} is the normalized root mean square error (NRMSE) of in-cylinder pressure.

3.6.1.1 Step 1: Estimate Combustion Parameters for Wiebe Function

The first step was the MATLAB calculation to estimate the mass fraction burned (MFB) profile with the measured cylinder pressure, using the principle that the percent of fuel burned is approximately equal to the percent of pressure rise due to the heat release from combustion [92]. Once the MFB profile was obtained, combustion phasing (CA50), combustion duration (CA10-90) could be calculated directly. Then a fitting based the functional form of Eq. 3-6 was conducted to find the Wiebe exponent (m_{wiebe}). The Wiebe function describing mass fraction burned vs. crank angle for SI combustion is given by Eq. 3-6.

$$x_b = 1 - \exp \left[-a \left(\frac{CA - CA10}{CA10 - 90} \right)^{m_{wiebe}+1} \right] \quad Eq. 3-6$$

Where:

x_b is the mass fraction burned;

CA is the crank angle in degree;

CA10 is the start of combustion defined as 10% fuel burned;

α is a parameter dependent on combustion efficiency;

3.6.1.2 Step 2: Initial Full Engine Model Simulation

The full engine model included all the components of the 2L EcoBoost engine such as intercooler, turbocharger, direct-injection etc. The purpose of this step was to calculate the residual gas fraction, wall temperatures and fuel evaporation profile which are important inputs to the reverse run model in next step.

The full engine model is predominantly governed by three sub-models:

1. **Flow model:** such as air flow through compressor, intercooler, intake runners, throttle body, manifold and intake valves etc. The geometry and material of this components affect the pressure drops and flow velocity. These components are normally calibrated by matching the measured pressures at relevant positions.
2. **Thermal model:** such as heat transfers through intercooler, through cylinder head, during combustion etc. These can be generally calibrated with measured temperatures. But unlike pressures, temperatures at different positions in a same control volume can be different and not all temperatures are measurable, for example the temperatures in the intake ports of cylinder head. In this case, thermal condition can be verified by matching the mass flow rate because heat transfer can affect the density of fluid.
3. **Combustion model:** the combustion burn rate is calculated using the combustion model. This part can be calibrated by matching the in-cylinder pressure with measured in-cylinder pressure. However, flow model and thermal model can also affect the in-cylinder pressure, so flow model and thermal model need to be calibrated before adjusting any parameters of combustion model.

The flow models for all components were developed with the measured geometry of the test engine. The measured pressures on the intake side were used to calibrate the flow models. Temperatures at the inlet and outlet of the intercooler and inside the manifold were calibrated to match the measured values. The turbocharger was modelled with factory data and calibrated to reproduce compressor-out pressure. A throttle controller was also incorporated, so it could adjust throttle position to match the measured manifold pressure.

Another important part in this step is fuel evaporation model that takes account of fuel distillation curve, injector geometry, and mass flow rate of injection. It calculates how much fuel is evaporated at each time step of calculation. Should not be considered, fuel would remain in liquid state and evaporation will not start until being consumed by combustion, so volumetric efficiency, charge temperature and combustion temperature will be affected. In this step, the fuel evaporation model was developed with injector geometry provided by the manufacturer and with fuel distillation curves measured by the fuel supplier.

In this step, a semi-predictive combustion model was used. The semi-predictive model in GT-Power takes CA_{50} , CA_{10-90} and m_{wiebe} that have been estimated in Step 1 as inputs to simulate combustion and to calculate combustion burn rate which was used in the non-predictive model used in the final step of the simulation.

Wall temperatures, such as cylinder wall temperature, piston temperature and cylinder head temperature were not specified in this step as these data were not available and not measured. Instead, the wall temperature solver was used to calculate wall temperatures based on the thermal conditions coupled with combustion. The wall temperature solver in GT-Power is based on finite element method and requires detailed engine geometry which was provided by the manufacturer of the engine. Only the heat transfer through intake ports was adjusted in this step. Although the manifold pressure and temperature were calibrated, the mass of air entering cylinders is very sensitive to the density of itself, which is affected by the temperature increase through intake ports and valves of cylinder head. The mass of trapped air influences the mass of fuel injected, and therefore total energy released, and in-cylinder pressure are affected. As demonstrated by Figure 3-20, simulated pressures are different when using different heat transfer multipliers for intake ports. In the simulation, h_{port} was adjusted until trapped fuel mass matched measured fuel mass and NRMSE was less than 5%. Heat transfer during combustion (h_{comb}) was not adjusted in this step because adjusting two parameters at one time would complicate the calibration.

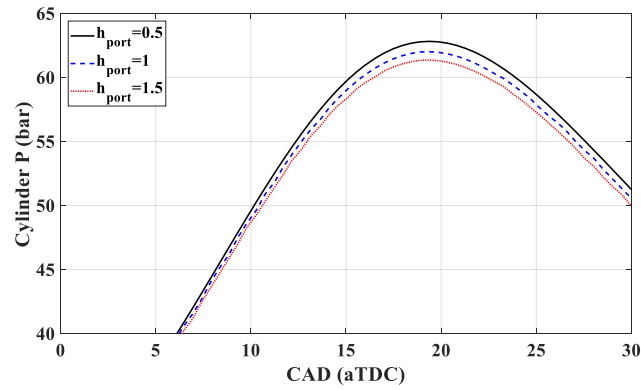


Figure 3-20 Simulated cylinder pressure for 3000RPM, 12bar BMEP, normal temperature condition using different h_{port} .

Results for simulations using different multipliers for heat transfer through intake ports (h_{port}) are summarized in Table 3-6. As shown, changing h_{port} affects volumetric efficiency and hence fuel mass trapped. Fuel evaporation is also influenced as h_{port} affects the charge temperature. However, wall temperatures are insensitive to the change of h_{port} because wall temperatures are primarily affected by combustion process while h_{port} directly influences the gas exchange process during the intake stroke.

Table 3-6 Results from simulations for 3000RPM, 12bar BMEP, normal temperature condition using different h_{port} .

	$h_{port}=0.5$	$h_{port}=1.0$	$h_{port}=1.5$
η_{vol} (%)	102.8	101.4	100.2
m_{fuel} (mg)	43.5	42.9	42.4
$\chi_{residual}$ (%)	6.09	6.14	6.18
$\chi_{fuel\ gas\ @IVC}$ (%)	80.6	83.6	85.9
T_{wall} (cylinder, piston, head) (K)	(429,471,532)	(429,471,531)	(429,471,530)

Once model was able to reproduce all measured parameters and the NRMSE was less than 5%, the simulated results of residual gas fraction, volumetric efficiency, evaporation profile and wall temperatures were recorded for the reverse run model in next step. If the NRMSE was greater than 5%, h_{port} needed to be adjusted until the NRMSE was less than 5%. For all cases, the NRMSE was always lower than 5% when the simulated fuel flow matched the measured fuel flow rate.

3.6.1.3 Step 3: Reverse Run Model

As indicated by its name, reverse run model is a back-calculation process that starts from IVC and ends at EVO, where the measured cylinder pressure is used as an input while combustion burn rate is the output. It is worth noting that the MFB calculated in Step 1 is slightly different from that obtained from the reverse run simulation. The former uses the Rassweiler-Withrow assumption [92] and does not consider the heat loss while the later uses the energy equations and takes accounts of heat loss and fuel evaporation. In reverse run, heat loss is calculated with the provided wall temperatures and fuel evaporation is accounted with imposed evaporation profile that comes from Step 2. Results from Step 2 were used to set up the initial conditions for reverse run. During the reverse run simulation, the solver iterated the combustion burn rate at each step and calculated the in-cylinder pressure until the calculated pressure matched the measured pressure. Then it proceeded to next time step and repeated this calculation until EVO. An example is given in Figure 3-21 where the measured in-cylinder pressure is compared with simulated pressure from reverse run model and it shows the simulated pressure well aligns with the measured pressure with the initial parameters from Step 2.

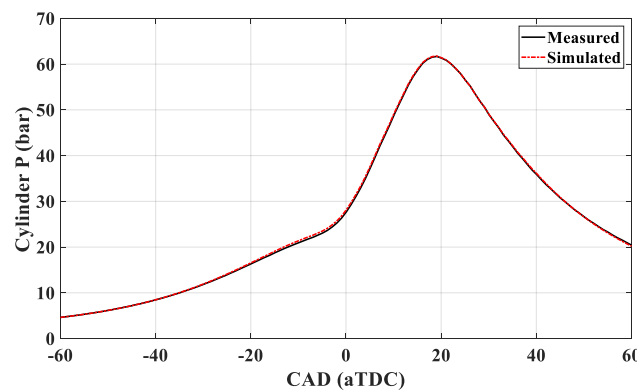


Figure 3-21 Measured cylinder pressure vs. simulated cylinder pressure from reverse run model for 3000 RPM, 12 bar BMEP, normal temperature condition.

3.6.1.4 Step 4: Final Full Engine Model Simulation

The calculated burn rate profile from the reverse run simulation was imposed into the final full engine model. The full engine model in this step is slightly different from the one used in Step 2. In this step, a non-predictive combustion model was used, which requires the prescribed combustion burn rate profile that had been calculated from Step 3.

All parameters used in Step 2 were preserved except the heat transfer multiplier during combustion (h_{comb}). The adjustment of h_{comb} was only applied to the combustion process to

avoid the influence on volumetric efficiency. As suggested by the GT-Power manual, a typical range of this value is from 0.8 to 1.2. An example of its effect on pressure trace is given in Figure 3-22 where the pressure is lower with higher h_{comb} . The target in this final step was to reproduce in-cylinder pressure with NRMSE less than the COV. The reason behind this was that the measured pressure traces for consecutive cycles at a given engine operating conditions had cyclic variation that was characterized by COV. The COV for stable combustion is typically less than 3% so the convergence criterion in this step is stricter than the one of Step 2. The calculated NRMSE for simulations using different h_{comb} is listed in Table 3-7 and it shows when $h_{comb}=1.0$, the simulation result meets the criterion $NRMSE < COV$. So the final results from this simulation were adopted for further analysis.

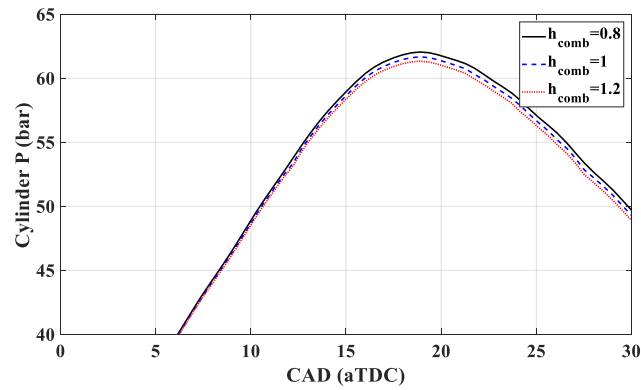


Figure 3-22 Simulated cylinder pressure for 3000 RPM, 12 bar BMEP, normal temperature condition using different h_{comb} .

Table 3-7 Results of NRMSE from final full engine simulation using different h_{comb} .

	$h_{comb}=0.8$	$h_{comb}=1.0$	$h_{comb}=1.2$
Experiment COV (%)	2.41		
NRMSE (%)	2.44	2.29	3.08

3.6.2 GT-Power Modelling

The calculation of end gas temperature by GT-Power uses the two-zone combustion model where the cylinder is divided into a burned zone and an unburned zone from the start of combustion [6]. The heat release from combustion is determined by the chemical equilibrium and the burn rate and it assumes no heat release in the end gas until the unburned fuel-air mixture is transferred to the burned zone.

The GT-Power simulation does not consider fuel chemistry and thus is unable to simulate the LTHR or ITHR during end gas compression. Recent studies showed that these heat releases could affect the pressure-temperature trajectory of SI combustion [54], especially when using PRFs as the fuel. However, the impact of these heat releases on the end gas temperature is considered to be minor in this work. This can be partially verified by the results in Ref. [54], which measured the pre-spark heat releases for a 99 RON gasoline (containing 80 vol.% saturates and 20 vol.% aromatics) in a similar GTDI engine. At 2000 RPM and 20 bar IMEP, the pre-spark heat release was observed to increase with intake temperature but below 70°C none was detected. Given the similar engine setup and a less paraffinic fuel used in this work, it is reasonable to estimate that the 92 RON E10 gasoline should produce less pre-ignition heat release at 2000 RPM, 16 bar BMEP with an intake temperature of 43°C. The likelihood to produce such heat release at other conditions should be even lower for the higher K values. With further compression by the flame, the end gas reactions might produce detectable amount of heat release. Estimation of such heat release will require a gasoline surrogate and a chemical kinetic model that is validated for engine applications, which, however, based on our recent work [93], still requires major efforts for development.

Given the uncertainty introduced by including chemical kinetics and the small effect of LTHR/ITHR of gasoline on the calculation of unburned gas temperature, only the GT-Power modelling results are used in the present study.

3.7 Vehicle Modelling

The vehicle modelling was performed with Autonomie, a MATLAB-based software for automotive system design, simulation and analysis [94]. Autonomie provides an interface where user can define, build and modify all sub-systems of a vehicle. The calculation of the Autonomie is conduct by commanding Simulink and StateFlow in MATLAB. The in-built library of Autonomie offers many validated plant models such as torque converter, tires, chassis etc. which makes vehicle modelling more straightforward. Once the vehicle model was complete, various driving cycles were implemented and all the operating points of each component were logged in a second by second fashion. The engine operation over different driving patterns were therefore derived, from which the distributions of K values were determined.

The vehicle modelling followed the hierarchy tree in Figure 3-23. The baseline was a conventional vehicle that was first built based on a midsize SUV (Ford Edge MY19) equipped with a 2L EcoBoost engine and an 8-speed automatic transmission, and was calibrated to reproduce engine operation and gear shifting events of vehicle tests data using the method proposed by ref. [95]. Then the conventional vehicle was hybridized into a full hybrid vehicle (HEV) with P2 configuration. Engine was downsized to a 1.5L 3-cylinder engine and each cylinder was assumed to be the same as the one of 4-cylinder engine. By doing so, the combined power of HEV was similar to that of the baseline vehicle. Also, since K values measured in this study is a function of BMEP (independent of displacement volume) and RPM, it is reasonable to assume that removing one cylinder from 4-cylinder engine would not change K value for a given BMEP and RPM. The ESS and motor were sized to make the HEV produce the same or better performance as the baseline vehicle. The vehicle control was optimized to achieve at least 35.7% fuel consumption reduction on the standard EPA 2-cycle procedure. This target of fuel consumption reductions were based on ref. [62] that benchmarked the fuel consumption benefits offered by electric drive powertrains for meeting 2025 Corporate Average Fuel Economy (CAFE) regulations.

The next level of hybridization was the plug-in powertrains with the same 3-cylinder engine. The vehicle model of a plug-in hybrid with 64 km (40 mile) AER (PHEV64) was developed. The electric drivetrain was sized to achieve 40-mile AER on UDDS cycle as well as to maintain the same or better performance than the conventional vehicle. The vehicle control was optimized to achieve 68.6% fuel consumption reduction relative the baseline vehicle (based on ref. [62]).

The full details of the Autonomie modelling of powertrains are provided in Section 6.2 of Chapter 6.

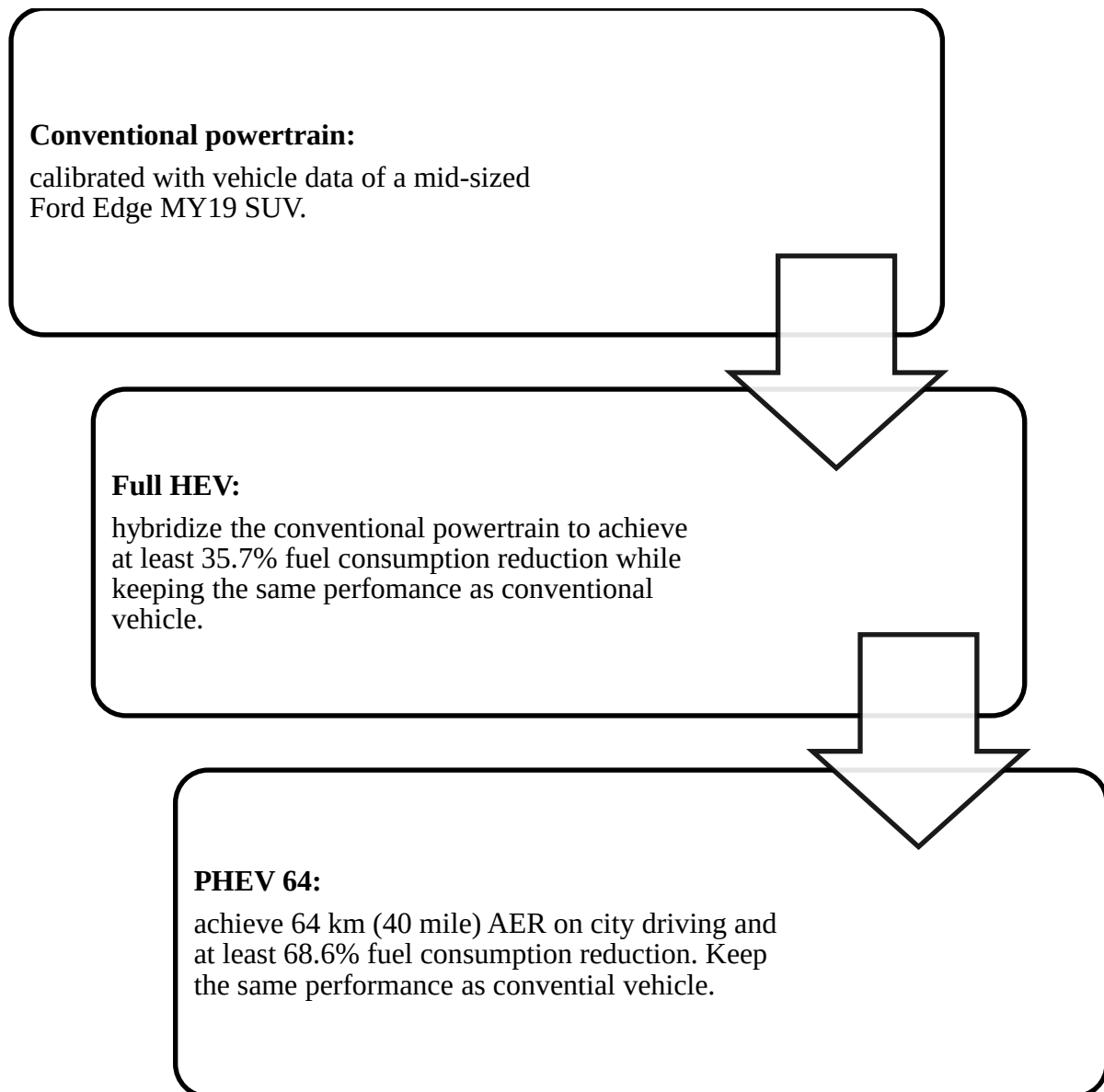


Figure 3-23 Hierarchy tree for vehicle modelling. The targets for fuel consumption reductions are based on [62]

4 Evaluation of Methods for Determining Octane Index and K value

In this chapter, methods for determining octane index and K values are first reviewed. With the literature data from a single-cylinder research engine [90], K values under different engine operating conditions are determined with different methods and the comparisons of these methods are made. Following the comparisons of methods, the effects of engine design and operation parameters on K values are investigated.

4.1 Introduction of Literature Data

The raw data was from the single-cylinder engine tests reported in [90]. A summary of test conditions is given by

Table 4-1. Stoichiometric air-fuel mixture and a constant intake temperature were used. Valve overlap was kept constant of 20° with IVO at 10° bTDC and EVC at 10° aTDC resulting in no scavenging effect and thus in-cylinder lambda was consistent with exhaust lambda. The coolant temperature was maintained at 100°C to be consistent with octane number rating on CFR engine. There was no turbocharger fitted on the test engine, and to mimic the turbocharging effect of modern GTDI engines, a 25 mm orifice was installed downstream of the exhaust port to create the restriction imposed by the turbine of turbocharger. The intake pressure was controlled by an external compressor to supply desired intake boosting.

The engine was specially designed to have three different fueling methods: a side-mounted DI, a port fuel injection (PFI) and a customized form of upstream fuel injection (UFI) among which the UFI produced the most homogeneous mixtures and had the least charge cooling effect. For all three different fueling methods, the air temperature was controlled to be 52°C . The data for two engine speeds (1500 RPM and 2000 RPM) and two compression ratios (10:1 and 14:1) was used for study. At each operating condition, the spark timing was swept to reach trace knock condition and this practice was kept even though the spark timing was more advanced than MBT timing i.e. engine was not knock-limited but over-advanced.

Table 4-1 Summary of engine and test condition

Engine	Single-cylinder SI engine
Fuel delivery	UFI, PFI and DI
Compression ratio	10:1 and 14:1
Valve timing	Constant timings IVO=10° bTDC and EVC=10° aTDC
Engine speed	1500 RPM and 2000 RPM
Intake temperature	52 °C
Intake pressure	Up to 2.5 bar (through external compressor)
Combustion phasing (SA or CA50)	Always adjusted to trace knock condition

The fuel matrix consisted of ethanol-gasoline blends and iso-octane. The ethanol-gasoline blends were prepared in such a way to blend base gasoline of RON from 82 to 98 with 0% to 75% v/v ethanol. The resulted ethanol-gasoline fuels yielded a wide range of RON, S and HoV as reported in [90, 96]. It should be noted that the RON and S (or MON) of the ethanol-gasoline blends are closely correlated as shown in Figure 4-1 where all the ethanol-gasoline points fall into a straight line with R^2 of RON-S linear regression being 0.95. However, the RON and S of iso-octane depart from the linear correlation of ethanol-gasoline blends which substantially reduces the correlation between RON and S, dropping the R^2 of RON-S linear regression from 0.95 to 0.68. This effect is important for calculating K via regression methods as demonstrated in this chapter.

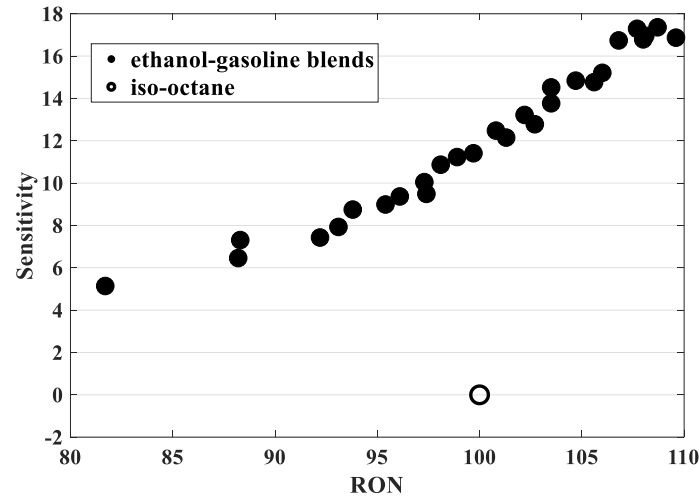


Figure 4-1 The RON and S of all test fuels in the engine experiment from [90].

4.2 Numerical Methods

Four methods for determining OI and K value were investigated including two regression methods: linear regression and nonlinear regression, and two PRF methods: PRF method via direct comparison and PRF method via interpolation.

To keep the consistency of previous studies on the calculation of OI and K, the definition of engine operating condition is based on engine speed, engine compression ratio, fueling method and intake pressure while the indicator of anti-knock ability is KLSA.

4.2.1 Regression Methods

4.2.1.1 Linear Regression Method

The linear regression method was first used when the concept of OI and K was proposed by Kalghatgi [36, 37] where the KLSA of different fuels tested at the same engine operating condition, was found to fit best with a linear combination of fuels' RON and MON, as given by Eq. 4-1.

$$KLSA = a \cdot RON + b \cdot MON + c \quad \text{Eq. 4-1}$$

In Eq. 4-1, the coefficients a , b and c were considered to be independent of the fuel's RON and MON and were determined by linear regression of the obtained KLSA, RON and MON data from a set of fuels.

Rearranging Eq. 4-1 gives Eq. 4-2:

$$KLSA = (a + b) \cdot \left(\frac{a}{a + b} RON + \frac{b}{a + b} MON \right) + c \quad \text{Eq. 4-2}$$

With $OI = (1-K) \cdot RON + K \cdot MON$, the Eq. 4-2 can be rewritten as Eq. 4-3 and Eq. 4-4:

$$KLSA = (a + b) \cdot OI + c \quad \text{Eq. 4-3}$$

$$K = \frac{b}{a + b} \quad \text{Eq. 4-4}$$

As shown by the equations above, to obtain the values of OI and K using linear regression, a set of data of KLSA, RON and MON are required i.e. a series of fuels of different RON and MON must be tested at a same operating condition. To be more specific, at least three different fuels need to be tested at the same operating condition as there are 3 unknowns in Eq. 4-1. An example of this linear regression method using data from [90] is shown by Figure 4-2 where the KLSA can be fitted by linear regression with the corresponding OI and K. The number of points in Figure 4-2 (a) and (b) are 8 and 12 respectively which are only subsets of the entire fuel matrix shown by Figure 4-1 because not all the fuels were tested under these two conditions.

It should however be noted that the regression method requires a carefully formulated fuel set where the RONs and octane sensitivities are sufficiently uncorrelated because the determination of K relies on the knowledge of coefficients a and b which are independent of each other in Eq. 4-1 and this in turn requires RON and MON be independent of each other for regression. Not meeting this requirement would reduce the OI to a function of the RON only, and thus potentially yield problematic K values from the regression. In this dataset, although the ethanol-gasoline blends have correlated RON and S values, the inclusion of iso-octane that is a non-sensitive fuel in the fuel matrix decouples the RON and S. For example, for fuels in Figure 4-2(b), which is a subset of those of Figure 4-1, the R^2 value of the RON-S linear regression drops from 0.96 to 0.15 after including iso-octane into the fuel matrix. Other fuels than iso-octane could also be used, provided their RON and S do not align with those of the rest fuels. Ideally, the fuel set should consist of fuels with evenly distributed and uncorrelated RON and S, instead of relying on a few fuels to break an existing RON-S correlation.

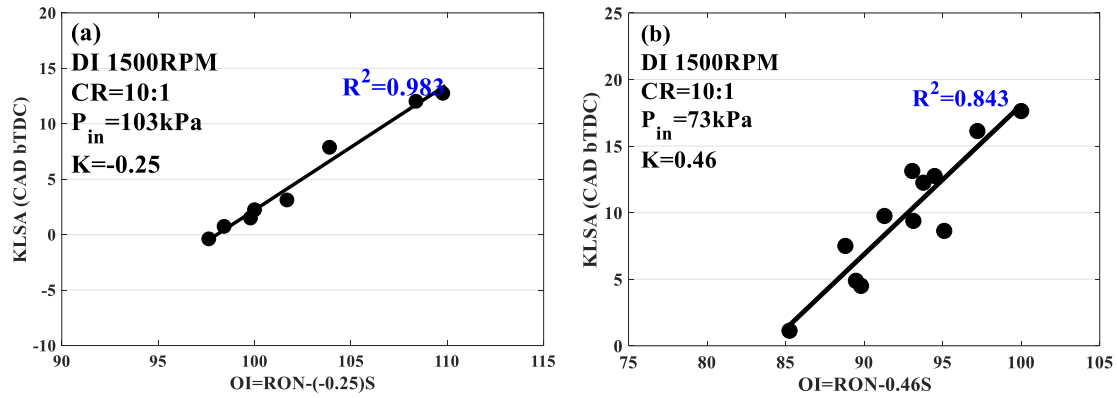


Figure 4-2 K determination using the linear regression method with data from two operating conditions. The fuels used here are subsets of those in Figure 4-1.

To demonstrate the importance of using properly decorrelated fuel set, a comparison of K values determined from fuel sets with and without iso-octane is shown in Figure 4-3 over a range of intake pressures. It is evident that including iso-octane has a major impact on some of the K values, with erratic results ($K > 4$ and $K < -2.5$) obtained at 100 kPa - 125 kPa conditions when iso-octane is excluded from the fuel matrix. This finding is consistent across the range of intake pressures studied. Iso-octane is therefore always included in all fuel sets further studied for K calculation using regression methods.

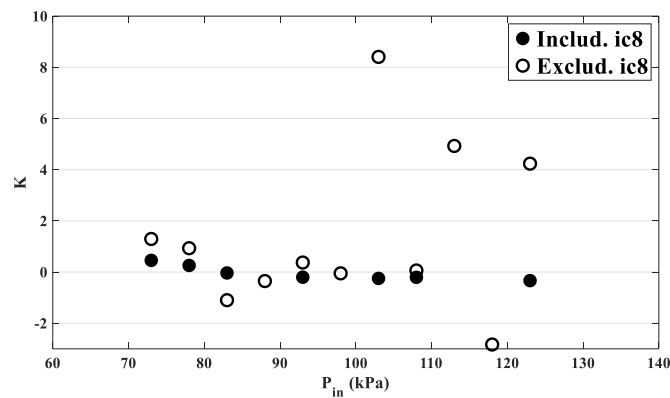


Figure 4-3 Variation of K with intake pressure at DI 1500 RPM and CR=10:1 condition using the linear regression method with dataset including iso-octane and excluding iso-octane.

4.2.1.2 Non-Linear Regression Method

Similar to Eq. 4-3, a second order non-linear relation between KLSA and OI (Eq. 4-5 and Eq. 4-6) were used for determining the K value in previous studies [34, 43].

$$KLSA = \alpha \cdot OI^2 + \beta \cdot OI + \gamma \quad \text{Eq. 4-5}$$

$$KLSA = \alpha \cdot (RON - K \cdot S)^2 + \beta \cdot (RON - KS) + \gamma \quad \text{Eq. 4-6}$$

As shown by Eq. 4-6, the final determination of K (and hence OI) was through solving four unknowns in the equation i.e. α , β , γ and K which can be obtained from the OI producing the best fit for Eq. 4-5. This quadratic regression was applied to the same experimental data sets as that in Figure 4-2 and results are shown in Figure 4-4. The OI and K in Figure 4-4(a) are similar to those obtained by linear regression method in Figure 4-2(a), while the results in Figure 4-4(b) are of difference from those by linear regression in Figure 4-2(b). In Figure 4-4(b), a single point, the iso-octane data, in this regression skews the fit into a trend that KLSA decreases with higher OI which is not physically meaningful. The erratic K value, +1.28, fitted from the quadratic regression, produces no OI in the range of 85-100, in contrast with the case in Figure 4-2(b) for the same data. Figure 4-4(b) demonstrates that the quadratic correlation of KLSA-OI could be problematic as there are both increasing part and decreasing part on a parabola but physically KLSA should increase with OI. Removing the outlying iso-octane point does not solve the issue because when this fuel is not part of the test set, erratic results similar to those in Figure 4-3 can be resulted.

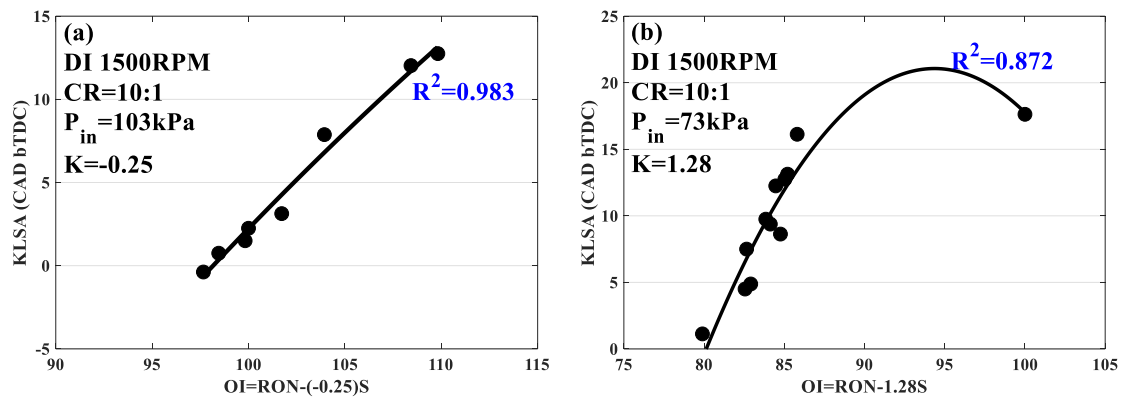


Figure 4-4 K determination using the quadratic regression method with the same data sets in Figure 4-2.

4.2.2 PRF Methods

The PRF method was first used by Mittal et al. [40] who determined the OI of a gasoline (and thus K) by matching the antiknock performance of the test gasoline with PRFs. The method exploits the basic concept that fuels of the same OIs have same anti-knock performance at a given engine operating condition. For example, when a sensitive fuel ($S > 0$) and a PRF exhibit the same anti-knock performance, the OIs of the two fuels are same. Since PRFs by definition have zero octane sensitivity ($\text{RON} = \text{MON}$, $S = 0$), the OIs of PRFs are always equal to the RON or MON values of them. Therefore, the OI can be directly obtained from the ON of the PRF.

The K value for this specific operating condition can then be determined using Eq. 4-7 with the knowledge of the RON and MON of the test fuel (with $S > 0$).

$$K = \frac{RON - OI}{S} \quad \text{Eq. 4-7}$$

One significant advantage of this approach is that PRF method does not require specially designed test fuel sets as the regression methods do. Rather, K can be determined with data from a single test fuel and PRF(s). By matching the antiknock performance of the test fuel with different PRFs at different operating conditions, the dependence of K on engine operating conditions can be investigated. The test fuel must be sensitive fuels with $S \neq 0$ otherwise K value will be infinity as indicated by Eq. 4-7. This method often requires more than one PRF to match the test fuel at a given engine operating condition. To reduce the number of these fuels, PRF calibration curves can be established to enable interpolation of the test fuel to the nearest PRFs, so that OI (and K) could be determined across a range of conditions.

4.2.2.1 PRF Method via Direct Comparison

This method is to find a PRF matching the knock limit of a test fuel under the same operating condition. However, application of this method is limited for the AVL-Ford data due to the fact that only one PRF (iso-octane) was tested in the raw data set. Only a few cases were found where test fuels and iso-octane were tested at similar engine operating conditions and with the same KLSA. For this subset of test fuels, the OI=100 and hence K can be determined using the PRF method. An example of using this method is shown in Figure 4-5 where the data was from intake pressure sweep tests of iso-octane and a gasoline B98E0 (RON98 gasoline blended with 0 v/v% ethanol). At intake pressure of 100 kPa, the KLSA of iso-octane and B98E0 are very close and thus the OI at this point is considered to be 100, with which the K value is determined to be -0.27 by Eq. 4-7. Since the K value is obtained through direct comparison with PRF(s), this is identified as the PRF direct comparison method.

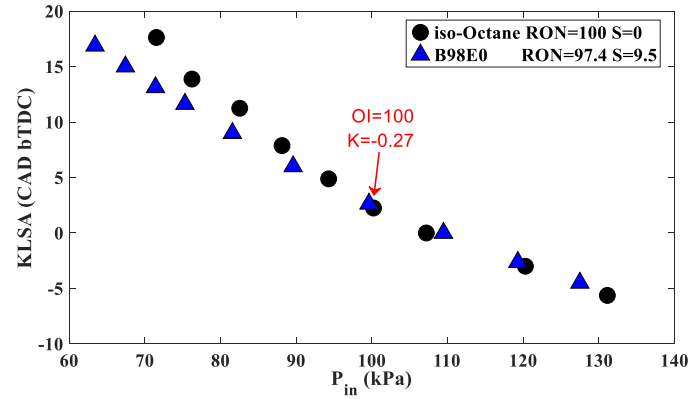


Figure 4-5 K determination using PRF direct comparison method with data at DI 1500RPM CR=10:1 and intake pressure sweep conditions.

4.2.2.2 PRF Method via Interpolation

To make full use of the iso-octane data for this study, a variant of the PRF method was developed. Here a third-order polynomial was formulated to correlate KLSA and P_{in} (as shown by Eq. 4-8) for each fuel at a given compression ratio, fueling method, and engine speed.

$$KLSA = a \cdot P_{in}^3 + b \cdot P_{in}^2 + c \cdot P_{in} + d \quad \text{Eq. 4-8}$$

The intersection of the polynomials for a test fuel and iso-octane at a given P_{in} (or any other appropriate engine operating parameter) should correspond to the condition where the OI = 100. The K value can then be determined from the RON and S of the test fuel at the intersection point while the corresponding P_{in} can be obtained by solving the polynomial equations. Third order polynomials were used in this study as they were found to give reasonable fit of the available data. Of course, this method could equally use other polynomials for other data sets if they provided a better representation.

The method is illustrated in Figure 4-6, where the polynomials of experimental points for iso-octane and a gasoline (B98E20), are observed to intersect at $P_{in}=91.55$ kPa, which yields K value of -0.09. This method does not require that iso-octane and the test fuel be experimentally tested at the intersection point, as required by the PRF direct comparison method. Rather, the polynomial fitting and interpolation allow calculation of K with more sparse data sets.

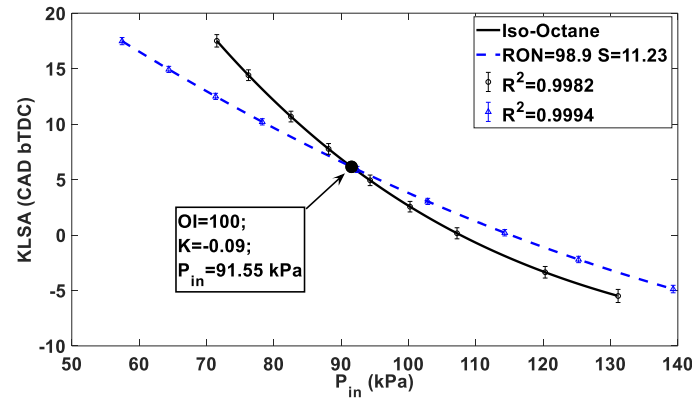


Figure 4-6 K determination using the PRF interpolation method. The polynomial curve of iso-octane intersects with that of a gasoline B97E20. The error bars show the error of the polynomial fitting relative to the experimental data.

4.3 Results and Discussion

4.3.1 Comparing Different Methods for Determining K

The results from linear regression and non-linear regression are compared first. Figure 4-7 shows the K values calculated with two regression methods at two different fueling conditions. The results match well at most conditions except for two points around $P_{in}=70$ kPa where K values from nonlinear regression are 1.3 and 1.4 at DI and PFI conditions respectively. The results from non-linear regression at $P_{in}=70$ kPa are isolated from the overall decreasing trend with increasing intake pressure, indicating the results from non-linear regression could be erratic. The nonlinear regression results for these two points are shown in Figure 4-4(b) and Figure 4-8 where the fitting curves are skewed by a single point (iso-octane) resulting KLSA decreases with higher OI at the right part of the parabola which has been discussed in Section 4.2.1.2. Based on these results, the nonlinear regression method is not used further for the comparison and only K values calculated with linear regression method are used.

Evaluation of Methods for Determining Octane Index and K value

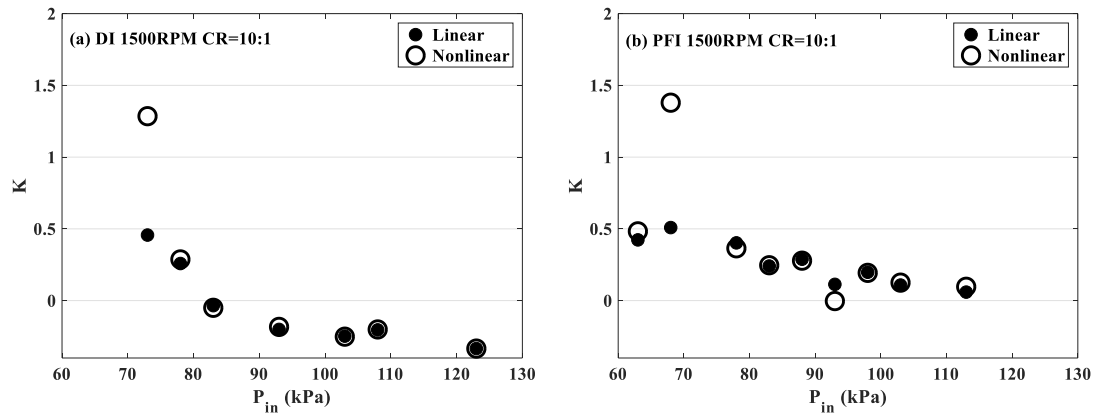


Figure 4-7 Comparison of results from linear regression and non-linear regression methods with data from (a) DI 1500 RPM CR=10:1 and (b) PFI 1500 RPM CR=10:1.

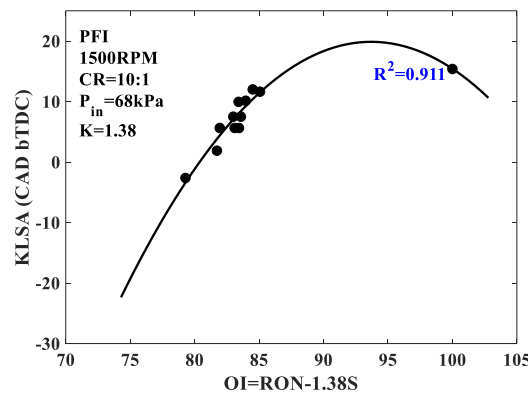


Figure 4-8 Nonlinear regression at PFI 1500 RPM CR=10:1 and $P_{in}=68$ kPa.

A comparison of the three methods other than nonlinear regression method for determining K is now conducted. The K values from these three methods are shown in Figure 4-9 for various operating conditions. Figure 4-9(a) shows for DI fueling condition, K values from three methods are overall similar but the difference can be up to 0.3 (at $P_{in}=83$ kPa). The difference is smaller at PFI fueling condition where the largest difference is 0.2 (at $P_{in}=93$ kPa) as shown by Figure 4-9(b). The K values from the three methods agree closely at UFI condition as shown by Figure 4-9(c), where the difference in K is less than 0.1. These differences are primarily between the linear regression method and the PRF interpolation method. The PRF direct comparison method yields only one or two points in each case, but with the K values generally consistent with the other methods.

Despite the overall similarity of the three methods, particularly in the mean trends of K vs P_{in} , the K values appear to fluctuate more significantly around the virtual trendline with the linear regression method than with the PRF interpolation method. This is particularly evident in Figure 4-9(b), where frequent non-monotonic K variation with P_{in} is observed for linear

regression method. As discussed early, this might be related to the non-ideal fuel set used in this study, with the RON and S being correlated for all fuels except iso-octane.

After comparing the results of K values from different methods, the strength and weakness of each method are summarized below.

1. Fuel set requirement. The regression methods require a set of fuel blends of which the RON and S are not correlated; Otherwise the K values are subject to significant error. Since most hydrocarbons blend more or less linearly with octane number, formulating such a fuel set requires special expertise and blending streams, which limits the application of the regression methods. In contrast, the PRF methods do not have this requirement but only requires a sensitive fuel and a few PRFs tested at the same operating condition.
2. Accuracy of K. The PRF-based methods use the octane numbers of PRFs as the OI reference, which is rigorous in theory. If the direct comparison scenario is applicable, exact K values can be obtained. Otherwise, some type of interpolation, e.g. PRF interpolation, needs to be used. The Regression method, on the other hand, depends on the assumed OI vs KLSA correlation, which can be linear or non-linear, and depends on the curve fitting quality of the regression.
3. OI range for determining K. A key advantage of regression method is that the range of OI is not constrained to values less than 100 as is the case for the PRF method. OI above 100 can be found with modern engines and fuels. Should an analogue to a PRF Method be used for OIs above 100, the mixture of iso-octane and n-heptane cannot of course be chosen and another insensitive reference fuel of high octane number is required.

Based on the above considerations and the fact that only few K values can be determined by the PRF direct comparison method, the PRF Method via interpolation is considered as most suitable for this dataset and is therefore used for further analysis.

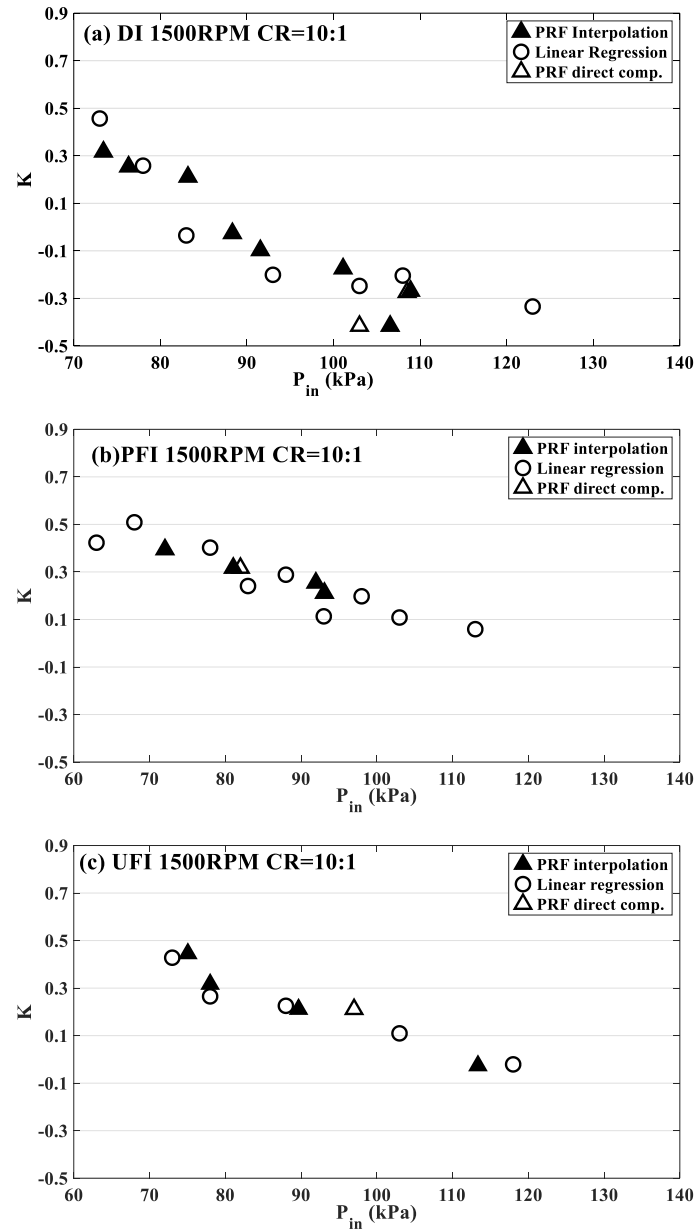


Figure 4-9 Variation of K with intake pressure for (a) DI, (b) PFI and (c) UFI at 1500 RPM and CR=10:1 conditions using PRF interpolation method, linear regression method and PRF direct comparison method.

4.3.2 Effects of Engine Operating Conditions on K

The variation of K with engine operating conditions is investigated for engine load, fueling method, engine speed, and compression ratio. The K values reported are determined using the PRF interpolation method. However, instead of using the P_{in} - KLSA curves to match test fuels with isooctane (as shown in Figure 4-6), the net mean effective pressure (NMEP) - CA50 curves at the corresponding conditions are used for fuel matching. Replacing P_{in} with NMEP

is intended to enable better comparison of K between engines with variable cam timing. Because the engine torque is directly related to engine BMEP and thus NMEP, but NMEP may be different at a constant P_{in} depending on the valve timings. Also, CA50 is indicative of combustion phasing and correlates more directly with end gas conditions than KLSA.

In most cases, K determined from the P_{in} - KLSA matching points is very close to that obtained from the NMEP - CA50 matching points, because the test fuel intersects with isooctane at a very similar, interpolated operating condition. Consistency of the K determined using the two pairs of matching parameters is therefore examined in Figure 4-10, where very similar trends are observed. This is to be expected since the original engine experiments [90] feature close correlation between P_{in} and NMEP due to fixed cam timings. It is noted that test fuels could intersect with isooctane on the P_{in} - KLSA curves, but not necessarily on the NMEP - CA50 curves, which creates disparity in the number of K data shown in Figure 4-10.

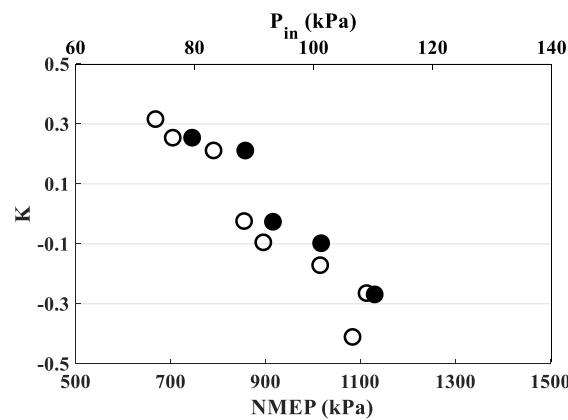


Figure 4-10 K values determined from the matching points on the CA50-NMEP curves (solid circles) and on the KLSA- P_{in} curves (open circles) with data from DI 1500 RPM CR=10:1 condition.

Given that PRF interpolation method is limited to OI=100, the K results presented here are only for a limited range of test conditions in the raw data set, and high-boosting conditions where iso-octane was the least knock-resistant than all other test fuels, are not included.

4.3.2.1 Effect of NMEP

NMEP has a major impact on K because the variation of in-cylinder pressure and temperature directly impacts end gas temperatures [38]. A decreasing trend of K with increasing NMEP is observed in all cases, as shown by Figure 4-10 and Figure 4-11. Recalling that NMEP and P_{in} correlate strongly in the present study, this trend is consistent with that reported by others for both throttled and boosted operation [37, 40, 43, 54].

The pressure impact on K was explained by Kalghatgi [14], as K is directly related to the charge temperature when the gas is compressed to a given pressure, e.g. $P = 15 \text{ bar}$ ($T_{\text{comp}15}$). A higher $T_{\text{comp}15}$ generally corresponds to a higher K for the operating condition. Increasing intake pressure will reduce this temperature and thus decrease K. A recent study by Szybist et al. [54] showed that LTHR and ITHR started emerging at high-load condition due to the higher pressure and this change was more distinct for non-sensitive fuels than for sensitive fuels, which made sensitive fuels more knock-resistant i.e. K value was lower at high-load condition.

As will be noted throughout this thesis, K decreases with engine load (characterized by P_{in} or NMEP or BMEP) consistently in all cases, regardless of other operating parameters that vary at the same time. This indicates the dominant impact of engine load on K.

4.3.2.2 Effect of Fueling Method

Most previous studies on K appear to have used a single type of fueling method. This study examines DI, PFI and UFI on the same engine. This is thought to be a significant feature of these experiments, since several engine parameters are expected to be affected by these differing forms of fueling, particularly the charge cooling and volumetric efficiency. In turn, these may affect end gas conditions and therefore engine knock.

Figure 4-11 shows that at a given NMEP, K for DI is generally lower than those for PFI and UFI. This is particularly clear at 2500 rpm (Figure 4-11(b)). To mark the important differences in engine operation, a dashed line is used to indicate the nominal MBT timing (defined as $CA_{50}=7.8$ and 7.1 CAD aTDC for 1500 and 2500 RPM respectively), which demarcates the knock-limited cases and over-advanced cases for isooctane and the matched test fuels. Note that when fuels of lower OIs are used at the same operating conditions, i.e. at same K-factors, the combustion could still be knock-limited. In other words, the indicated “overly advanced” and “knock limited” are only for $OI = 100$ fuels.

The lower K with DI is most likely due to the stronger charge cooling associated with DI, and greater with ethanol blends, which reduces the charge temperature during compression. The differences between the three fueling methods are nonetheless significantly smaller at 1500 rpm, which is thought to be because most K values at this engine speed were obtained at throttled conditions. With small quantities of fuel injected, the charge cooling from fuel vaporization is less significant relative to in-cylinder heat transfer and other effects. If this is the case, different fueling methods may have limited impact at throttled, low speed conditions.

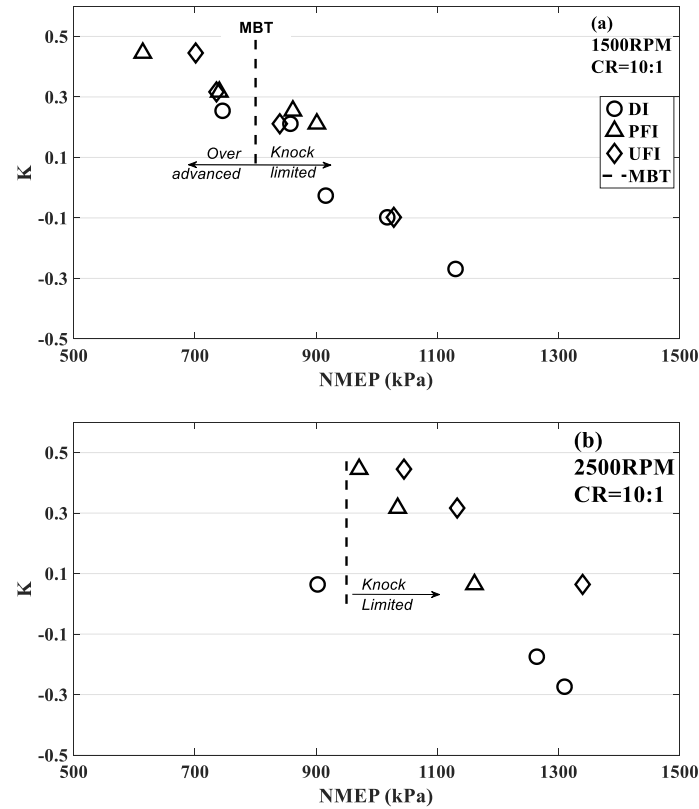


Figure 4-11 The effect of engine fueling on K at (a) 1500 RPM CR=10:1 and (b) 2500 RPM CR=10:1 conditions. The dashed line indicates the MBT limit with knock-limited combustion on the right and over-advanced combustion on the left.

Other findings come to light that K values are less than 0.5 for all knock-limited conditions at compression ratio of 10:1 indicating RON contributes more to OI than MON does and this conclusion is consistent with previous studies [37, 46, 97]. However, K can be positive when combustion is knock-limited especially at 2500 RPM and K value can be close to 0.5 at PFI 2500 RPM condition as shown in Figure 4-11(b), which infers the importance of higher MON value for knock suppression. Though K value is lower at DI condition than that at PFI condition and DI has increasing penetration in the market, the vehicles with PFI still have a large share, as shown by Figure 4-12. Furthermore, as PFI-DI dual-injection system becomes a promising technology on modern gasoline engines [98], PFI condition where K is more positive is therefore still important in the short to medium term. Therefore, there is uncertainty if the MON requirement in modern SI engines can be relaxed without first conducting a comprehensive evaluation of the significance of MON.

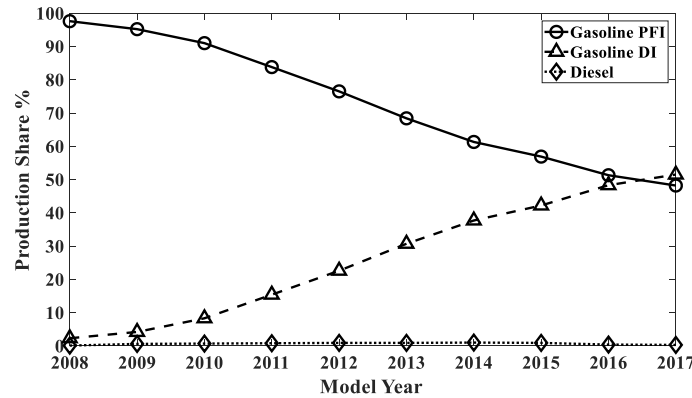


Figure 4-12 Production share of engine fuel delivery technologies on light-duty vehicles in US market from MY 2008 to MY 2017 [17].

4.3.2.3 Effect of Engine Speed

Direct comparisons of the 1500 and 2500 rpm cases are conducted in Figure 4-13 for each fueling method. These are the same data as in Figure 4-11 but plotted differently. A separate reference line for MBT is used for the regrouped data at each engine speed. It is evident that increasing the engine speed leads to higher K, regardless of the fueling method used. This can be generally explained by the less time available for heat transfer to take place at higher engine speeds, shifting the temperature-pressure curve to the higher temperature side i.e. higher charge temperature at a given pressure compared with lower RPM condition. In addition, the residence time of the end-gas at higher RPM is shorter, reducing the time elapsed in the low-temperature chemistry regime where the autoignition of PRFs is promoted, and therefore K is higher [29]. The impact of engine speed on K appears to grow from DI, PFI to UFI. Specifically, increasing engine speed from 1500 rpm to 2500 rpm increases the K by ~ 0.1 with the DI fueling, but this difference increases to ~ 0.5 with UFI. Such variation is likely because with DI, the heat loss difference from 1500 to 2500 rpm is somewhat dampened by the charge cooling effect, therefore resulting in smaller differences in the charge temperature and K in comparison with the UFI cases.

Evaluation of Methods for Determining Octane Index and K value

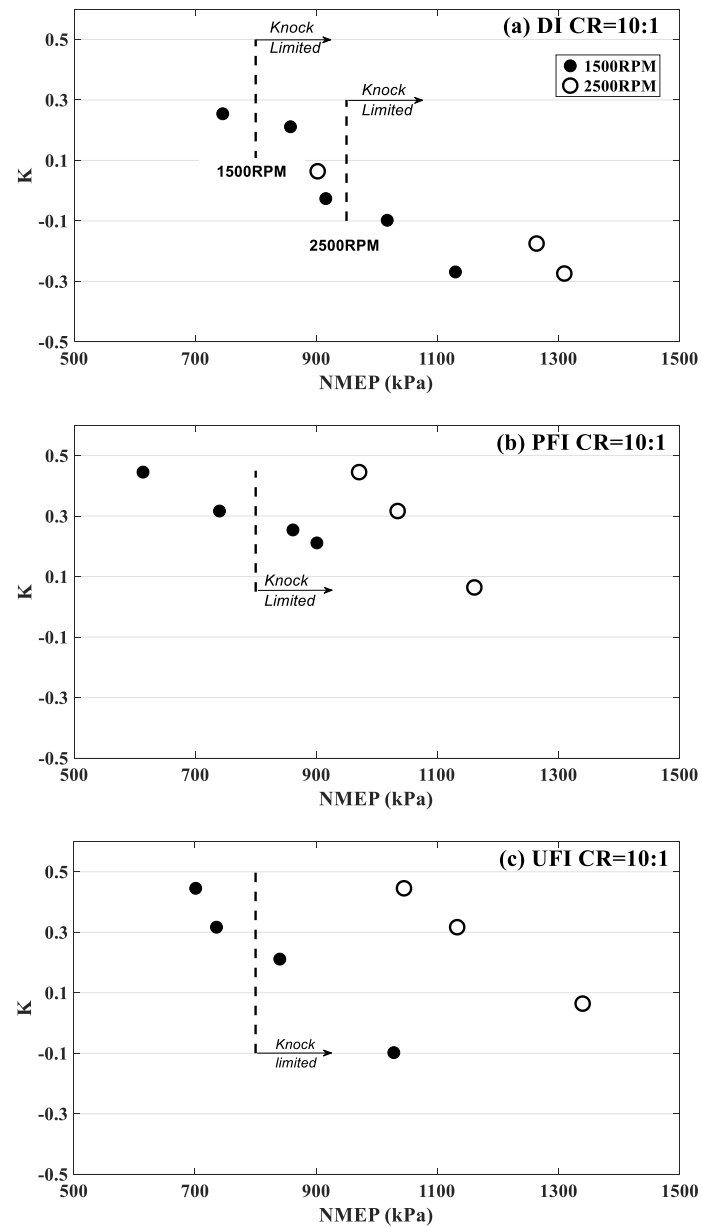
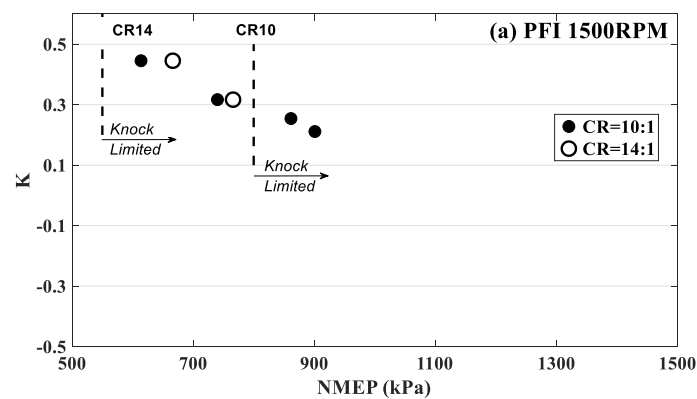


Figure 4-13 The effect of engine speed on K for (a) DI, (b) PFI and (c) UFI CR=10:1 conditions. The dashed line indicates the MBT limit for iso-octane with knock-limited combustion on the right side and over-advanced combustion on the left side.

4.3.2.4 Effect of Compression Ratio

The effect of compression ratio (10:1 and 14:1) is compared in Figure 4-14 for PFI at 1500 RPM and UFI at 2500 RPM. The K values are very similar at both compression ratios, which is consistent with earlier work [5], even though that study did not consider throttled conditions. This insensitivity to compression ratio is nonetheless not a surprising result, since compression ratio increases both compression temperature and pressure, and therefore its impact on the charge temperature at a given pressure is not straightforward. For example, previous experiments in a DI engine [8] showed that K is lower at higher compression ratio.

Despite K values are insensitive to compression ratio, it should be noted that iso-octane (OI=100) is more knock-limited at compression ratio of 14:1 than at compression ratio of 10:1 and combustion can be knock-limited even at low-load condition when compression ratio is increased to 14:1 as shown by Figure 4-14(a). The K values at NMEP=6 bar and CR=14:1 is close to 0.5 which indicates the MON is important for improving OI and thus suppressing knock at this condition. Considering the primary effect of increasing compression ratio on improving engine efficiency, future high-efficiency SI engines will be of higher compression ratio and fuels must be optimized for these engines. Traditionally, engine is calibrated to avoid knock at high-load condition where K is negative and combustion phasing can benefit from fuels of high RON and S. But for engine of high CR, combustion can be knock-limited at part-load where K is positive and efficiency penalty can be caused when using fuels of low MON (high S).



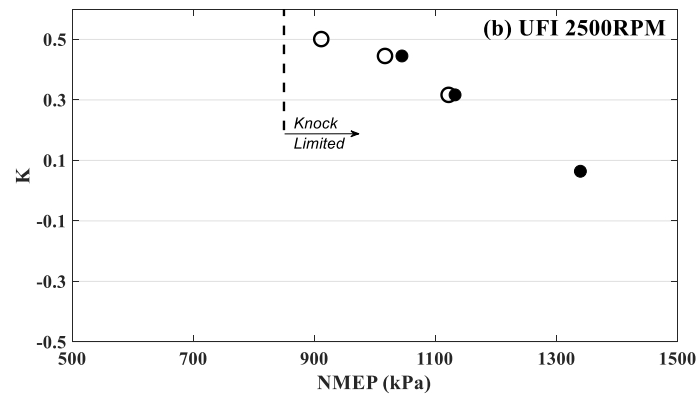


Figure 4-14 The effect of compression ratio on K for (a) PFI 1500 RPM and (b) UFI 2500 RPM conditions. The dashed line indicates the MBT limit for iso-octane with knock-limited combustion on the right side and over-advanced combustion on the left side.

4.4 Summary

In this chapter, four different methods for determining OI and K are compared with experimental data from literature. Regression methods require specially designed fuel matrix of uncorrelated RON and MON while PRF methods only need a sensitive fuel and PRFs to be tested. The results from four methods are consistent at most conditions. The PRF methods produce results of better accuracy due to the rigorous definition that octane number of a PRF equals to its OI. The range of OI is limited to 100 when using PRF method while regression methods do not have this limit. The effects of engine operating conditions on K are investigated with results from PRF interpolation method. K values decrease with higher load, or lower engine speed or fuel delivery of better utilizing HoV but K values are insensitive to the change in compression ratio. Also, K values are positive at some knock-limited conditions especially for higher compression ratio and PFI cases, indicating MON should also be considered at these conditions.

However, it must be noted that the results present in this chapter are limited particularly for the investigation of effects of engine operating conditions on K because the original data set was not intended for studying OI and K. Therefore, a more comprehensive study on OI and K was conducted this thesis and is introduced in Chapter 5 where K values and knock-limited OI were determined throughout the entire operation map of a modern GTDI engine.

5 Octane Index and K values in a Modern Boosted DISI engine

This chapter presents the experimental results of OI and K measured on a 2.0L 4-cylinder Ford EcoBoost engine and investigates the interplay between K and the thermodynamic states of the unburned gas. As introduced in Chapter 3, K values over the engine operation map were determined by matching the CA50 of an EPA Tier 3 Certification gasoline with different PRFs at trace knock condition. It is worth emphasizing that engine operation in the present study was different from that of studies in previous literature where the engine was controlled by varying one operating parameter at a time. By contrast, the engine operation in this study used the production operating map at all conditions for such parameters as valve timing, fuel injection timing, fuel rail pressure and boost control. Previous literature focused on low-speed and high load conditions, but the present study covers the entire engine operating range. In the chapter, the results are divided into two parts: the first part presents experimental results of K measurement and the second part analyses the relationship between K and the end-gas state.

5.1 Repeatability Test

A reference test was conducted regularly to ensure the consistent performance of the engine and thus the repeatability of the K measurement throughout the experimental campaign. In the repeatability test, K was measured at 1500 RPM, 6.5 bar BMEP, and a normal temperature condition ($T_{\text{manifold}} = 38^{\circ}\text{C}$, $T_{\text{coolant}} = 90^{\circ}\text{C}$). Figure 5-1 shows the CA50 at trace knock that was measured at different dates for gasoline and PRFs. Despite the deviation in CA50, $\sim \pm 1$ crank angle degree (CAD) from the mean, the difference in CA50 between gasoline and PRF in the same test was controlled to be less than 0.5 CAD. In Figure 5-2, the measured K values from the repeatability tests are plotted, showing ± 0.03 variation from the mean value. The 95% confidence interval from the repeatability test is ± 0.025 from the mean. The range of K found in the current work is from -1 to 1.1 so a 0.025 variation in K corresponds to an uncertainty of 1.2 % of the value of K.

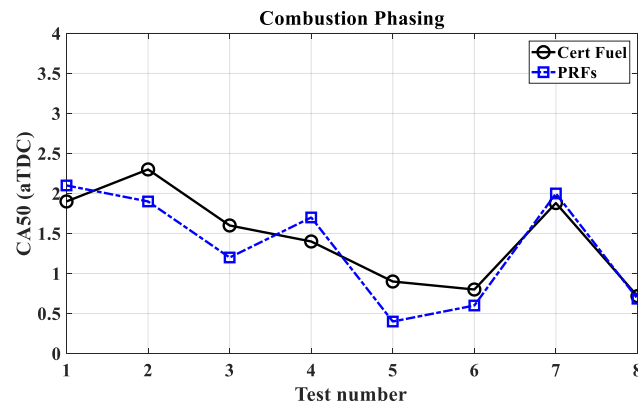


Figure 5-1 CA50 of the certification gasoline and PRFs at trace knock condition from repeatability tests conducted at different stages of project.

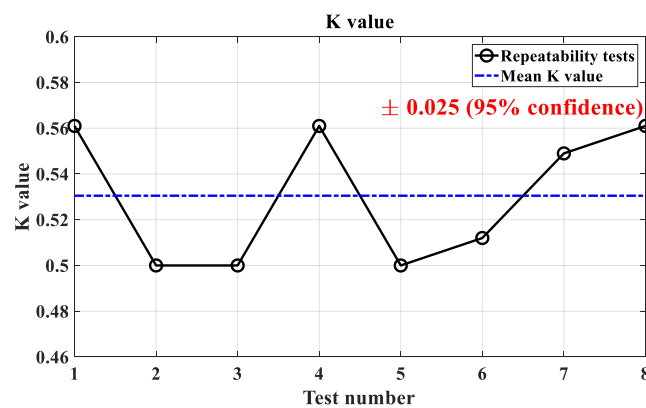


Figure 5-2 Measured K values from repeatability tests. Repeatability tests show 0.025 variation in K.

5.2 Results of Normal Temperature Tests

This section reports the experimental results for normal temperature conditions. This section is divided into three sub-sections and each represents a range of engine speed i.e. low-speed, medium-speed and high-speed. At each speed, load sweep results are presented, including intake pressure, combustion phasing, OI, K etc. In all the figures presented in this section, open markers indicate operating points where the engine was not knock-limited at MBT spark timing (spark timing was over-advanced to achieve trace knock), while closed markers indicate knock-limited operation.

5.2.1 Low-Speed Conditions: 1000-1500 RPM

The MAP is shown in Figure 5-3 for engine speeds of 1000 RPM, 1250 RPM and 1500 RPM. At 1000 RPM, there was no intake boosting due to the low enthalpy of the exhaust gas. From 1250 RPM, turbocharger provided boost at loads of 10 bar BMEP and above. At most

conditions in this speed range, for a given BMEP, intake pressures at different speeds were very close, with the difference less than 3 kPa. The exception to this is at 10 bar BMEP where the MAP at 1250 RPM was higher than that of 1500 RPM by 10 kPa. This difference was attributed to more retarded combustion phasing at 1250 RPM than at 1500 RPM (Figure 5-4), so the intake pressure was increased to compensate for spark retard and maintain 10 bar BMEP.

In Figure 5-4, at 1000 RPM and 1250 RPM, the lowest measured load was at 6 bar BMEP where trace knock occurred when CA50 was over-advanced to TDC. At 1500 RPM, the lowest BMEP that could be measured when CA50 was over-advanced to TDC was at 6.5 bar BMEP. As shown in Figure 5-4, combustion phasing was more retarded at lower speed or at higher load and at the highest loads of 1250 RPM and 1500 RPM, CA50 was very close to 30 °aTDC (the limit of stable combustion). However, this was not the factor limiting the highest load, because fuel enrichment could be used to increase the load when CA50 reached its limit. Figure 5-5 shows that lambda did not reach the enrichment limit ($\lambda=0.75$) at the highest load, so fuel enrichment was not a limiting factor to increasing load. In fact, the highest load at low-speed range was limited by the available enthalpy of the exhaust for the turbocharger. This is different from other studies using an external compressor, in which the intake pressure could be increased regardless of the available enthalpy of the exhaust. Stoichiometric combustion was achieved at most conditions (Figure 5-5), except for the 1250 RPM 12 bar BMEP condition, where fuel enrichment was used to mitigate knock intensity when CA50 reached the stable combustion limit (CA50=30 °aTDC). It should also be noted that with increasingly stringent emission regulations, fuel enrichment will not be tolerated, and future SI engines will operate at stoichiometry over the entire operating range [99].

The knock-limited operation is defined as the point when CA50 is retarded from the MBT timing that is given by Eq. 3-2. In Figure 5-4, the engine is knock-limited (solid points) from a MAP of 100 kPa at 8 bar BMEP for all three speeds. This is a part-load condition for this engine and it is already knock-limited, which is consistent with the findings in ref. [49]. It should be noted that the knock limit is dependent on the gasoline (91.6 RON certification gasoline) and engine (here, a 2.0L EcoBoost engine with 9.3:1 compression ratio) used in this work.

Octane Index and K values in a Modern Boosted DISI engine

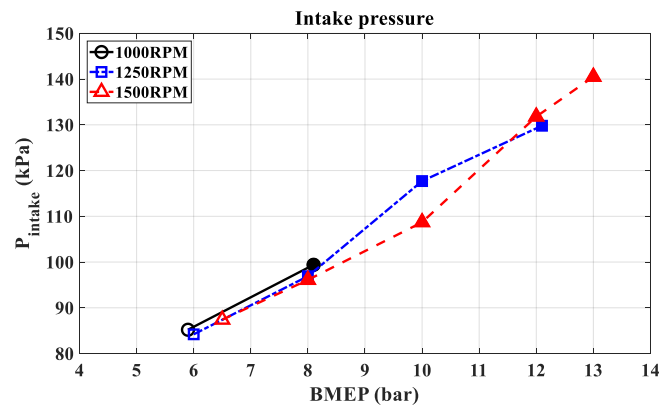


Figure 5-3 Intake manifold pressure of certification gasoline from load sweep at 1000 RPM, 1250 RPM and 1500 RPM. Solid points are for knock-limited conditions while hollow points are for over-advanced conditions and this convention lasts in all figures in this section.

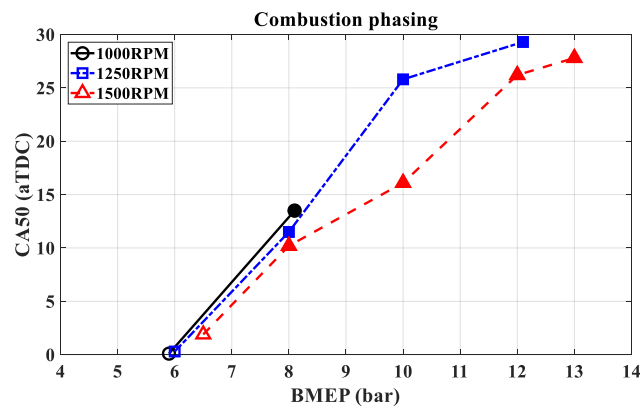


Figure 5-4 Combustion phasing of gasoline at trace knock condition from load sweep at 1000 RPM, 1250 RPM and 1500 RPM.

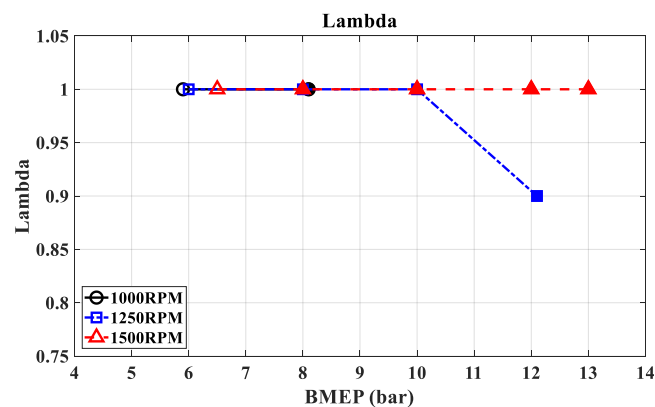


Figure 5-5 Exhaust lambda from load sweep at 1000 RPM, 1250 RPM and 1500 RPM.

The measured OI and K values are shown in Figure 5-6 and Figure 5-7 for the low-speed load sweeps. As shown, OI of the certification gasoline is always higher at lower speed or higher load condition and accordingly, K values are lower at those conditions. However, it should be noted that the effect of BMEP is much stronger than that of speed on OI and K. The knock-limited OI begins from 90 at 1500 RPM and 8 bar BMEP and goes higher at lower RPM or

higher load conditions. As shown in Figure 5-7, K value can be 0.4 – 0.6 at 6 bar BMEP, but combustion phasing is over-advanced from MBT timing, i.e. the engine is not knock-limited at this condition. However, the knock limit is dependent on the engine and fuel as mentioned above. If a higher compression ratio or another gasoline of lower octane rating is used, the over-advanced conditions may become knock-limited. For knock-limited conditions, the K values in low-speed conditions range from slightly positive 0.2 to negative -0.6. These values suggest that RON is much more important than MON in terms of the contribution to knock resistance. However, this does not mean that a lower MON will always improve the fuel's anti-knock performance e.g. for the cases with positive K values.

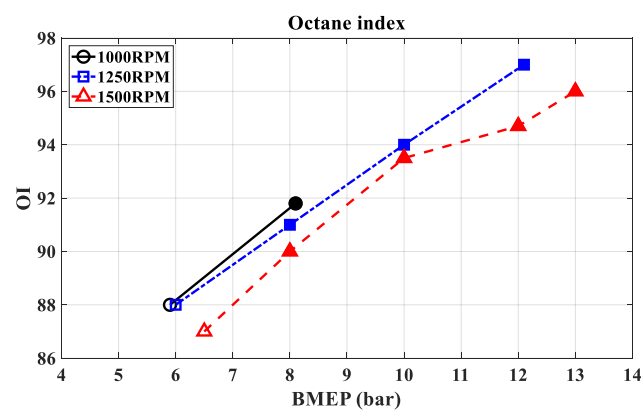


Figure 5-6 Measured octane index of gasoline from load sweep at 1000 RPM, 1250 RPM and 1500 RPM.

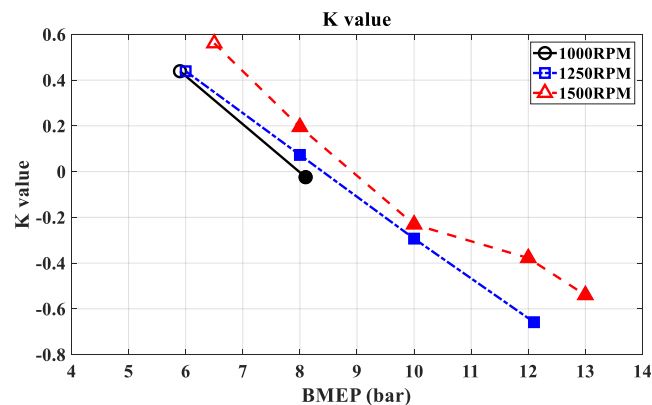


Figure 5-7 K values from load sweep at 1000 RPM, 1250 RPM and 1500 RPM.

5.2.2 Mid-Speed Conditions: 2000-3000 RPM

The MAP is shown in Figure 5-8 for load sweeps at 2000 RPM, 2500 RPM and 3000 RPM. The intake pressures at 3000 RPM were lower than those at lower speed conditions across the range of 12 to 18 bar BMEP. Typically speaking, friction at higher speed is increased over that of lower speed, so for a given BMEP, IMEP should be higher at higher engine speeds. Given

that IMEP is normally a linear function of intake pressure, manifold pressure is supposed to be higher at higher engine speed when BMEP is fixed. There are several reasons for this unexpected engine behavior. Firstly, as given in Figure 5-9, valve overlaps at 3000 RPM were much lower than those at 2000 RPM and 2500 RPM. As those lower speed operating points were boosted, the scavenging effect was stronger at 2000 RPM and 2500 RPM, which lowered the volumetric efficiency. Secondly, as shown in Figure 5-10, CA50 was less retarded at 3000 RPM compared with the other two speeds owing to shorter residence time for the in-cylinder end-gas at higher RPM condition, thus combustion phasing was closer to MBT timing.

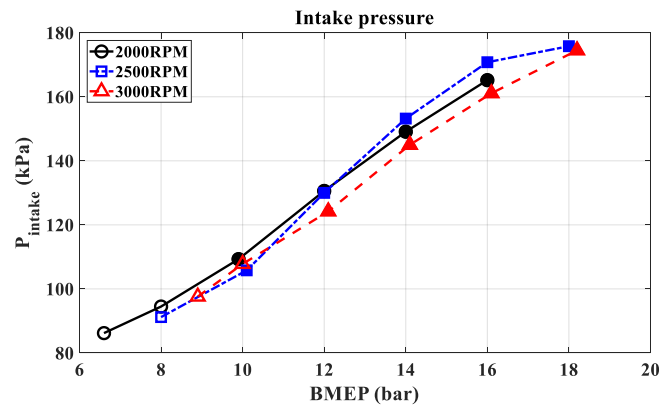


Figure 5-8 Intake manifold pressure of certification gasoline from load sweep at 2000 RPM, 2500 RPM and 3000 RPM. Solid points are for knock-limited conditions while hollow points are for over-advanced conditions.

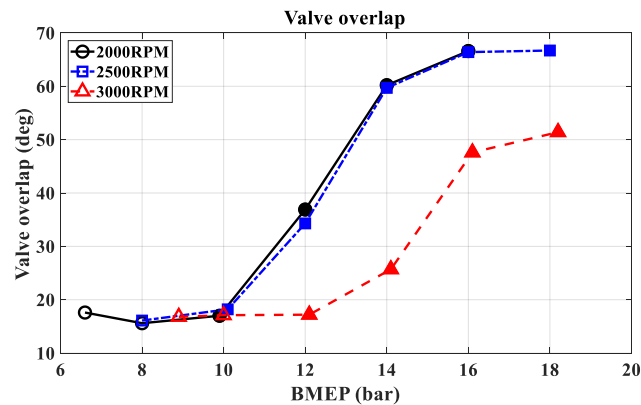


Figure 5-9 Valve overlap from load sweep at 2000 RPM, 2500 RPM and 3000 RPM.

As indicated by the solid points on the figures, the engine became knock-limited at higher loads, (10 bar BMEP for 2000 RPM and 2500 RPM and 12 bar BMEP for 3000 RPM) compared with low-speed conditions in which knock-limited operation starts from 8 bar BMEP. The lowest measured loads (where the CA50 was set to close to TDC, as shown by Figure 5-10) were higher as well, especially for 2500 RPM and 3000 RPM conditions where the lowest achievable loads were 8 bar and 8.9 bar BMEP respectively. At 2000 RPM, the highest load was 16 bar

BMEP, lower than those at the other two speeds, and this was not limited by the enrichment limit, as combustion was still stoichiometric (Figure 5-11). Rather the highest load at 2000 RPM was constrained by the maximum OI that can be produced by the PRF blending system. As shown in Figure 5-13, OI reached 98.5 at 2000 RPM 16 bar BMEP: if load was increased to 18 bar BMEP, OI would be higher than 100, as inferred from the measurement of OI=99.5 at 18 bar 2500 RPM. As the fuel blending system did not use any octane boosting additives such as TEL, it was unable to measure the K values at some of the peak load conditions. However, these conditions account for negligible fractions in standard drive cycles, as will be discussed in Chapter 6.

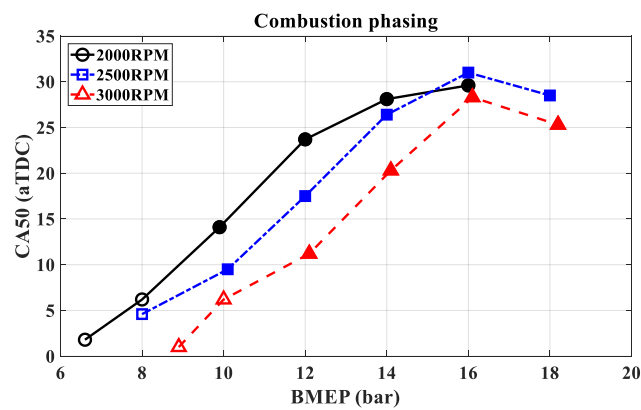


Figure 5-10 Combustion phasing at trace knock from load sweep at 2000 RPM, 2500 RPM and 3000 RPM.

Exhaust lambda and exhaust temperature are shown in Figure 5-11 and Figure 5-12 respectively. Stoichiometric combustion was achieved through the load sweep of 2000 RPM, while fuel enrichment was used at high load of 2500 and 3000 RPM. At 14 bar BMEP and engine speeds of 2500 RPM and 3000 RPM, the exhaust temperature was 900 °C and no fuel enrichment was required. Moving to higher load conditions, combustion phasing needed to be retarded to avoid severe knock intensity, while exhaust enthalpy increased due to the higher fuel consumption rate, both of which caused higher exhaust temperatures. To protect the turbine without increasing knock intensity, fuel enrichment was applied to lower the exhaust gas temperature. At 18 bar BMEP, combustion was richer at 2500 RPM than at 3000 RPM and this was because knock was more likely to happen at lower engine speed. Engine operation at high load and high engine speeds always required a carefully selected combination of spark retard to avoid severe knock (maintaining a CA50 no later than 30 °aTDC) and fuel enrichment both to prevent knock and to cool exhaust gases to protect the turbocharger hardware. Fuel enrichment was only used when spark retard alone could not produce stable, trace-knocking

combustion or the exhaust gas temperature exceeded the continuous operating limit of the turbine ($\sim 900^\circ\text{C}$).

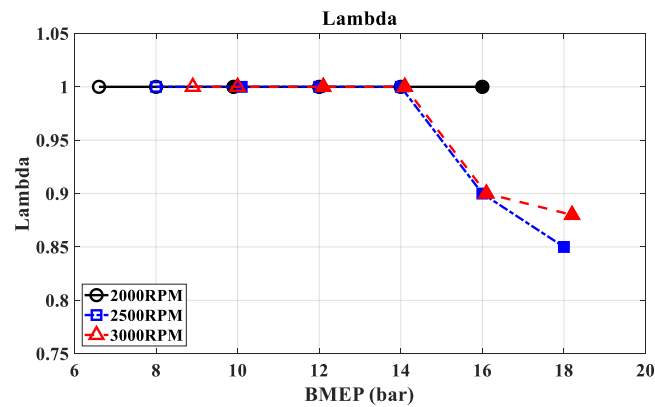


Figure 5-11 Exhaust lambda from load sweeps at 2000 RPM, 2500 RPM and 3000 RPM.

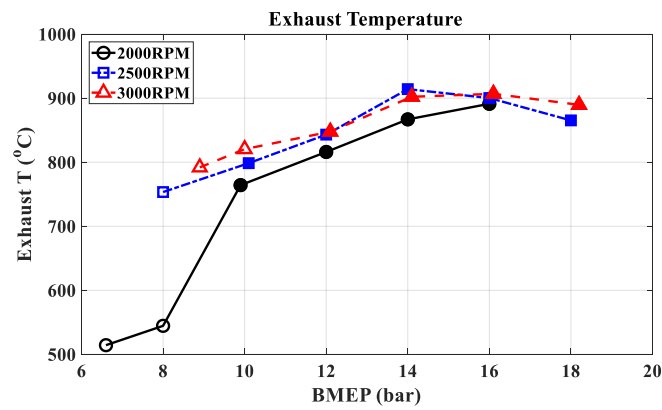


Figure 5-12 Exhaust gas temperature measured before turbine from load sweep at 2000 RPM, 2500 RPM and 3000 RPM.

The measured OI and K are shown in Figure 5-13 and Figure 5-14 respectively. Although the engine was less knock-limited at higher engine speeds, the lowest knock-limited OIs were almost identical for all speeds, which are approximately $\text{OI}=90$. K values were very positive at part-load conditions, and at the lowest loads, K is $+0.6$ indicating MON was more important than RON. However, those conditions were not knock-limited for the test engine with $\text{CR}=9.3:1$ and 91.6 RON gasoline as indicated by the open markers in Figure 5-14. At knock-limited conditions, the highest K value was approximately 0.2 and was similar to that at low-speed.

Octane Index and K values in a Modern Boosted DISI engine

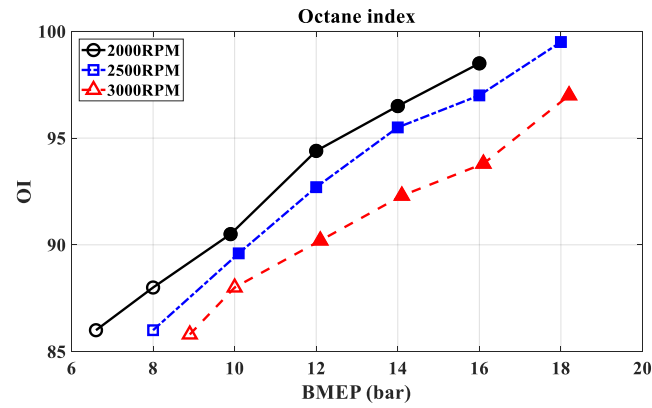


Figure 5-13 Measured OI from load sweeps at 2000 RPM, 2500 RPM and 3000 RPM.

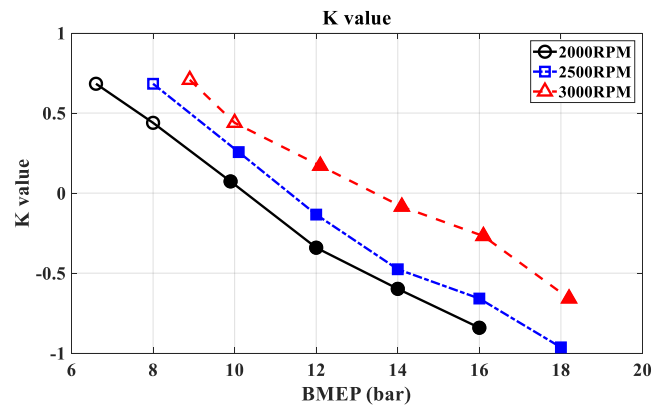


Figure 5-14 Measured K values from load sweeps at 2000 RPM, 2500 RPM and 3000 RPM.

5.2.3 High-Speed Conditions: 4000-5000 RPM

High-speed operation is differentiated from low or mid-speed operation due to higher friction, higher exhaust temperatures and shorter residence time for the in-cylinder end-gas. As shown in Figure 5-15, almost all points are at boosted conditions because part-load, high speed conditions were knock-free in the tested engine setup. MAP at 5000 RPM was always higher than MAP at 4000 RPM, which is due to richer combustion (Figure 5-16) and higher friction mean effective pressure (FMEP). Fuel enrichment was used extensively at high-speed conditions due to the high exhaust gas temperature as shown in Figure 5-17.

Octane Index and K values in a Modern Boosted DISI engine

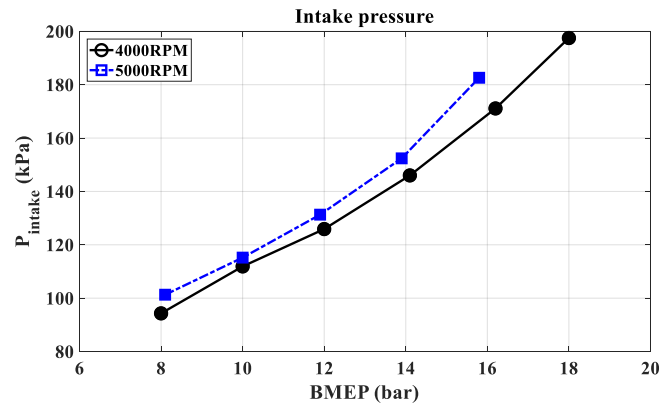


Figure 5-15 Manifold pressure from load sweep at 4000 RPM and 5000 RPM.

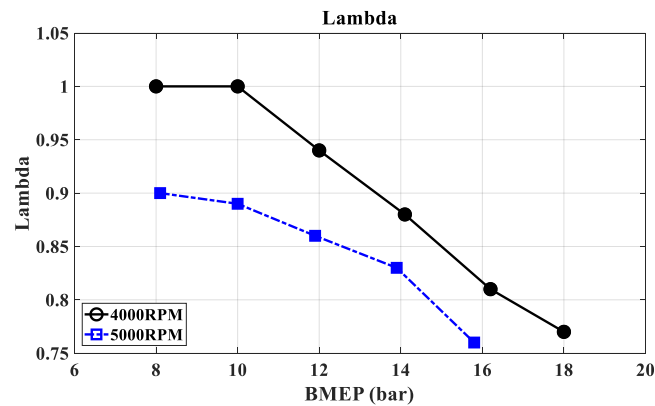


Figure 5-16 Exhaust lambda from load sweep at 4000 RPM and 5000 RPM.

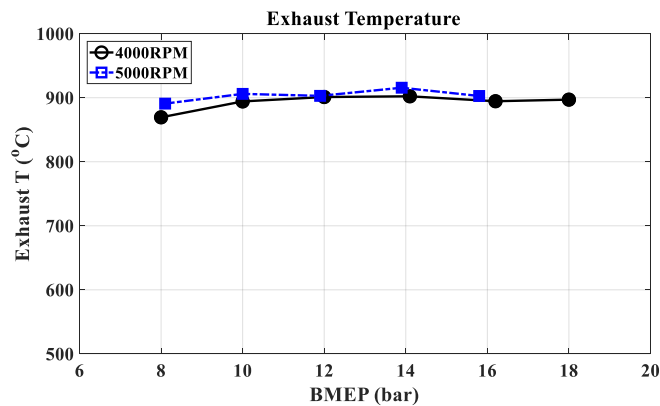


Figure 5-17 Exhaust temperature from load sweep at 4000 RPM and 5000 RPM.

Combustion phasing at the trace knock condition is shown in Figure 5-18. Surprisingly, the engine was more knock-limited at higher engine speed, which was different from the observations at low- and mid-speed conditions. This may indicate that the residence time effect is less significant at high engine speeds. At speeds approaching the engine's revolution limit, the time for heat transfer is reduced and fuel flow rate is higher, resulting in higher temperature and pressure that induces the hot-ignition process. However, at 12 bar and 14 bar BMEP, CA50

Octane Index and K values in a Modern Boosted DISI engine

values at 4000 RPM and 5000 RPM were similar. This may be due to the high fuel enrichment, complicating the assessment of the effect of engine speed.

As shown in Figure 5-18, the lowest load was 8 bar BMEP where engine combustion was knock-limited. Lower loads were possible with over-advanced CA50, but these tests were not conducted at high engine speeds because an engine is unlikely to run at low loads and high speeds during real world vehicle operation. The highest loads achievable in the tests were constrained by the enrichment limit as shown by Figure 5-16 where lambda at the highest load was close to 0.75.

The measured OIs are plotted in Figure 5-19, and it is clear that the overall OIs of 4000 RPM and 5000 RPM are very similar overall. Knock-limited OI starts from 88, which is slightly lower than the low- and mid-speed cases. Accordingly, K values for 4000 and 5000 RPM are similar, ranging from -0.7 to 0.5. The knock-limited K at these speeds are very positive, as high as 0.5, meaning RON and MON contribute equally to knock resistance. K becomes negative at high load conditions as seen with other engine speed load sweeps.

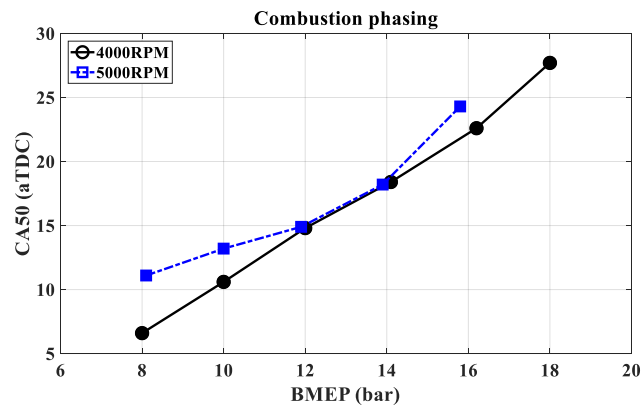


Figure 5-18 Combustion phasing at trace knock from load sweep at 4000 RPM and 5000 RPM.

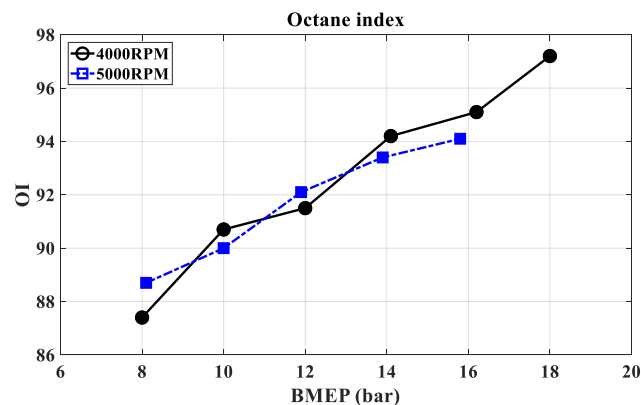


Figure 5-19 Measured OI from load sweep at 4000 RPM and 5000 RPM.

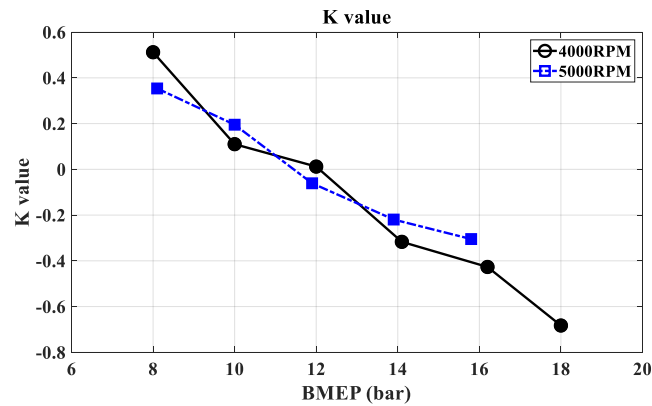


Figure 5-20 K values from load sweep at 4000 RPM and 5000 RPM.

5.2.4 Results of Normal Temperature K-Map

The final experimental matrix of engine operating conditions is summarized in Figure 5-21. The range of conditions does not encompass the full range of engine operation in Figure 3-14. Much of the low load range is truncated because the engine requires excessive over-advancing of the spark to achieve trace knock. The highest load of 20 bar BMEP in Figure 3-14 is not achievable due to the limits of combustion phasing, fuel enrichment and the PRF number. The interpolated K map for engine operation at the normal temperature condition is shown in Figure 5-22. The contour in Figure 5-22 is calculated using the thin-plate harmonic (TPH) spline method and reason for using method can be found in Appendix B.1 of the thesis.

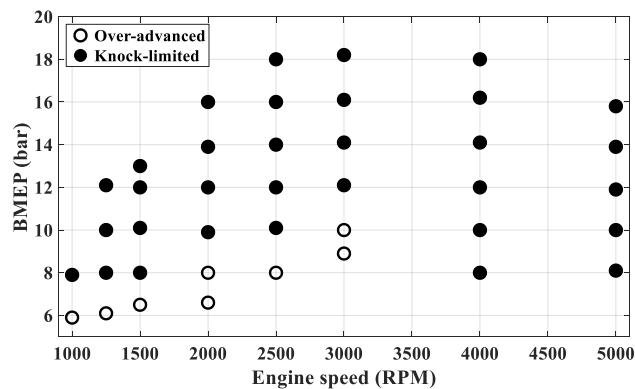


Figure 5-21 Final matrix of engine operating conditions for normal temperature tests. Solid points are for knock-limited conditions while hollow points are over-advanced from MBT.

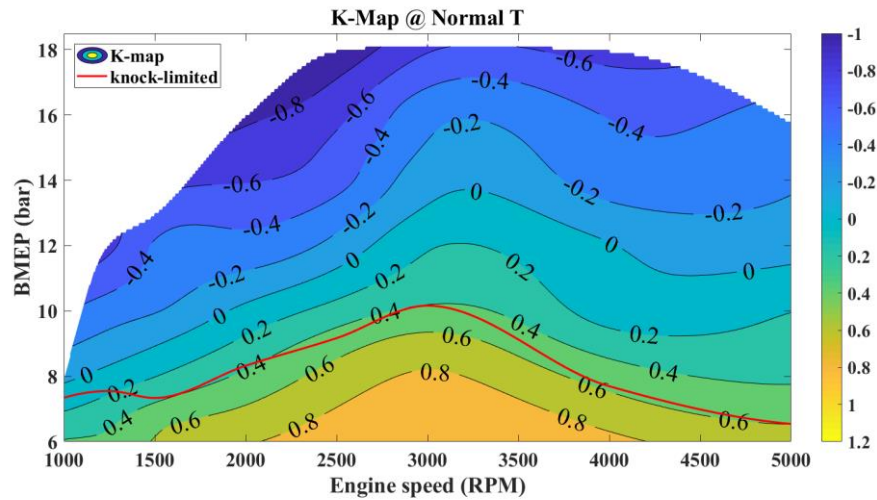


Figure 5-22 Normal operating temperature K map. Conditions above the red line are knock-limited conditions.

5.3 Results of High Temperature Tests

5.3.1 Mid-Speed Conditions: 2000-3000 RPM

The measured manifold pressure is shown in Figure 5-23 for 2000 RPM and 3000 RPM high temperature conditions. Similar to normal temperature conditions, at the same load, intake pressures at different speeds were almost identical. Only difference was at 12 bar BMEP, where the MAP at 2000 RPM was slightly higher than at 3000 RPM due to the more retarded combustion phasing (Figure 5-24) and more fuel enrichment (Figure 5-25) at 2000 RPM.

In Figure 5-24, CA50 was retarded from MBT timing at 8 bar BMEP for both 2000 RPM and 3000 RPM conditions. At the highest loads at these two speeds, fuel enrichment was used as CA50 approached 30 °aTDC (In Figure 5-24 and Figure 5-25). At 3000 RPM, combustion was richer, not only because CA50 was close to the limit, but also because exhaust temperature was approaching the turbine operating limit as shown in Figure 5-26.

Octane Index and K values in a Modern Boosted DISI engine

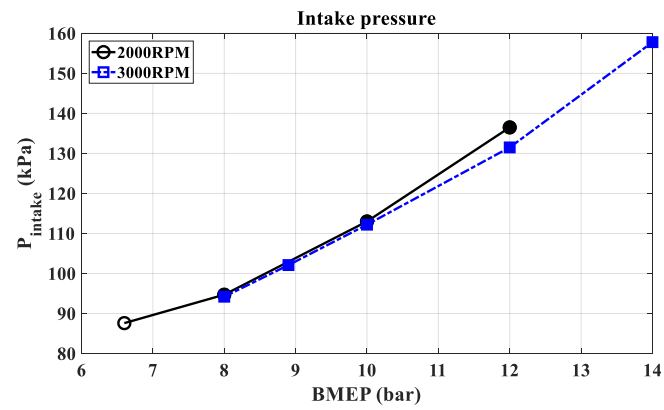


Figure 5-23 Manifold pressure from load sweep at 2000 RPM and 3000 RPM high temperature conditions. Solid points are for knock-limited conditions and open markers are for over-advanced conditions.

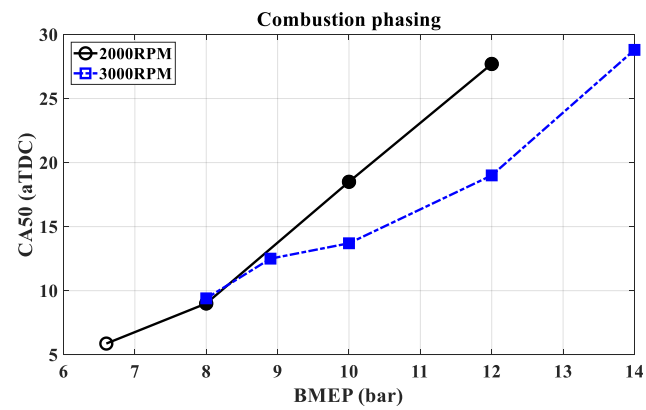


Figure 5-24 Combustion phasing at trace knock from load sweep at 2000 RPM and 3000 RPM high temperature conditions.

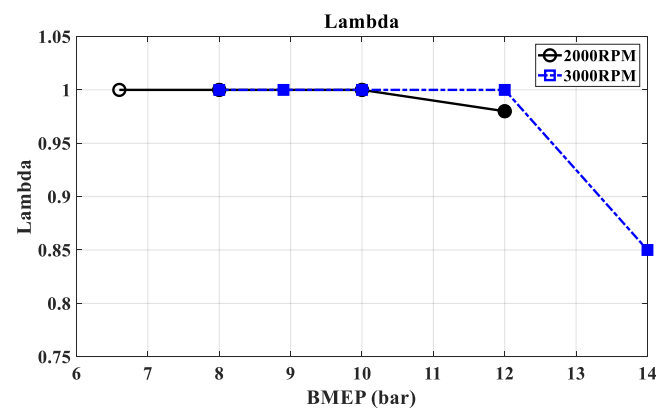


Figure 5-25 Exhaust lambda from load sweep at 2000 RPM and 3000 RPM high temperature conditions.

Octane Index and K values in a Modern Boosted DISI engine

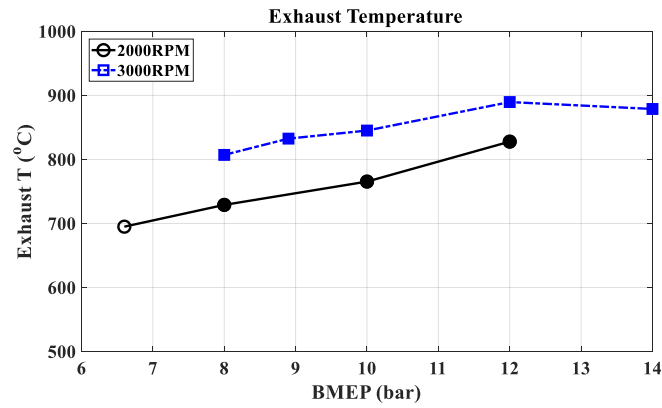


Figure 5-26 Exhaust temperature from load sweep at 2000 RPM and 3000 RPM high temperature conditions.

The measured OI and K are plotted in Figure 5-27 and Figure 5-28. The lowest knock-limited OI, around 86 at 2000 RPM and 82 for 3000 RPM, were much lower than those at normal intake air temperatures (where OI= ~ 90), and accordingly, the maximum knock-limited K values were very positive (greater than 0.5 at both speeds). In particular, at 3000 RPM and 8 bar BMEP, K was greater than 1, in which MON had a dominant effect on knock resistance.

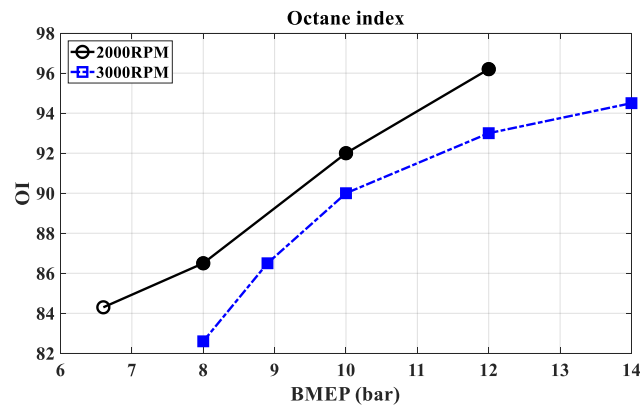


Figure 5-27 Octane index from load sweep at 2000 RPM and 3000 RPM high temperature conditions.

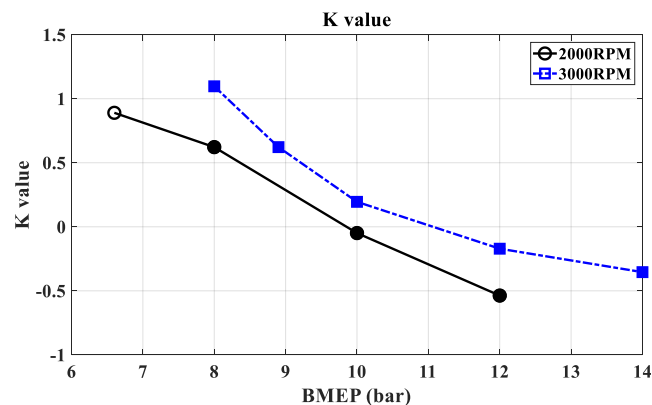


Figure 5-28 K values from load sweep at 2000 RPM and 3000 RPM high temperature conditions.

5.3.2 High-Speed Conditions: 4000-5000 RPM

Figure 5-29 shows the MAP at high temperature conditions, and similar to what was observed at normal intake air temperature, the MAP was higher at 5000 RPM than at 4000 RPM for a given load. This was primarily due to more retarded combustion phasing at the 5000 RPM condition as shown in Figure 5-30. With the exception of 8 bar BMEP at 4000 RPM, all the conditions shown in Figure 5-31 were enriched because of the high exhaust temperatures (Figure 5-32). The measured OI and K are plotted in Figure 5-33 and Figure 5-34 respectively. For the 8 bar and 10 bar BMEP conditions, OI and K at the two engine speeds were nearly identical, and this is consistent with the results at normal intake air temperature. Considering the results of Figure 5-28, the knock-limited K was always greater than 0.5 at the 8 bar BMEP condition across all speeds, i.e. MON was more important than RON at these conditions.

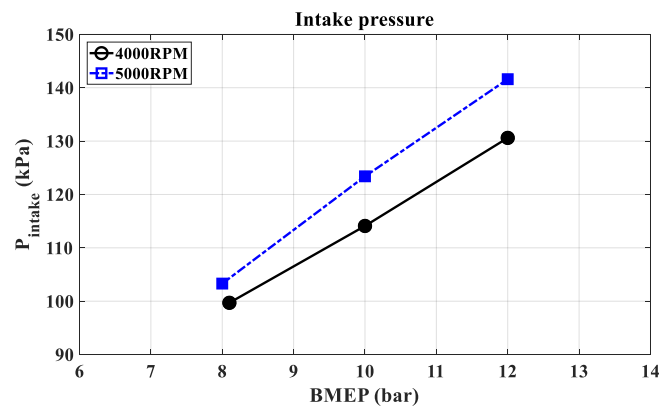


Figure 5-29 Manifold pressure from load sweep at 4000 RPM and 5000 RPM high temperature conditions.

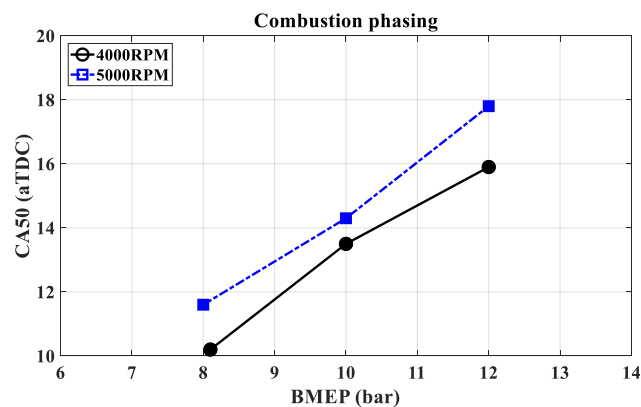


Figure 5-30 CA50 from load sweep at 4000 RPM and 5000 RPM high temperature conditions.

Octane Index and K values in a Modern Boosted DISI engine

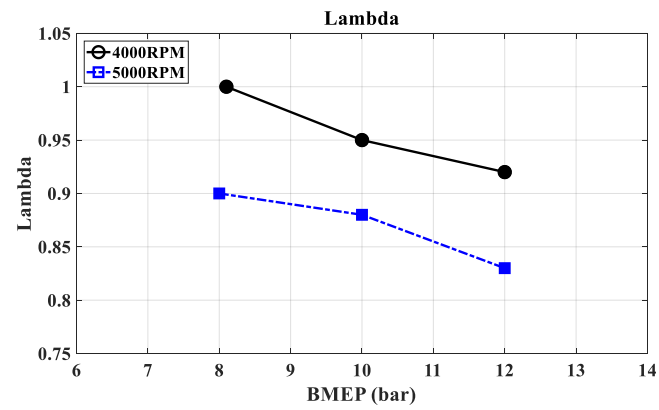


Figure 5-31 Exhaust lambda from load sweep at 4000 RPM and 5000 RPM high temperature conditions.

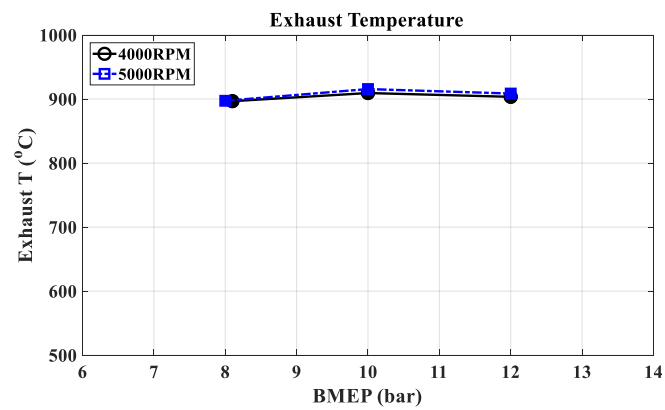
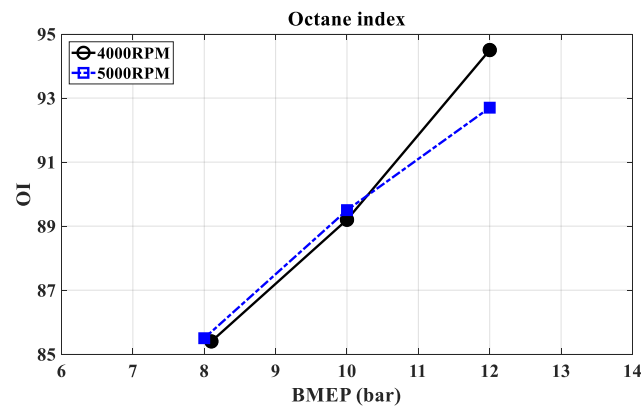


Figure 5-32 Exhaust temperature from load sweep at 2000RPM and 3000RPM high temperature conditions.



Octane Index and K values in a Modern Boosted DISI engine

Figure 5-33 Octane index from load sweep at 4000RPM and 5000RPM high temperature conditions.

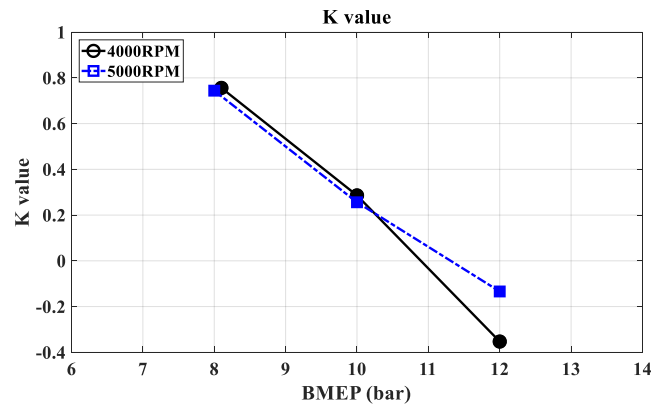


Figure 5-34 K values from load sweep at 4000 RPM and 5000 RPM high temperature conditions.

5.3.3 Results of High-Temperature K-Map

The K map for the high temperature operation is presented in Figure 5-35. The same interpolation method (TPH spline) was used for generating the contour as shown in Figure 5-22. Comparing Figure 5-35 and Figure 5-22, at part load conditions (~8 bar BMEP), the K values at the higher temperature are higher than at normal temperature conditions. In addition, as indicated by the flat contour across the speed range, the effect of engine speed on K at high temperature is less pronounced as that at normal temperature. These effects on K is investigated in Section 5.4.

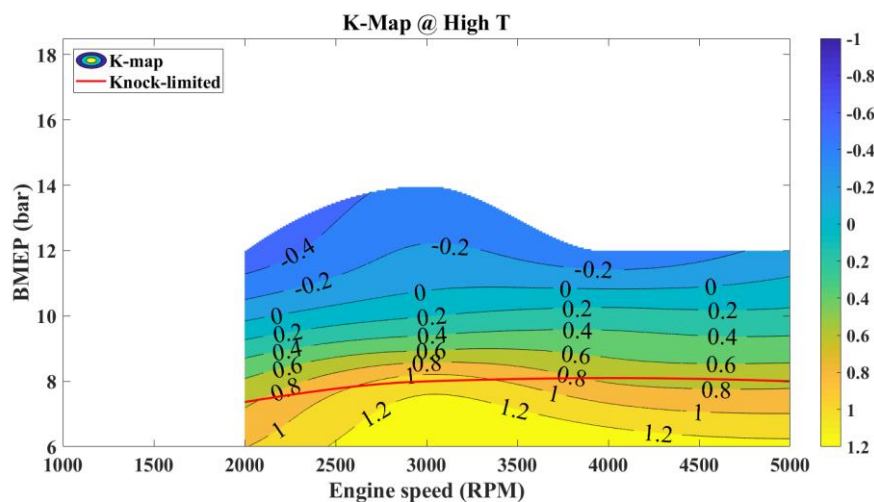


Figure 5-35 High-temperature K map. Conditions above red line are knock-limited conditions.

5.4 Effect of Engine Operating Conditions on K

Although the variation of K values over a range of engine operating conditions have been investigated in Section 4.3.2, the range was limited to relatively low speeds and loads. More importantly, the test engine was a single-cylinder research engine with fixed valve timings and fuel injection timings, and there was no turbomachinery used to generate boost. This part aims to understand how K changes with operating conditions for a modern, multi-cylinder production engine running with an OEM optimized configuration.

5.4.1 Effect of Engine Speed

The dependence of K on engine speed at normal temperature (intake temperature 38°C and coolant temperature 90°C) is investigated in this sub-section. Combustion phasing at trace knock is plotted in Figure 5-36 at two different engine loads. At 12 bar BMEP, CA50 became less retarded with increasing engine speed in the low- and mid-speed ranges and then combustion phasing became more retarded with higher speed from 3000 to 5000 RPM. The trend was different at high load conditions where fuel enrichment was utilised differently for different speeds. As generally anticipated, for a given load, the engine is less knock-limited at higher engine speed (decreasing CA50 towards MBT operation), which is consistent with the trend shown from 1250 to 3000 RPM. The reason for this trend is that the residence time for the end-gas autoignition reactions is shorter at higher engine speed, so autoignition is less likely to happen [27-29]. However, this cannot explain the non-monotonic trend of CA50 from 3000 RPM to 5000 RPM at 12 bar BMEP, which was also observed in ref. [20]. To address this, measured cylinder pressures and modelled unburned gas temperatures for a speed sweep from 3000 RPM to 5000 RPM, at 12 bar BMEP conditions are shown in Figure 5-38. As shown in Figure 5-38, both the unburned gas temperature and cylinder pressure at high speed are lower than that at 3000 RPM and resistance time for autoignition is shorter at high speed condition. Those effects at high speed are inhibiting autoignition process. However, autoignition can be promoted by fuel enrichment at a given pressure or temperature due to the increased overall reactivity of the mixture [100]. These results suggest that the trace knock combustion phasing at high speed is dictated by competing effects of resistance time (engine speed), thermal condition (pressure and temperature) and fuel-mixture strength. The results at 12 bar BMEP indicates the promoting effect of fuel enrichment on autoignition is greater than the other two inhibiting effects at high engine speed condition.

Octane Index and K values in a Modern Boosted DISI engine

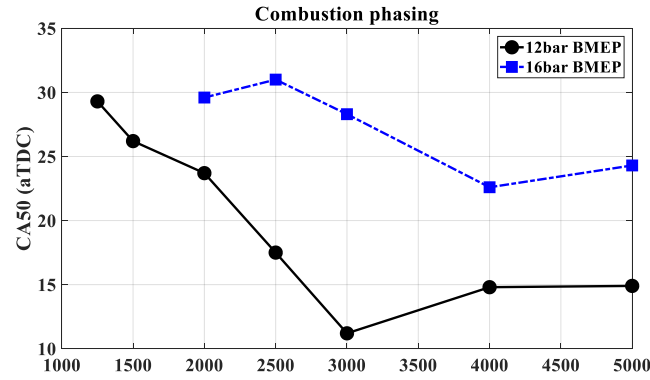


Figure 5-36 CA50 at trace knock from speed sweeps at part- and high-load, normal temperature conditions.

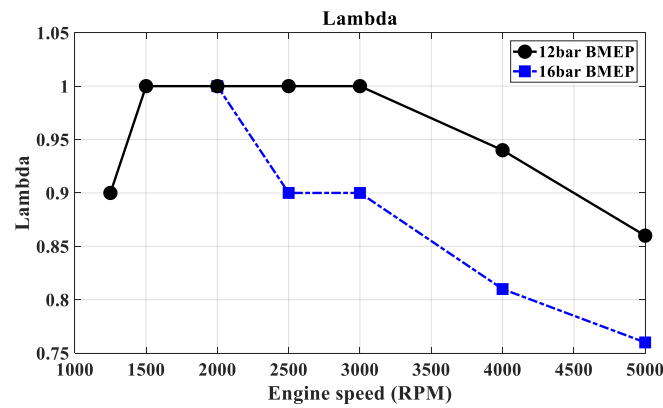


Figure 5-37 Exhaust lambda from speed sweeps at part- and high-load, normal temperature conditions.

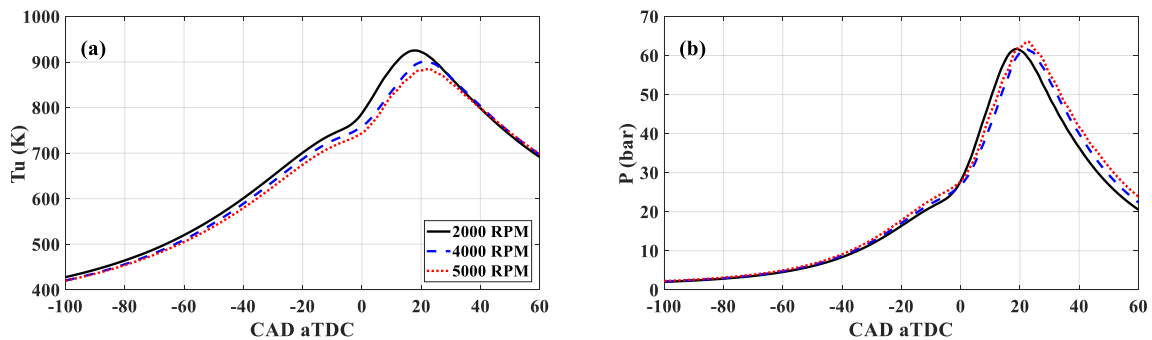


Figure 5-38 (a) unburned gas temperature and (b) cylinder pressure from 3000 RPM to 5000 RPM at 12 bar BMEP, normal temperature condition.

Figure 5-39 shows the K values at different speeds for a part-load condition and a high-load condition. Regardless of the load, K increased with engine speed when the speed was lower than 3000 RPM and became insensitive to engine speed when the speed was higher than 3000 RPM. In ref. [29], Westbrook et al. concluded that lower speed resulted in longer residence

time at low temperature where PRFs exhibited low-temperature reactivity, promoting the autoignition process. On the other hand, sensitive fuels like gasoline showed weaker low-temperature reactivity, so the autoignition process was less promoted by the increased residence time than for PRFs. Consequently, K should be lower. This can explain the increasing trend of K with engine speed when speed is lower than 3000 RPM, but it cannot characterize the trend at high-speed conditions. A possible reason could be that when speed is high enough, residence time at the low-temperature condition is too short for low-temperature chemistry to promote autoignition, therefore increasing engine speed past a certain threshold would not further impact low-temperature oxidation and K would not change. However, this explanation needs more support from kinetic modelling which is not included in the present study.

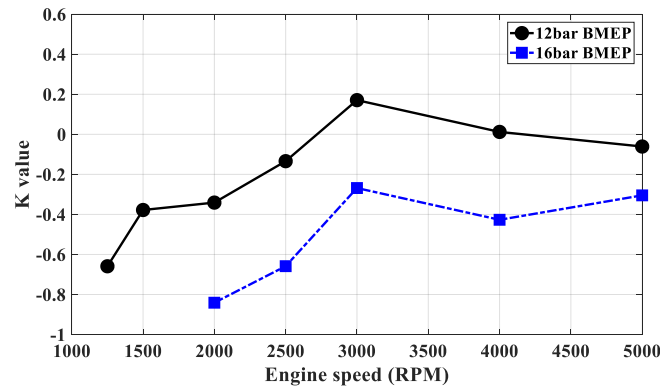


Figure 5-39 K values from speed sweeps at part- and high-load, normal temperature conditions.

In addition, another contributor to the non-monotonic behavior shown in Figure 5-40 is the increasing friction at higher engine speed, which can be inferred from Figure 5-40. To produce the same BMEP, the cylinder pressure during combustion process (characterized by the gross indicated mean effective pressure or GIMEP), increased at higher engine speed. Here, the GIMEP increases more sharply from 3000 RPM to 5000 RPM than at lower engine speeds. This may partially explain why K decreased from 3000 RPM to 5000 RPM.

Octane Index and K values in a Modern Boosted DISI engine

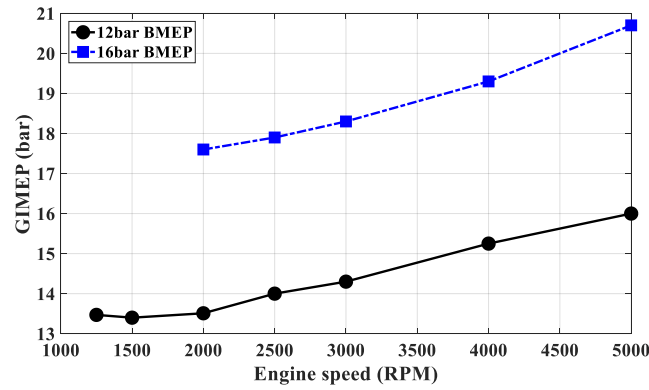


Figure 5-40 GIMEP corresponding to 10 bar and 16 bar BMEP at different engine speeds.

The non-monotonic change of K with engine speed could also relate to the end-gas temperature. Figure 5-41 shows the simulated end-gas temperatures from 2000 RPM to 5000 RPM at a constant load (12 bar BMEP) and the temperature is plotted as a function of mass fraction burned to better reflect the end-gas condition during the combustion process. At 2000 RPM where K is the lowest, the unburned gas temperature during the main combustion stage (CA20 – CA80) is lower than at other speeds, due to the more retarded CA50. The unburned gas temperature is the highest at 3000 RPM and K reaches a maximum value at this speed. The unburned gas temperature decreases with engine speed at 3000 – 5000 RPM, mainly due to the stronger fuel enrichment used in the experiments. Correspondingly, K decreases with engine speed from 3000 RPM to 5000 RPM. This relationship between K and end gas temperature during the combustion event suggests that K is a physically meaningful quantity in the context of end gas autoignition. This connection is further explored in subsequent discussion.

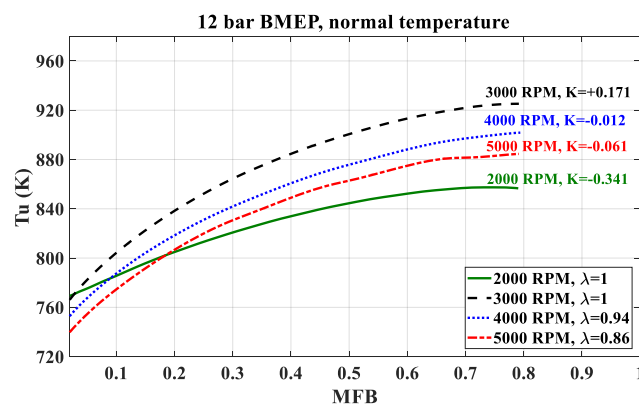


Figure 5-41 Simulated unburned gas temperature as a function of the mass fraction burned (MFB) at 2000 – 5000 RPM, 12 bar BMEP and normal operation temperature.

5.4.2 Effect of Increased Intake Air and Coolant Temperatures

Increasing intake air temperature and coolant temperature created an in-cylinder environment where autoignition was more likely to occur. As demonstrated by Figure 5-42b, combustion phasing at an engine speed of 2000 RPM was more retarded at the high temperature condition compared with that at the normal temperature condition. However, the intake pressure only showed a negligible increase at 12 bar BMEP (Figure 5-42a) which was due to the fuel enrichment (Figure 5-42c) and retarded CA50. Although it is not shown here, this effect was consistent at other speeds. The differences in K at the two temperature conditions, however, were not monotonic as shown in Figure 5-42d, where K at the high temperature condition shows a stronger dependence on BMEP than at the normal temperature condition. As a result, the former is higher at 8 bar BMEP but lower at 12 bar BMEP, than that at the normal temperature condition. At other speeds, this crossover between K values was also observed (results are omitted here).

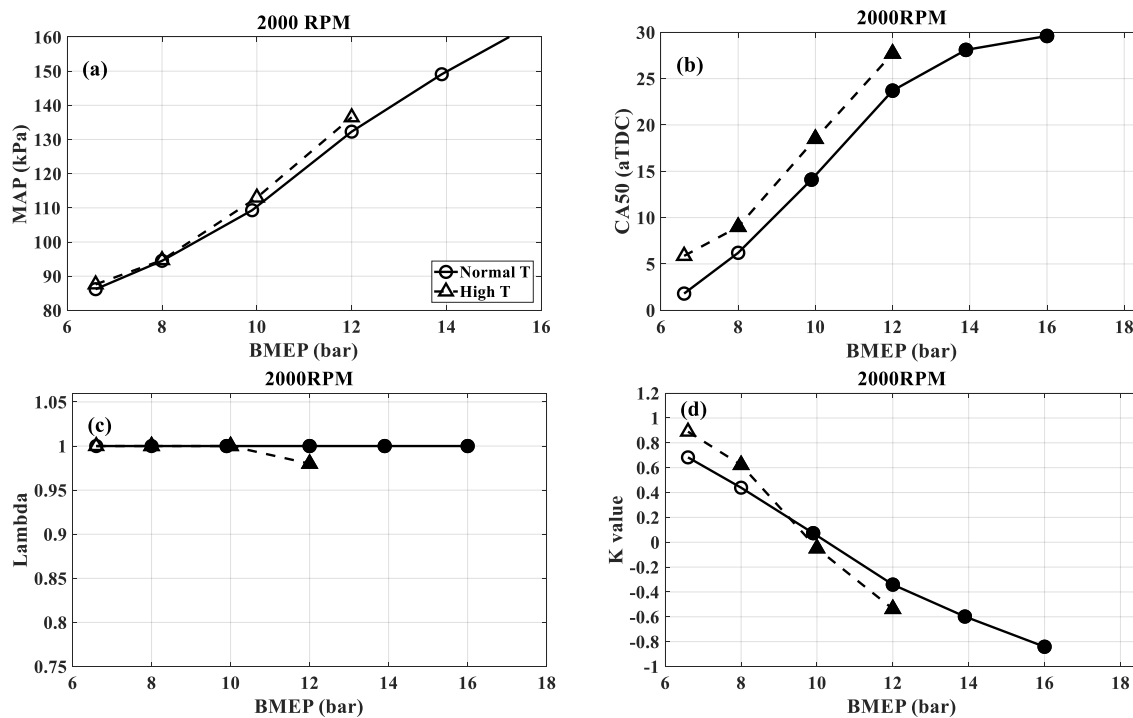


Figure 5-42 Results of (a) intake pressure, (b) CA50, (c) exhaust lambda and (d) K value from load sweeps at normal temperature and high temperature, 2000 RPM conditions.

GT-Power combustion modelling is used to further investigate this unintuitive phenomenon. As charge temperature increases, the unburned gas temperature also increases and knock is promoted. Consequently, more combustion retard and/or fuel enrichment is required to control knock, which reduces the end gas temperature during the combustion process. These two

competing effects that both impact end gas temperature complicates the analysis of the change in K. An example of this phenomenon is shown in Figure 5-43 for the unburned gas temperatures near the crossover point at 2000 RPM. At 8 bar BMEP (to the left of the crossover), the end gas temperature of the high temperature case is consistently higher than at normal temperature, despite the more retarded combustion timing, and therefore the higher temperature condition has a higher K value. Passing the crossover at 12 bar BMEP, the increased charge temperature at the high temperature condition cannot compensate for the temperature decrease caused by the retarded combustion phasing, resulting in a lower end gas temperature from 10 to 35°CA aTDC, which is the period where the flame-compressed end gas is most likely to autoignite [101-103]. The lower end gas temperature during this process therefore leads to a lower K value for the high temperature case. Following this point, it means the K value can be affected by the combustion phasing that has a significant effect on the end-gas temperature, which is consistent with the findings in the recent literature [104, 105].

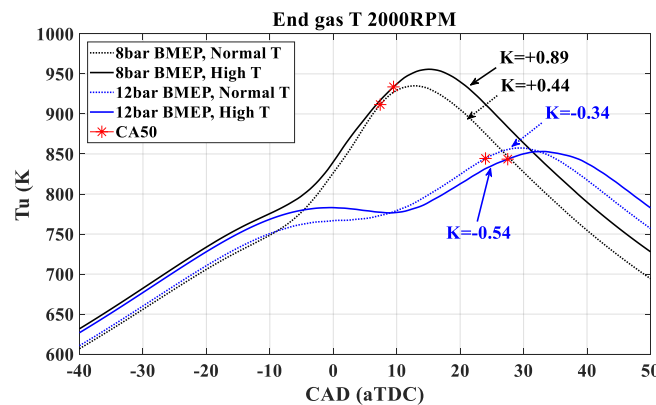


Figure 5-43 Unburned gas temperatures from GT-Power modelling for conditions at 2000 RPM.

5.5 End-Gas States and Their Correlation with K

The end-gas conditions affect the autoignition process of the fuel. However, the autoignition of different fuels do not respond to end-gas conditions in the same manner and this can result in a variation of K. This can be explained by a conceptual diagram in Figure 5-44. The gasoline of RON 91 and MON 83 shows the same resistance to autoignition as PRF91 at the RON condition and as PRF 83 at the MON condition. When the engine condition changes the end-gas condition to a region where the autoignition of PRF 91 is more likely to happen than that of gasoline, the OI of gasoline will be higher than 91 and K will become negative. PRFs have more pronounced low- and intermediate-temperature oxidation pathways than sensitive fuels like gasoline [28, 29, 106], and the heat release (LTHR/ITHR) from this oxidation promotes

the hot-ignition process (i.e. autoignition) [50]. As demonstrated in HCCI engines, higher pressure can induce significant enhancement of these pathways, so there are more favorable conditions for hot-ignition[107, 108]. Qualitatively, K decreases as low- or intermediate-temperature oxidation is promoted by the end-gas state. As discussed in ref.[50], higher pressure or lower temperature or longer resistance time increases the difference in low temperature reactivity between a non-sensitive fuel and a sensitive fuel of the same RON, and consequently K shifts to lower values at these operating conditions.

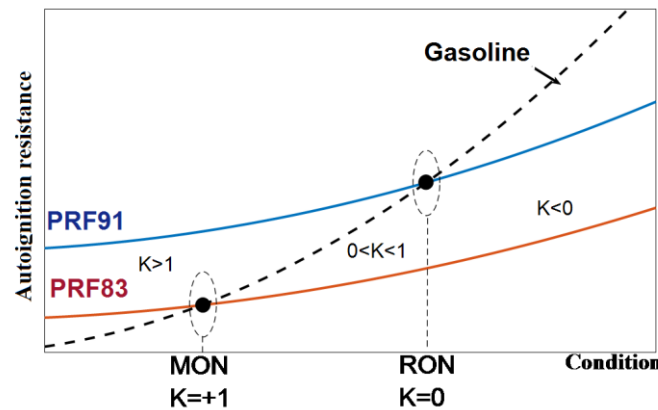


Figure 5-44 Conceptual diagram of the relationship between K and the different responses of fuels to engine operating conditions in knock resistance.

In the following sections, the relationship between K and end-gas conditions are investigated with the results from GT-Power modelling. Although chemical kinetics are not incorporated in the GT-Power modelling, with the calculated end-gas temperature and measured cylinder pressure, it is possible to deduce the relationship between K and end-gas state though analyzing the effects of temperature and pressure on autoignition process.

5.5.1 Temperature-Pressure Trajectory in End-Gas

A common practice to understand the fundamental of K is to correlate K value with the pressure-temperature trajectory of the unburned gas as in [34, 38, 54]. In these studies, it was generally concluded that K was lower when the T-P trajectory shifted to lower temperature or to higher pressure at a particular point of the engine cycle, i.e. temperature at a given compression pressure was lower, which is favorable for low-temperature chemistry. This does explain the decreasing trend of K with increasing load at a given engine speed in the present study as demonstrated by Figure 5-45, which clearly shows the T-P trajectory shifts to lower temperatures while K is decreasing.

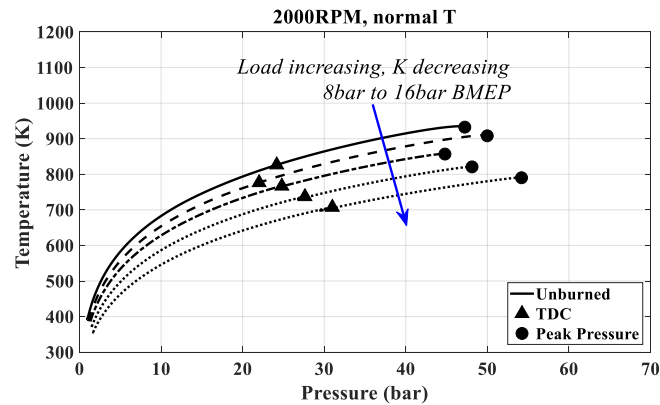


Figure 5-45 Temperature-pressure trajectories for load sweep at 2000 RPM normal T condition.

Figure 5-46 shows the T-P trajectories for both the normal and high temperature conditions at 2000 RPM. At 8 bar BMEP, the T-P profile shifts to the higher temperatures, which is consistent with the findings from literature. By contrast, at 12 bar BMEP, T-P evolutions for the normal temperature conditions aligns with that for the high temperature condition, although K (-0.54) at the high temperature condition is lower than K (-0.34) at the normal temperature condition. This discrepancy reveals that the shift in T-P trajectory is not sufficient to capture trends in K over a wide range of engine operating conditions. As described in [53], one potential reason for this is that the end point of the trajectory is not considered. The pressure and temperature in the later stage of compression varies depending on many engine configuration and operating parameters, all of which affect autoignition significantly.

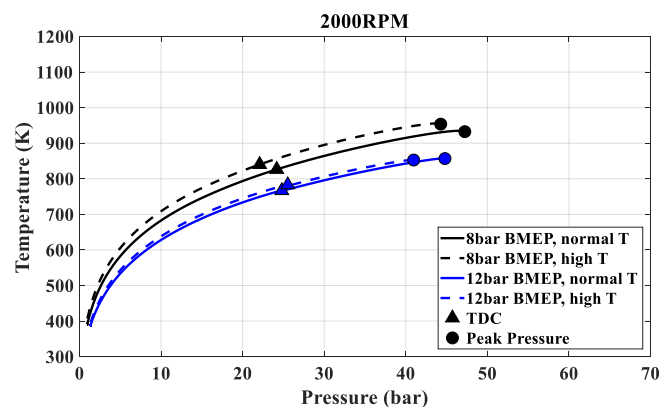


Figure 5-46 Temperature-pressure trajectories for different temperatures and loads at 2000 RPM.

The T-P trajectory shift also does not explain the effect of engine speed on K . It is shown in Figure 5-39 that K changes with engine speeds at a given load. The T-P trajectories for a speed sweep at 10 bar BMEP is displayed in Figure 5-47, where T-P trajectories for different speeds align, and only the 5000 RPM curve shows a slight deviation from the other three due to fuel enrichment. For those conditions, temperatures at a given pressure are almost identical but K

values are very different ($K = -0.3 \sim 0.4$, as given in Figure 5-39). This finding is consistent to that of ref. [89] - changing the RPM does not significantly alter the T-P trajectory, rather, it affects the time elapsed at a certain temperature and pressure. Therefore, trends in K with changing engine speed will not be captured by an analysis of T-P trajectory shifting.

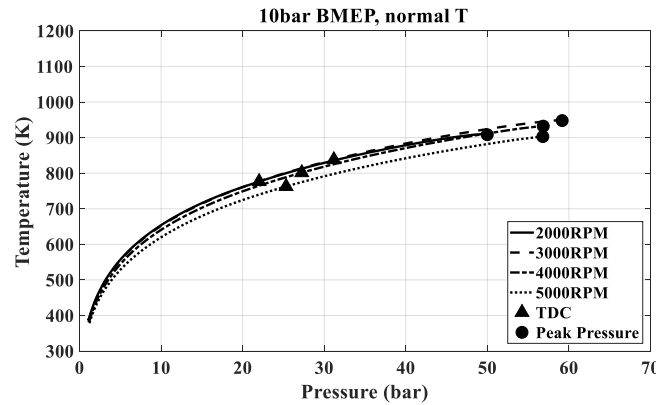


Figure 5-47 Temperature-pressure trajectories for speed sweep at 10 bar BMEP normal T condition.

Another method to correlate end-gas state to K is through the use of a single parameter such as T_{comp15} , which is the unburned gas temperature at 15 bar in-cylinder pressure. It correlates well with K in HCCI engines [52, 109] and has been shown to have some relevance to K in SI engines [38, 41]. With the abundant results of K values and results from GT-Power modelling, T_{comp15} for various conditions were calculated and are plotted in Figure 5-48. In addition to the points from the EcoBoost engine tests with the certification gasoline, the standard RON and MON conditions (red points) from a CFR engine are also included. It is worth repeating that K at the RON and MON conditions are defined as 0 and 1 respectively. The test fuel for the CFR engine tests was TRF91-45 (composition is given in Table 5-2) that closely mimics the RON and sensitivity of the certification gasoline (Table 5-1). In Figure 5-50, there is a general increasing trend of K with T_{comp15} and the two points from the CFR engine tests also fall onto the trendline. However, there are many dispersed points around the trendline resulting in a somewhat weak correlation ($R^2 = 0.746$) using a simple linear fit. The data at 4000-5000 RPM agree more closely with the fitted line, whereas the scattering is mostly due to data at 2000 RPM. This difference might be attributed to the complicated impact of engine speed on end gas autoignition as shown in Section 5.4.1, especially for the effects of resistance time that greatly affects end gas autoignition but may not affect T_{comp15} correspondingly at different RPMs.

Table 5-1 Octane numbers of TRF91-45 and EPA Tier 3 certification gasoline (cert fuel).

	RON	MON	S
TRF91-45	91.2	83.6	7.6
Certification gasoline	91.6	83.4	8.2

Table 5-2 The composition of TRF91-45 used as a gasoline surrogate for CFR engine test.

Composition	Iso-octane	N-heptane	Toluene
Vol. %	34.7	20.3	45

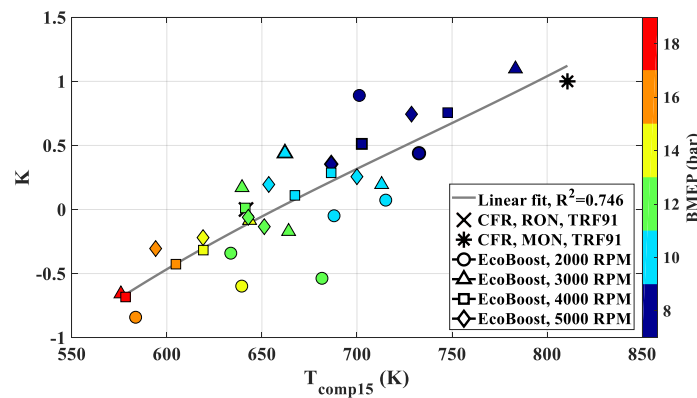


Figure 5-48 T_{comp15} for various conditions on EcoBoost engine tests as well as CFR engine test. The shapes of the markers represent for different engine speeds and colors stand for engine loads.

As mentioned previously, T_{comp15} correlates well with K in HCCI engines, but the results shown in Figure 5-48 suggest this is not the case for a production SI engine. Autoignition in both HCCI and SI engines are primarily controlled by chemical ignition kinetics, and in both cases autoignition is caused by the compression of unburned gas [110]. In HCCI engines, the autoignition process is not influenced significantly by the effects of turbulence, mixing or turbulent flame propagation [11], so the unburned gas temperature at compression of 15 bar is a reasonable predictor of the unburned gas condition where chemical reactions related to autoignition begin to occur. By contrast, compression of the end-gas in an SI engine is influenced substantially by turbulent flame propagation, and the position of T_{comp15} in the engine cycle might occur before ignition or during the early stages of combustion. Therefore, T_{comp15} will not necessarily capture the effects of flame-induced compression on autoignition in SI engines. If it is assumed that K is a physically meaningful factor which is related to

autoignition, then a parameter that correlates end-gas state to K must be related to the thermodynamic states of the end gas at some point close to the onset of the autoignition.

5.5.2 Relationship between End-Gas Temperature and K

The end gas temperature effect on K can also be explained by comparing the different responses of autoignition chemistry of gasoline and PRF to temperature change. As previously mentioned, PRFs and other non-sensitive fuels have low-temperature oxidation pathways that produce modest LTHR, promoting the autoignition in the end-gas [11, 27]. However, the magnitude of LTHR can be reduced with increased temperature and end gas reactions will enter the NTC region, such that the autoignition process of the end-gas is inhibited [111, 112]. LTHR or ITHR of sensitive fuels like gasoline and ethanol are much weaker as compared to PRFs and their autoignition is mostly promoted by increased temperature. In addition to the difference in low-temperature chemistry, the autoignition of non-sensitive fuels like PRFs have greater resistance to temperature in the high-temperature chemistry regime when compared with sensitive fuels [55]. Revisiting Figure 5-44, it can be concluded that K is higher when end-gas temperature is higher.

The gas temperature before combustion, at IVC is shown in Figure 5-49 where temperature at IVC is nearly uncorrelated with K ($R^2=0.576$). The temperature at IVC for the EcoBoost engine is in a narrow range of 350 – 440 K as the intake air temperature was well controlled across the speeds and loads. At this low temperature range, no chemical reactions related to autoignition can happen. Although temperature at IVC indicates the initial temperature of the compression process, the end-gas temperature is greatly affected by other parameters such as combustion phasing, engine speed and mixture strength which cannot be fully characterized by the IVC temperature.

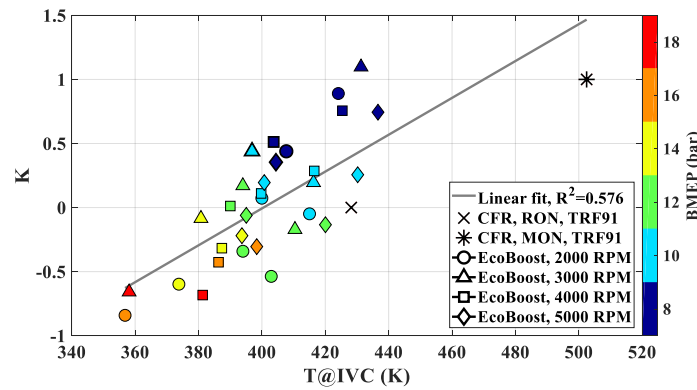


Figure 5-49 Linear fitting of K vs. unburned gas temperature at IVC.

The relationship between K and end-gas temperatures from the start of combustion (spark timing) to the end of combustion (CA90) are investigated by assessing the R^2 of linear fitting of K and end-gas temperature. As shown in Figure 5-50, at the ignition point, the temperature appears uncorrelated with K, whereas an increasingly stronger correlation is observed until CA70. The R^2 is nearly 0.89 from CA60 to CA90, indicating that the end-gas temperature in the later stage of combustion is more relevant to K.

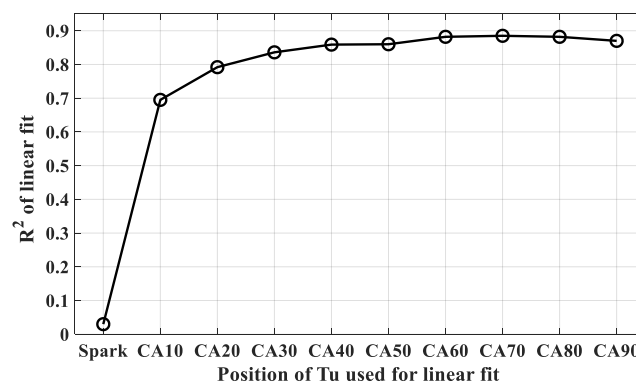


Figure 5-50 R^2 of the linear fitting of K and end-gas temperatures at different position during the combustion process.

It is interesting to note that K and the unburned gas temperature at ignition are nearly independent from each other, with an $R^2 = 0.03$ (Figure 5-51). This can be explained by Figure 5-52, where the temperature at CA50 is used to characterize the end-gas temperature during the main combustion process. A lower temperature at the spark can lead to either a higher temperature at CA50 (e.g. 10 bar vs 14 bar BMEP cases) or a lower temperature at CA50 (e.g. 18 bar vs. 14 bar BMEP cases). In the former case, the higher CA50 temperature is mainly due to the more advanced combustion phasing, whereas in the latter case the lower CA50

temperature is primarily due to the stronger fuel enrichment. The variation of combustion retard and fuel enrichment complicates the connection between spark timing temperature and the end gas temperature at the later stage of combustion, leading to the poor correlation between K and spark timing temperatures.

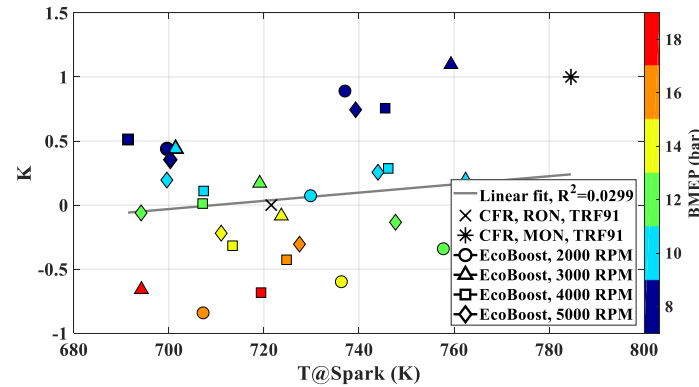


Figure 5-51 Linear fitting of K vs. unburned gas temperature at spark ignition.

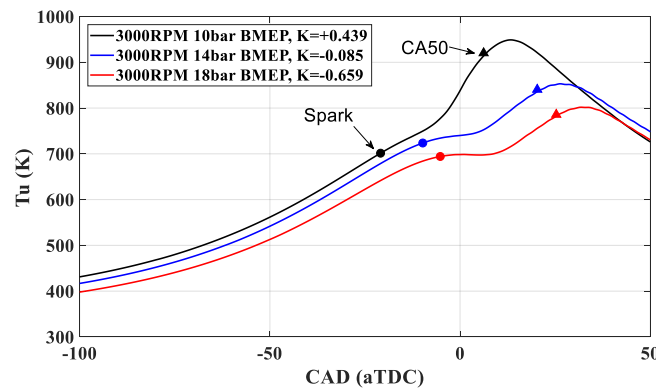


Figure 5-52 End-gas temperatures at different loads at 3000 RPM normal temperature condition.

The best correlation with K occurs when using the end-gas temperature at CA70, which is shown in Figure 5-53. The two points from the CFR engine using a different fuel also follow the trendline, suggesting some degree of independency of engine design and fuel composition for this correlation. The strong correlation of K with end-gas temperatures at later stage of combustion, particularly from CA60 to CA80, can be attributed to the following factors.

- Firstly, end-gas autoignition is primarily driven by oxidation chemistry at low- to intermediate-temperatures where temperature is the predominant parameter controlling the process. If this is the case, knock should then first appear late in any burn that commences close to knock limited spark timing since this is the hottest part of the cycle and has the most direct impact on knock. Indeed, previous studies have reported that knock occurred near CA60 to CA80 in SI engines [101-103].

- Secondly, end-gas temperatures at CA60 - CA80 encapsulate all the thermochemical effects that occur early in the cycle (i.e. the impact of all engine operating parameters are lumped together in the end gas temperature at this CA location). For example, engine speed affects the time for heat transfer; but this effect on autoignition cannot be captured by temperatures early in the cycle. However, the engine speed effect will manifest in the end-gas temperature in the later phase of combustion.

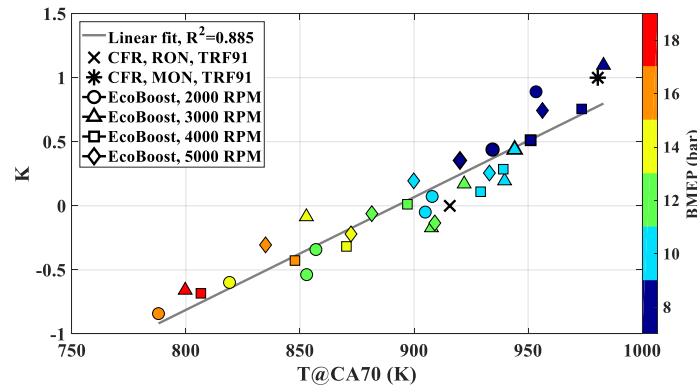


Figure 5-53 Linear correlation of K and unburned gas temperatures at CA70.

5.5.3 Relationship between Cylinder Pressure and K

It is apparent that K decreases with higher pressure, and many engine operating parameters affect the cylinder pressure. The intake pressure affects the initial pressure of compression stroke, spark timing affects the initial pressure of flame-induced compression and combustion duration determines pressure rise rate during the combustion process. Another regression analysis using the data from the K mapping experiments is now presented to relate K to pressure at different points in the engine cycle and determine if the pressure at a specific point in SI engines is correlated with K values.

The pressure at IVC defines the initial pressure of the piston-induced compression before combustion. In Figure 5-54, it shows a decreasing trend with K as expected. But its correlation to K is weak with the R^2 of a linear fitting less than 0.5. Most scattered points are for the low engine speed conditions where resistance time (engine speed) effect is critical for autoignition reactions, however this effect on K cannot be captured by the pressure at IVC. Another possible reason is that the temperature at IVC is very low (350-440 K, as shown in Figure 5-49) and there is no autoignition reactions happening at this low temperature. Therefore, the pressure at this point has no direct impact on the autoignition process.

Octane Index and K values in a Modern Boosted DISI engine

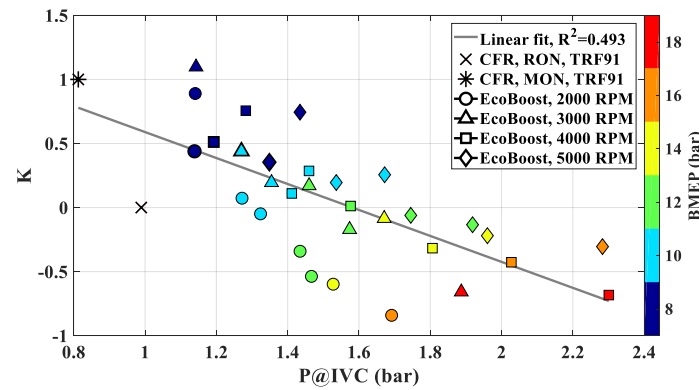


Figure 5-54 Linear fitting of K vs. pressure at IVC.

The correlation between K and pressures during the combustion process is examined in Figure 5-55. K correlates best with the cylinder pressure at the ignition timing, but the correlation with pressures at later timings becomes consistently worse with R^2 showing a decreasing trend later in the combustion process.

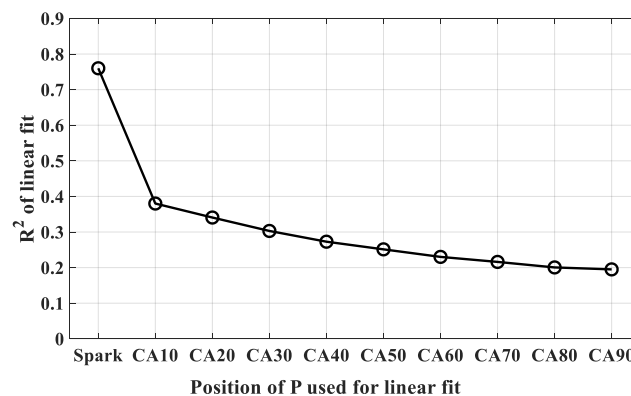


Figure 5-55 R^2 for linear fitting of K and cylinder pressures during the combustion process.

The relationship between K and the pressures at the spark is examined in Figure 5-56. Compared with Figure 5-54, the correlation is much stronger. As already mentioned, flame-induced compression plays a dominant role in the end-gas autoignition and the pressure at spark defines the initial pressure of this compression process. Also, the temperature at the spark is typically around 700-800 K (shown in Figure 5-51) where low-temperature oxidation is most likely to happen. Given that pressure effect is significant for the low-temperature oxidation and that the low-temperature oxidation affects K, the in-cylinder pressure at the spark should be reasonably well correlated with K. Notice that the result for the CFR engine at the RON condition is lower than the fitted line in Figure 5-54, suggesting there could be other effects that are not characterized by the pressure at spark. One plausible reason is that the engine speed

for the RON condition is 600 RPM, which is much lower than the speeds of EcoBoost engine tests. Lower engine speed allows for a longer residence time for end-gas reactions, and low-temperature oxidation is sensitive to this time due to the slow reaction rates of some key reactions in the low-temperature chemistry regime. For a given pressure at spark, the low-temperature oxidation becomes stronger when residence time is longer (lower RPM) therefore the K value will be lower.

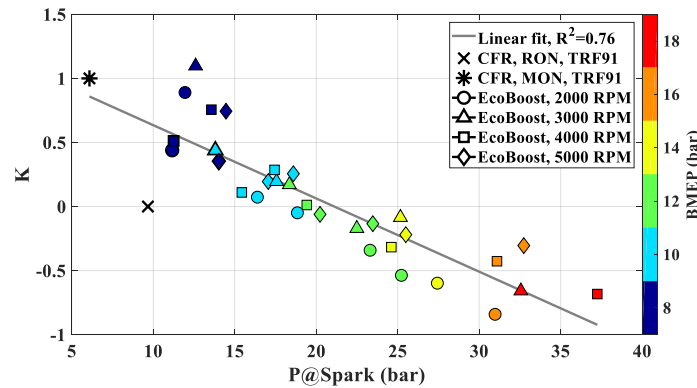


Figure 5-56 Linear fitting of K vs. pressure at spark ignition.

The correlation of K with pressure at ignition is much weaker than that with the unburned gas temperature at CA60 - CA80. This is because the effect of pressure on K is mainly associated with the pressure effect on low- and intermediate-temperature oxidation that is also sensitive to other factors, especially the residence time (engine speed). As already mentioned, end-gas temperature in the later stage of combustion can lump these effects on the autoignition process.

As shown in Figure 5-57, the pressure in the later phase of combustion (CA70) is not correlated to K especially for the low engine speed condition. Temperatures at these points are higher than those at spark and the time available before the end of combustion is limited, so the temperature-driven, high-temperature autoignition chemistry that has faster reaction rates becomes more important than the low-temperature oxidation.

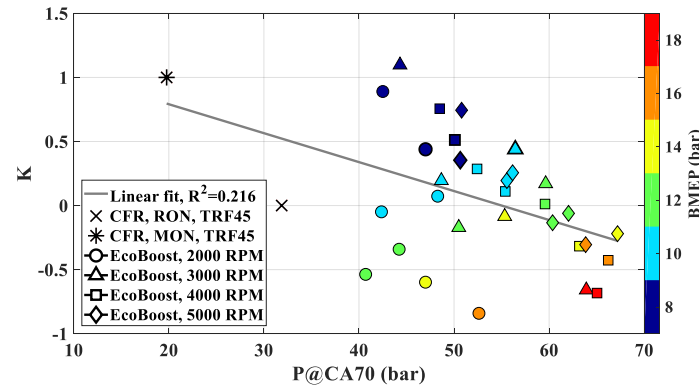


Figure 5-57 Linear fitting of K vs. pressure at 70% fuel burned.

5.6 Summary

In this chapter, experimental results of K over normal-temperature and high-temperature engine operating maps are presented, including over-advanced and knock-limited conditions. Knock-limited K ranges from positive to negative through the load and speed range of the engine. At normal temperature conditions, K increases with engine speed until 3000 RPM and then slightly decreases. In contrast, at high temperature conditions, the effect of engine speed is not significant. K values from high-temperature tests are higher than those from normal-temperature at low load conditions, but this trend is reversed at higher load conditions. The relationship between K and end-gas conditions is investigated using results from engine combustion modelling. The comparison of the unburned gas temperature and pressure trajectories is not well correlated with K through the operating range of the EcoBoost engine. Further analysis shows the in-cylinder pressure at ignition timing has moderate correlation with K because of its relationship with low-temperature reactivity. End-gas temperatures at the later phase of combustion (CA60 - CA80) are strongly correlated with K because they accurately characterize the thermal condition just before the onset of autoignition.

6 Significance of RON and MON for Different Powertrains on Various Driving Cycles

This chapter presents the results on the significance of RON and MON for light-duty vehicles with conventional and hybrid powertrain configurations. Using a combination of engine data from the K-mapping experiments, vehicle test data and vehicle modelling, the fuel efficiency loss caused by knock-limited operation over various drive cycles is quantified. The distributions of K based on fuel consumption and knock-limited fuel efficiency loss for different powertrains and drive cycles are calculated, from which the significance of RON and MON are evaluated.

6.1 Driving Cycles

Three standard US EPA drive cycles and two SAE J2807 tow-rating cycles were adopted in the present study. There are discrepancies between regulatory cycles and real-world driving, and there are more countries starting to include real-world driving tests to complement the standard drive cycle tests. However, the real-world drive cycles contain enormous diversity and they are less well defined as the standard drive cycles. The drive cycles used in the present study cover a wide range of driving conditions including mild city driving, steady-state highway cruising, aggressive high-speed driving and high-power demand towing, such that represent most driving conditions in the real world.

6.1.1 *Standard Environmental Protection Agency (EPA) Drive Cycles*

Real world driving consists of a wide range of driving behaviors depending on driving style, traffic conditions and region of the world. As the fuel economy and emissions ratings for a vehicle must be based on the demand over a drive cycle, several organizations have developed laboratory drive cycle tests that are representative of real-world driving. Three groups of driving cycles are widely used for fuel economy/emission measurements and regulations, including the US EPA cycles, European legislative cycles and Japanese legislative cycles. In this study, three US EPA cycles covering different driving conditions were used, which are summarized by Table 6-1. The vehicle speed profiles of these three cycles are plotted in Figure 6-1, Figure 6-2 and Figure 6-3.

Significance of RON and MON for Different Powertrains on Various Driving Cycles

Table 6-1 General information of EPA Certification Cycles

Cycle Name	Distance (m)	Duration (sec)	Mean Speed (kph)	Driving Characteristics
UDDS (FTP-72)	11997	1369	31.6	Urban
HWFET	1650	765	77.7	Highway cruising
US06	12894	596	77.9	High speed and aggressive

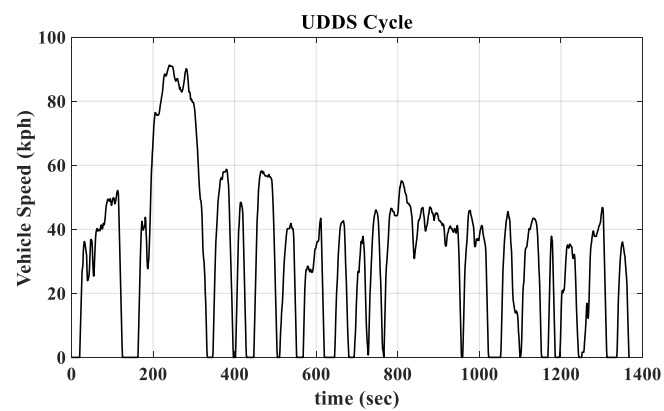


Figure 6-1 EPA Urban Dynamometer Driving Schedule (UDDS) cycle

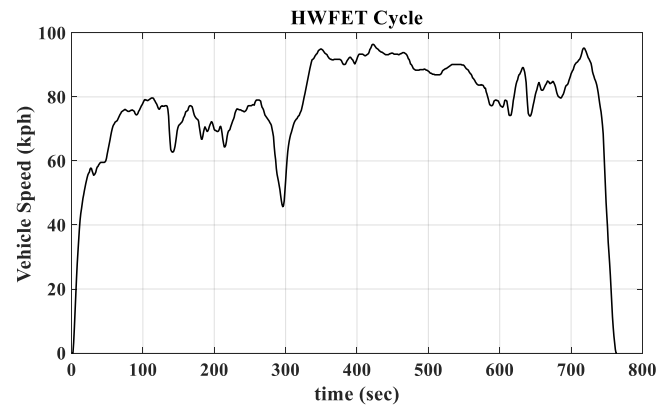


Figure 6-2 EPA Highway Fuel Economy Test (HWFET) cycle.

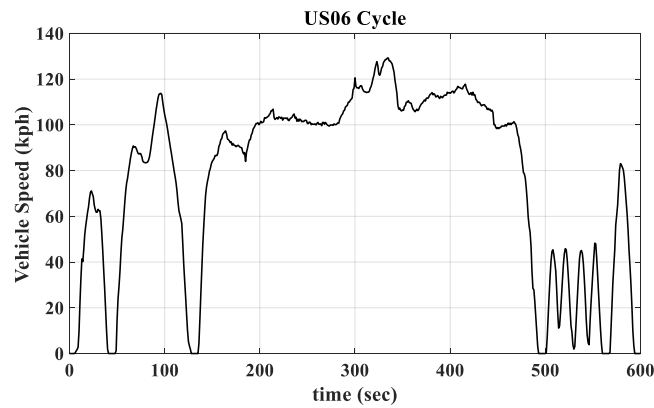


Figure 6-3 EPA US06 cycle.

The driving cycles listed in Table 6-1 are employed by EPA for fuel economy and emissions certification tests and the National Highway Traffic Safety Administration (NHTSA) for CAFE regulations. It should be noted that fuel consumption (FC) in L/100 km or fuel economy (FE) in miles per US gallon (MPG) in this study is based on the Unadjusted EPA 2-cycle procedures where two consecutive UDDS cycles are used to measure the city FC, and one HWFET cycle is used to measure the highway FC. The combined FC is calculated by weighting 55% of city FC and 45% of highway FC. This is different from the MPG values displayed on the window stickers of new vehicles. The window sticker MPG before 2008 was based on the Adjusted 2-cycle procedures where the city FE and highway FE from 2-cycle procedures were adjusted downward by 10% and by 22% respectively. This was to make up the discrepancy between consumers reported MPG and EPA measured MPG. Since 2008, the EPA has used 5-cycle procedures as an updated methodology for determining the certified MPG for all new vehicles in the US market. In the new 5-Cycle Procedures, more driving cycles are incorporated including US06 for aggressive and high-speed driving, SC03 for high temperature with air conditioning and FTP-75 with cold start.

6.1.2 Davis Dam Towing Drive

Due to the increasing usage of trailering, towing capacity has become a major marketing point of new vehicles. The SAE J2807 test method is used to rate GCWR of a vehicle and trailer combination, which is then used to calculate a maximum trailer weight rating [88]. The test practices require that the vehicle tow a trailer at a hot ambient temperature ($>38^{\circ}\text{C}$ or 100°F) drive through several tests including acceleration on level road, launch on a 12% grade, highway gradeability on the Davis Dam Grade, etc.

Two highway gradeability tests on the Davis Dam Grade were considered in this work. The vehicle speed profiles for those two tests are given in Figure 6-4. In these tests, a mid-sized Ford SUV equipped with a 2L EcoBoost engine was towing a 1591 kg (3500 lbs.) trailer on the Davis Dam Grade that has the variable grade ranging from 4% to 7%. Because of the high-power demand and high ambient temperature, this drive test represents one of the extreme driving conditions where the engine is more knock-limited.

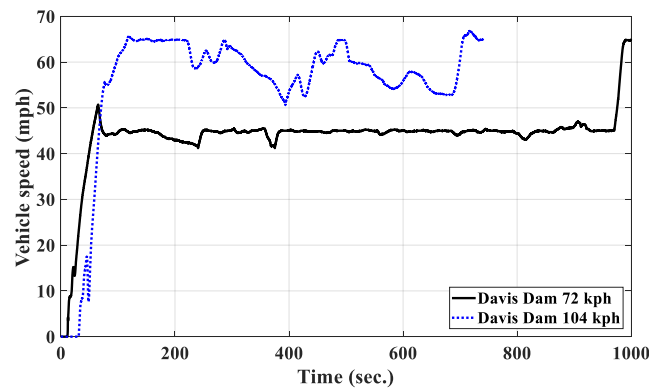


Figure 6-4 Vehicle speed of Ford SUV towing a 1591 kg (3500 lbs.) trailer in the highway gradeability tests on Davis Dam Grade (part of the SAE J2807 tow rating test).

6.2 Powertrain Configurations

The Ford Edge MY19 is used as the vehicle platform for all powertrain simulations in this study, as it represents a typical, mid-size SUV in the market. The vehicle test data for the conventional powertrain configuration was available from Ford and was used for analysis directly. The data for the hybrid and plug-in hybrid powertrains was not available (as there are no production Ford Edge of these powertrains), so vehicle modelling was used. The vehicle model of the conventional powertrain was first developed and calibrated with vehicle test data. Then, the electric-drive system was added to the calibrated vehicle model to hybridize the conventional powertrain.

6.2.1 Conventional Powertrain

The general specifications of the conventional vehicle are shown in Table 6-2 and the engine data was presented in Table 3-2. These parameters were imposed into the vehicle model. The experimentally measured fuel flow rates and engine torque at different operating conditions were imposed in the engine model to define the engine operating map for use in drive cycle simulations.

Table 6-2 General specifications of Ford Edge (MY19).

Engine	2L EcoBoost, 4-cylinder
Transmission	8-speed automatic
Gear ratios	4.69-3.31-3.01-1.92-1.45-1.00-0.75-0.62
Final drive ratio	3.805
Length	4.80 m (188.8 in.)
Width	1.93 m (75.9 in.)
Height	1.73 m (68.3 in.)
Ground clearance	0.203 m (8 in.)
Curb weight	1796 kg (3959 lb.)

The power output of the powertrain was calibrated using the reverse validation method: the vehicle model was validated by following the flow of power in the reverse order through the powertrain. The forward power flow is depicted in Figure 6-5, as engine power is distributed through the transmission system, through the final drive and then to the wheels. The power from the final drive is used to propel the vehicle through four types of resistance: rolling resistance, grading resistance, vehicle dynamics and aerodynamic loss. The rolling coefficients of the tires were pre-defined by the Autonomie database and are listed in Table 6-3. The grading resistance and vehicle dynamics depended on vehicle mass (Table 6-2). The only unknown was the aerodynamic loss that is defined by Eq. 6-1.

$$F_{aero} = \frac{1}{2} \rho A_f C_d (V + V_w)^2 \quad \text{Eq. 6-1}$$

Where:

- ρ is the air density;
- A_f is the frontal area;
- C_d is the drag coefficient;
- V is the vehicle speed;
- V_w is the wind speed.

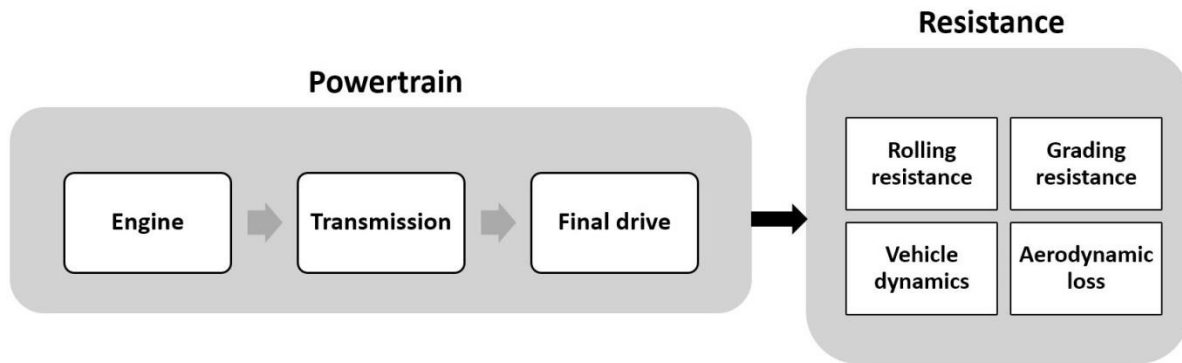


Figure 6-5 The simplified power flow of a conventional vehicle.

In Eq. 6-1, the frontal area, A_f , was calculated to be 2.953 m² with Eq. 6-2 and the vehicle dimensions listed in Table 6-1. The frontal area calculation is not as accurate as what would be required for a wind tunnel test, but as indicated by Eq. 6-1, the calibration of C_d can mask any errors in the frontal area. The density of air was determined in Autonomie with the ambient temperature (24°C or 75°F). Wind speed was zero in the simulations and the vehicle speed was described by the drive cycle. The drag coefficient was then calibrated by running the vehicle model on the HWFET cycle where vehicle speed was high and aerodynamic loss was significant. In Figure 6-6, the engine power from the vehicle test and vehicle modelling are compared, and it shows that the simulated power matches the tested power when the drag coefficient (C_d) is 0.345. This value is close to the value estimated by another source [113].

$$A_f = \text{width} * (\text{height} - \text{ground clearance}) \quad \text{Eq. 6-2}$$

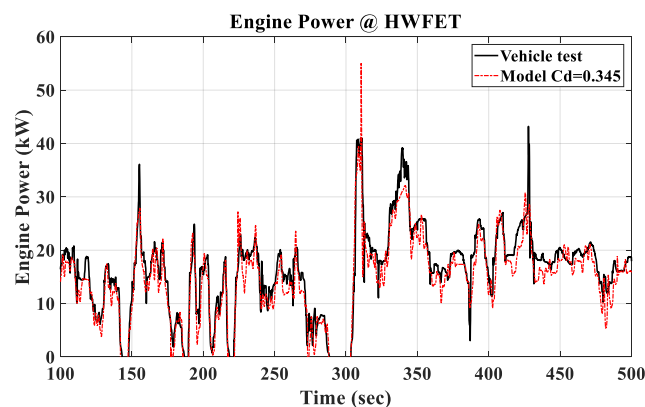


Figure 6-6 Comparison of engine powers from vehicle test and Autonomie modelling.

Table 6-3 Summary of parameters characterizing aerodynamic loss and rolling resistance.

Frontal area (m²)	2.953
Drag coefficient	0.345
Rolling resistance coefficient 1	0.009
Rolling resistance coefficient 2 (s/m)	0.00012

There are many combinations of engine speed and torque for a given power from the engine to service vehicle demand. The determination of the correct engine condition to match the simulated engine speed profile with that of the real vehicle drive cycle test requires accurate modelling of the vehicle's gear shifting strategy. Figure 6-7, Figure 6-8 and Figure 6-9 show engine power, speed and gear shifting in the UDDS cycle that was modelled using the default gear shifting strategy of Autonomie. The UDDS cycle is highlighted here because this cycle contains a significant number of transient acceleration events (as shown in Figure 6-1), and therefore more gear shifting events happen. This example therefore provides a reasonable assessment of the validity of the vehicle's transmission model in Autonomie. As shown, the simulated engine power using the calibrated C_d is consistent with the power from vehicle test. However, the simulated engine speed is different from that measured in vehicle test as shown in Figure 6-8. This is because the default gear shifting strategy of Autonomie cannot reproduce the shifting events of the Ford Edge. For example, in 200-300 seconds of the drive cycle, the transmission of the Autonomie model is at a higher gear than the vehicle test data, and consequently, the simulated engine speed is lower than the actual engine speed.

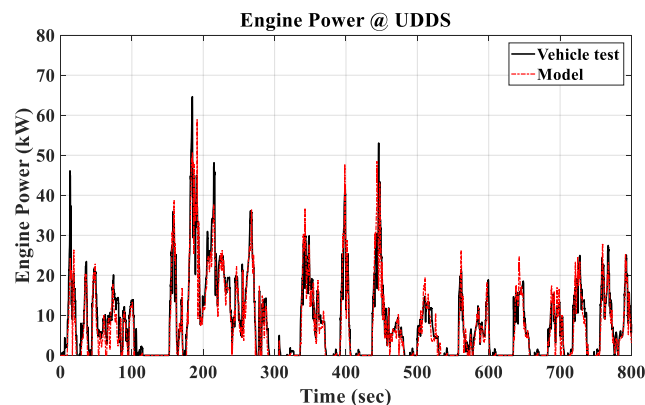


Figure 6-7 Engine power from vehicle test and Autonomie modelling for UDDS cycle.

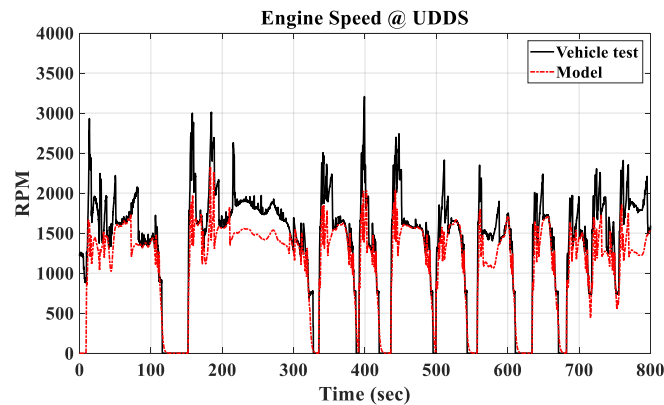


Figure 6-8 Engine speed from vehicle test and Autonomie modelling before adjusting gear shifting strategy for UDDS cycle.

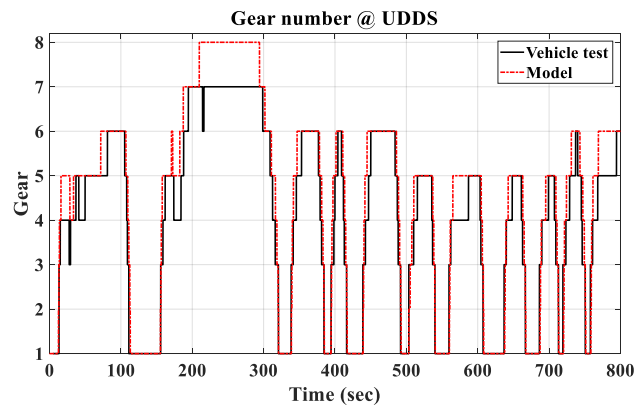


Figure 6-9 Gear shifting events from vehicle test and Autonomie modelling before adjusting gear shifting strategy for UDDS cycle.

To improve the fidelity of the vehicle modeling, the gear shifting control was calibrated using the method developed by Namdoo et al. in ref. [95]. The gear shifting strategy in Autonomie is a function of vehicle speed and acceleration pedal position, which is a linear function of wheel torque demand. The wheel torque demand was calculated by dividing wheel power by wheel rotation speed. In doing so, the gear shifting points of the vehicle test data in three drive cycles were obtained, with which the gear shifting strategy was adjusted in the Autonomie transmission model to match the vehicle test data. Using the updated gear shifting strategy, the model results match the vehicle test data well (Figure 6-10). When gear shifting is calibrated, both the simulated engine speed and simulated engine torque reproduce the real engine operation, as can be seen in Figure 6-11 and Figure 6-12.

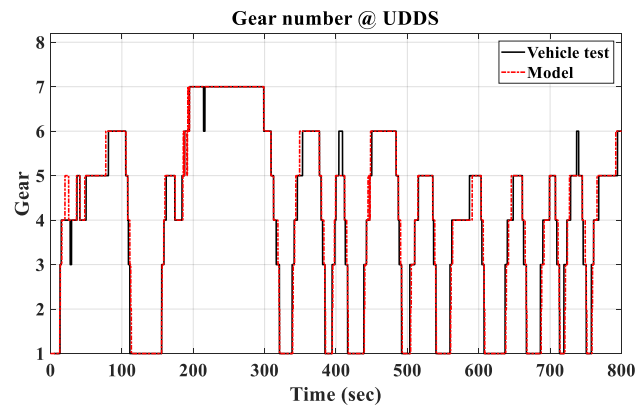


Figure 6-10 Gear shifting events from vehicle test and Autonomie modelling using the calibrated gear shifting strategy for UDDS cycle.

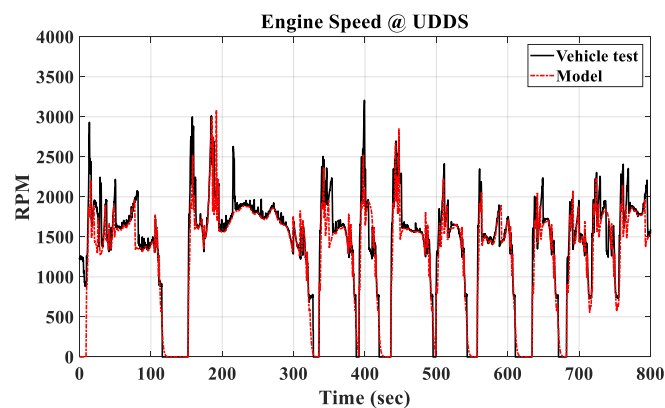


Figure 6-11 Engine speed from vehicle test and Autonomie modelling using calibrated gear shifting strategy for UDDS cycle.

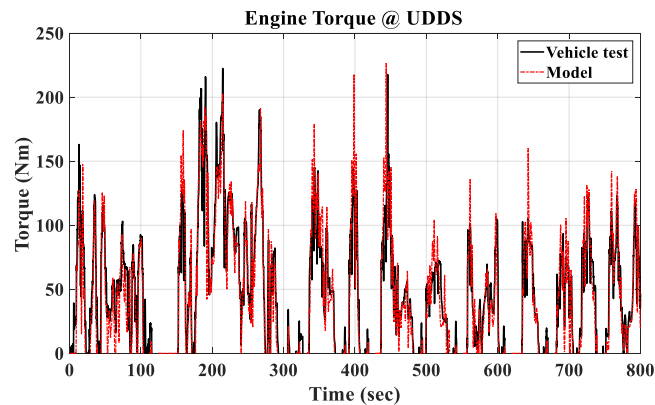


Figure 6-12 Engine torque from vehicle test and Autonomie modelling using calibrated gear shifting strategy for UDDS cycle.

After the calibration of the conventional vehicle model, vehicle performance and fuel economy were evaluated using Autonomie to set the baseline for further comparisons with the HEV and PHEV. The former was characterized by the 0-96 kph (0-60 mph) acceleration time and the latter was using the Unadjusted 2-cycle procedures. The results of these tests are listed in Table

6-4. However, as mentioned previously in Section 6.1.1, these fuel consumption results are not comparable with the reported values on the window sticker due to different methods used for the evaluation.

Table 6-4 Vehicle performance and fuel consumption of the conventional vehicle. Results were modelled using vehicle modelling.

0-60mph acceleration time	7.4 seconds
City fuel consumption	9.31 L/100km (25.27 MPG)
Highway fuel consumption	7.23 L/100km (32.54 MPG)
Combined fuel consumption	8.37 L/100km (28.10 MPG)

6.2.2 Full Hybrid Electric Vehicle

The calibrated conventional vehicle model was used for developing the hybrid vehicle model. The powertrain configuration was based on the P2 parallel hybrid architecture where an electric motor is placed between the engine and the transmission. The hybrid vehicle was developed to meet two targets:

1. Comparable or better vehicle acceleration performance than the conventional vehicle;
2. At least 35.7% reduction in fuel consumption relative to the conventional vehicle.

The fuel economy target is based on ref. [62] in which the fuel consumption reductions of hybrid vehicles were benchmarked to support 2025 US CAFE regulations.

The 2L, 4-cylinder EcoBoost engine was first downsized to a 1.5L, 3-cylinder engine with 75% of the output of the 2L engine. This was done to avoid the unnecessarily high combined power of the 2L engine and electric motor, as the goal was to generate similar performance as the conventional powertrain, and ultimately the increased performance from adding electrical components to the conventional powertrain would significantly increase vehicle cost. Engine downsizing by removing one cylinder does not change the geometry of each cylinder, therefore it is reasonable to assume that the combustion performance observed experimentally in each cylinder will be applicable to each cylinder of 3-cylinder model. As it has been shown in Chapter 5 that K is a function of engine speed and engine BMEP, and BMEP is independent

of the number of cylinders, the experimentally measured K-maps from the 2L, 4-cylinder engine are assumed to be valid for the 3-cylinder engine model.

Sizing an electric motor for the 3-cylinder engine required an estimation of vehicle weight from Table 6-5. With the vehicle weight estimated, the effect of peak motor power on vehicle acceleration performance was then examined. In this simulation, motor power was varied from 5 kW to 60 kW and for each case the 0-96 kph (0-60 mph) acceleration test was simulated. The results are plotted in Figure 6-13, showing that vehicle acceleration performance increases almost linearly with motor power and it is better than that of the conventional vehicle (7.4 seconds) when motor power is higher than 30 kW.

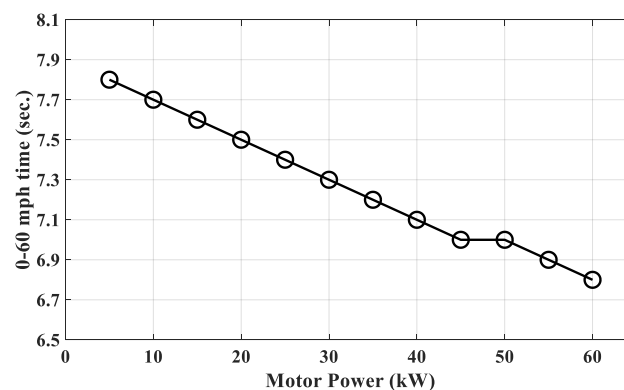


Figure 6-13 Effect of motor power on vehicle 0-96 kph (0-60 mph) acceleration performance for the P2 hybrid.

The other important consideration in sizing the motor is its capability as a generator during regenerative braking. The electric motor size has a significant impact on the energy that can be recovered during deceleration events, and therefore on the overall fuel economy over a drive cycle. Based on ref. [114], the motor power was sized to capture all the regenerative energy from a UDDS cycle. Figure 6-14 shows the power of wheels of the HEV during the UDDS cycle where negative values represents braking power or vehicle kinetic power. The maximum kinetic power during braking is about 35 kW during this cycle, and this motor size coincides with slightly improved acceleration performance shown in Figure 6-13. Ultimately, a motor of 35 kW peak power was chosen for the HEV configuration.

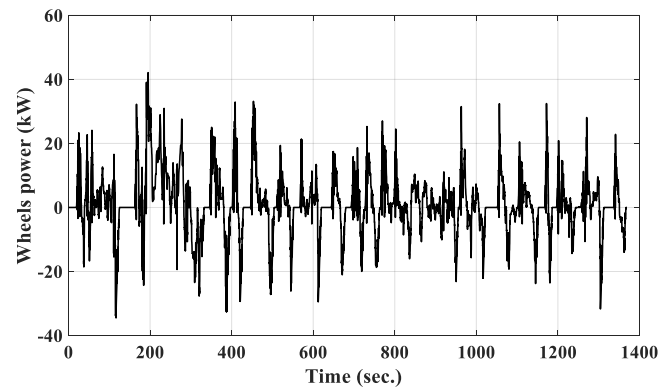


Figure 6-14 Power on wheels for HEV on UDDS cycle. Positive power means propulsion and negative power means braking.

The required power of the battery in this case would be 35 kW in order to drive the motor. Considering the battery loses some of its capacity after a period of time, an oversize factor was used to ensure the same performance at the end of life as the performance at the beginning. For the HEV battery, an oversize factor of 18% was used according to ref. [62], so the power of the battery was set at 41.3 kW. Because the HEV battery requires high power more than high energy storage, the standard Lithium-ion battery capacity of 6 Ah was sufficient, and the battery's energy was 1.89 kWh.

After sizing the propulsion components, the HEV mass was calculated by adding the masses of the motor, battery and inverter to the curb weight of the conventional vehicle and then accounting for the reduced mass of the engine due to downsizing (Eq. 6-3). The mass of each component in Eq. 6-3 was estimated with the data listed in Table 6-5. The final vehicle weight was determined to be 1845 kg. A summary of the results of the component sizing and vehicle weight is given in Table 6-6.

$$m_{hev\ curb} = m_{conv\ curb} + m_{mot} + m_{mot\ controller} + m_{battery\ pack} - m_{eng\ downsize} \quad Eq. 6-3$$

Table 6-5 Data sources of mass calculation for the HEV.

Component	Data source	Mass
Curb weight of conventional vehicle	Provided by Ford	1796 kg
Electric motor	1600 W/kg [62]	35 kW ÷ 1.6k W/kg=21.9 kg

Significance of RON and MON for Different Powertrains on Various Driving Cycles

Motor controller	13000 W/kg [62]	$35 \text{ kW} \div 13 \text{ kW/kg} = 2.7 \text{ kg}$
Battery pack (entire system, incl. packaging, cooling and control)	Energy: 150 Wh/kg Power: 1250 W/kg [115]	Evaluated by power $41.3 \text{ kW} / 1.25 \text{ kW/kg} = 33 \text{ kg}$
Engine weight reduction by downsizing	7% weight reduction with 25% downsizing ratio [116]	$141 \text{ kg} * 7\% = 9.9 \text{ kg}$

Table 6-6 The size of the electric drive system and the resulted vehicle mass of the HEV.

Motor power	35 kW
Battery power	41.3 kW
Battery capacity	6 Ah, 1.89 kWh
Vehicle mass	1845 kg

Rule-based control logic was used to simulate the operation of the hybrid system [117]. In this scheme, the engine power demand is the sum of the requested power at the wheels, plus or minus the power required to regulate the battery SOC at 50-60% (plus in the instance that the battery needs to be charged, and minus when the battery contributes power to the given demand). The engine starts when:

1. The demanded power is above a threshold (24 kW) for a predefined duration (2 s),
OR
2. The electric motor power is saturated (higher than 35 kW), OR
3. The battery SOC is lower than a predefined threshold (40% in the present study).

The engine is off when:

1. The demanded power is lower than a threshold (12 kW) for a predefined duration (1.7 s), AND
2. The electric motor is not saturated (lower than 35 kW), AND
3. The battery SOC is higher than a threshold (45%).

Among those parameters, only the thresholds of the demanded power were adjusted and optimized for achieving the best fuel economy in the EPA 2-cycle test. The rest of the parameters were based on default values in Autonomie. The operation of this rule-based controller in city driving (UDDS cycle) is demonstrated in Figure 6-16. The battery SOC is well regulated at 50-60% during urban driving conditions. Figure 6-16 shows a zoomed in view of the power of different components during the UDDS cycle. As shown during the times from 50 to 55 seconds, the motor power is negative and engine is shut off as regenerative braking is performed. From 60 to 80 seconds, pure electric drive is achieved with the engine off. From 85 to 90 seconds, demanded power is higher than the predefined threshold, so the engine starts providing propulsive power to wheels and charging power to motor.

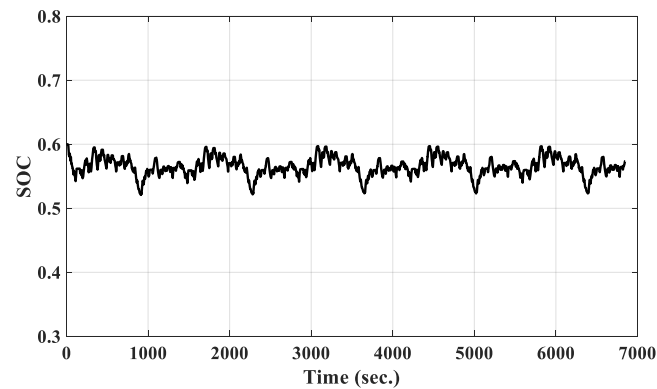


Figure 6-15 Battery SOC of the HEV over 5 consecutive UDDS cycles.

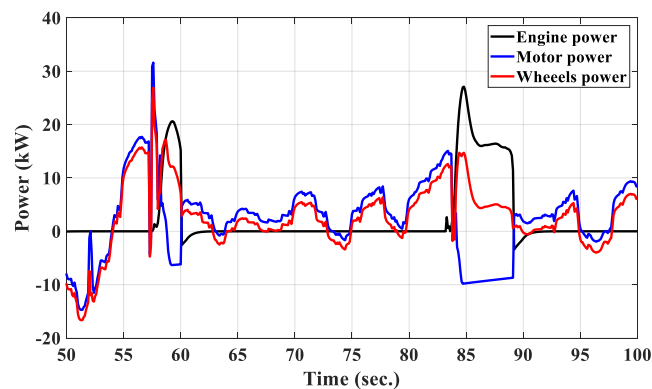


Figure 6-16 The engine power, motor power and wheels power of the HEV during the UDDS drive cycle.

After these steps, the EPA 2-cycle tests were simulated, and fuel economy was calculated following the SAE J1711 test procedures [118]. In this test, the battery SOC was controlled to be the same before and after the test cycles, so the net energy consumption was attributed to the combustion of fuel. As given in Table 6-7, significant fuel reduction was achieved in city

driving for the HEV compared with the conventional powertrain. Highway driving features more steady-state engine operation and less transient acceleration events, therefore the fuel reduction is less than that of city driving. Overall, 38.2% fuel reduction was achieved by the HEV, which is modestly higher than the fuel reduction target (35.7%).

Table 6-7 Fuel consumption and vehicle performance of the full hybrid vehicle.

	HEV	Improvement relative to conventional vehicle
City fuel consumption	4.81 L/100km (48.94MPG)	49.2 %
Highway fuel consumption	5.62 L/km (41.89MPG)	22.3 %
Combined fuel consumption	5.17 L/km (45.49MPG)	38.2 %
0-60mph acceleration	7.2 s	2 %

6.2.3 Plug-in Hybrid Electric Vehicle

The HEV model was used to develop a plug-in hybrid vehicle model with a 64 km (40-mile) AER, and this configuration is referred to as PHEV64. For a PHEV configuration, one of the most important features is zero-emission driving, where the electric motor provides all the power without assistance from the combustion engine. Although the HEV is also able to run in pure electric mode, the vehicle driving conditions and distance for that mode are limited due to the less powerful motor and small battery capacity. In comparison, the PHEV can achieve all-electric driving under a wide range of driving conditions for a longer distance.

For the PHEV configuration, the electric motor was sized to be able to follow the UDDS cycle and HWFET cycle in electric-only mode, as city driving and highway cruising are the most common driving conditions [119]. Unlike the sizing procedure for the HEV, the motor power in the PHEV must be sufficient to propel the vehicle with no assistance from combustion engine. Because of the inevitable losses that occur during power transmission through the clutch, gearbox and final drive, the power at wheels is less than that provided by the electric motor. The power requirement for propelling the vehicle would be underrated if wheel power was

used in sizing the electric motor. The demanded motor power to propel the PHEV through the UDDS and HWFET cycles was simulated, which is plotted in Figure 6-17. The HWFET driving requires less power than UDDS does because the UDDS cycle has more frequent acceleration events. The highest motor power demanded is 50 kW, and for the most of time power demand is less than 30 kW. Based on these results, an electric motor of 50 kW peak power was chosen for the PHEV64. It should be noted that the electric motors for parallel hybrid are generally of less power than those for series and power-split hybrids as ICE can assist the electric power in parallel when the power demand is high.

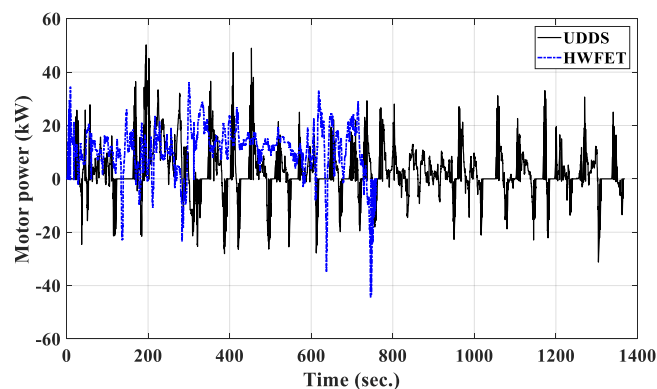


Figure 6-17 The demanded motor power for a PHEV running in pure electric mode on the UDDS cycle and HWFET cycle.

The power of the battery for PHEV64 was oversized by 16% to ensure the performance at the end of life. As a result, the battery of 59 kW power was chosen. Following the same method in ref. [62], the battery energy was determined by scaling the battery capacity to follow UDDS for 64 km (40 mile) in electric-only mode. A special control algorithm was used to enable the all-electric mode for this sizing exercise. Figure 6-18 shows the impact of battery capacity on AER. To achieve 64 km (40 mile) AER, 40 Ah capacity is required. Then, the storage capacity was oversized by 26% to ensure the AER after a long period of use [62] resulting in a 12 kWh battery. The summary of the component size is given in Table 6-8. Some similar vehicles in production are listed in Table 6-9 to confirm that the HEV and PHEV models are realistic. After sizing these components, the vehicle mass was calculated using Eq. 6-3 and data provided in Table 6-5. But it should be noted that the battery weight was evaluated with energy density instead of power density as PHEV battery requires high energy more than high power.

Significance of RON and MON for Different Powertrains on Various Driving Cycles

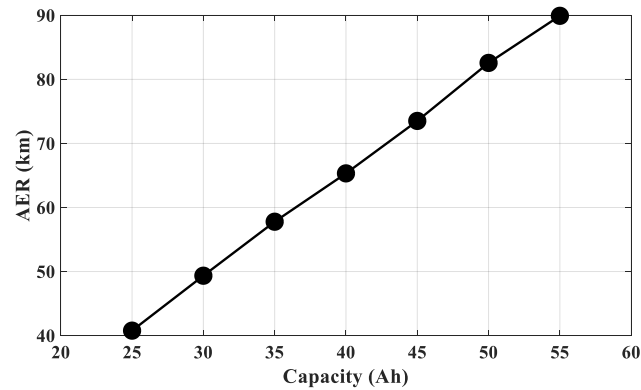


Figure 6-18 All electric ranges along UDDS cycle with different battery capacities.

Table 6-8 The size of the electric drive system and the resulted vehicle mass of the PHEV64.

Motor power	50 kW
Battery power	59 kW
Battery capacity	50.4 Ah, 12 kWh
Vehicle mass	1905 kg

Table 6-9 HEV and PHEVs in production.

Vehicle	Type	Engine power	Motor power	Battery size
Volvo XC90 T8 (parallel hybrid)	Large SUV	238 kW (2L i-4 GTDI)	65 kW	9.2 kWh (43-km AER)
BMW X1 xDrive30 Le	Compact SUV	100 kW (1.5L i-3 GTDI)	70 kW	14.7 kWh (60-km AER)
Geely Lynk & Co 01 HEV (parallel hybrid)	Mid-sized SUV	105 KW (1.5L i-3 GTDI)	40 kW	
Geely Lynk & Co 01 PHEV (parallel hybrid)	Mid-sized SUV	132 kW (1.5L i-3 GTDI)	60 kW	9.4 kWh (50-km AER)

Similar to the HEV configuration, the PHEV controller is also rule-based. However, the HEV only uses CS mode where the SOC of the battery is regulated at 50-60%, while the PHEV uses the CD mode first when battery SOC is high, and then it shifts to the CS mode when the battery SOC drops to 30%. This is demonstrated in Figure 6-19 where the simulated battery SOC of the PHEV64 drops continuously from 90% to 30% in the CD mode with very limited use of engine power. Once SOC drops to 30%, the vehicle controller shifts to CS mode where the SOC does not decrease further but varies in a small range around 30% SOC with more frequent use of engine power.

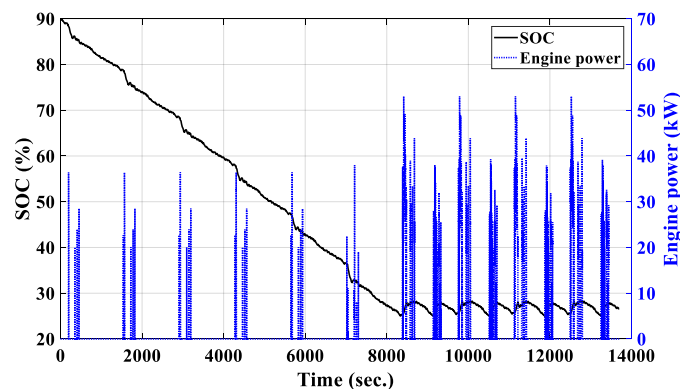


Figure 6-19 The battery SOC and engine power of PHEV64 over 10 consecutive UDDS cycles. Results are from the Autonomie simulation of the developed vehicle model.

Once the PHEV configuration was finalized, the vehicle acceleration test and the 2-cycle test were simulated to ensure the performance and fuel reduction targets were met. The fuel consumption was simulated using the SAE J1711 standard procedures, which dictates that the fuel consumption and electricity consumption in CD and CS modes are evaluated with the utility factor [118]. The utility factor is based on the probability of daily driving distance of US vehicles and is used to estimate the proportion of in-use utility of the CD operation. The results are listed in Table 6-10, which shows significant fuel reduction compared with the conventional vehicle. In the combined fuel consumption evaluation, a 74.7% fuel reduction was achieved, which exceeds the target set for this work. One notes that two energy sources are involved for the PHEV64, so to have a fair comparison with the conventional vehicle, electricity consumption was converted to the equivalent fuel consumption with the EPA electrical energy to fuel equivalence factor (8904 Wh/L). When the electricity consumption was included, the equivalent fuel consumption was 3.20 L/100 km, which was lower than that of conventional vehicle by 61.8%. The vehicle acceleration performance was enhanced (9.5% improvement) due to the stronger motor and larger battery pack.

Table 6-10 Fuel consumption and vehicle performance of the PHEV64.

	PHEV64	Improvement relative to conventional vehicle
City fuel consumption (CD+CS)	1.48 L/100km (159.06MPG)	84.1 %
City electricity consumption (CD+CS)	92.90 Wh/km (149.97Wh/mile)	N/A
Highway fuel consumption (CD+CS)	2.91 L/100km (80.92MPG)	59.8 %
Highway electricity consumption (CD+CS)	99.23 Wh/km (159.16Wh/mile)	N/A
Combined fuel consumption (CD+CS)	2.12 L/100km (110.88MPG)	74.7 %
Combined electricity consumption (CD+CS)	96.08 Wh/km (154.10Wh/mile)	N/A
Fuel consumption equivalent	3.20 L/100km (73.5MPGe)	61.8%
0-96 kph (0-60mph) acceleration	6.7 s	9.5 %

6.3 Distributions of K on Different Powertrains and Driving Cycles

In this section, the distributions of K for conventional vehicle, HEV and PHEV64 in different driving conditions are investigated. The normal temperature K-map was used for the standard EPA drive cycles and the high temperature K-map was used for Davis Dam vehicle tests. Using this information, the significance of RON and MON are quantified.

6.3.1 Calculation Method

6.3.1.1 Knock-Limited Fuel Efficiency Loss Calculation

Distributions of K were calculated for three categories, based on (i) amount of total drive cycle time, (ii) integrated fuel consumption and (iii) knock-limited fuel efficiency loss. The results are reported with K distributed into bins of 0.25 interval in K value.

The calculation of the first two categories are straightforward. The time spent and fuel consumed at each engine operating condition in a given drive cycle was first calculated, and then the experimentally determined K-maps (shown in Figure 5-22 and Figure 5-35) were used to transform the distribution of engine condition to a distribution of K. The calculation of fuel efficiency loss due to knock constraints required the calculation of knock-limited fuel efficiency loss (KLFEL), which is introduced in this section.

For a drive cycle, KLFEL is defined as the percent of the total fuel consumption that is used to suppress knock onset, quantifying the fuel efficiency penalty that is imposed by the knock constraints of the engine. If the engine is not knock-limited throughout a drive cycle, the KLFEL will be 0%, otherwise it will be positive. The following steps were used to calculate KLFEL.

1. At each time step t_i , determine the mass of fuel burned m_i and knock-limited CA50;
2. Calculate the fuel efficiency loss, η_i , (in percent of fuel consumption increase) due to CA50 retard from MBT timing (x) using the correlation (Eq. 6-4) from ref. [18].

$$\eta_i = 1 - 0.168 \left[\sqrt{(1 + 4.443 \cdot 10^{-3} \cdot x^2)} - 1 \right] \quad \text{Eq. 6-4}$$

3. Calculate the mass of fuel lost due to knock using Eq. 6-5, where λ_i is the actual exhaust lambda at t_i and $\lambda_{req,i}$ is the lambda requirement at MBT condition to control the exhaust temperature below 900°C.

$$m_{loss,i} = m_i \cdot \left(1 - \frac{\lambda_i}{\lambda_{req,i}} \eta_i \right) \quad \text{Eq. 6-5}$$

4. Calculate the fuel efficiency loss at time step t_i with Eq. 6-6.

$$KLFEL_i = \frac{m_{loss,i}}{\sum_{i=1}^n m_i} \quad \text{Eq. 6-6}$$

5. Calculate the KLFEL for entire drive cycle using Eq. 6-7.

$$KLFEL = \sum_{i=1}^n KLFEL_i \quad \text{Eq. 6-7}$$

6. Calculate the KLFEL weighted K_w for entire drive cycle with Eq. 6-8.

$$K_w = \frac{\sum_{i=1}^n KLFEL_i \cdot K_i}{KLFEL} \quad \text{Eq. 6-8}$$

The correlation used in Step 2 was developed by Ayala et al. [18] to quantify the effect of retarding CA50 on the fuel efficiency relative to the efficiency at MBT timing across a wide range of operating conditions and fuels. This correlation was validated by spark sweeps at different speeds and loads in this study. The relative fuel efficiency is expressed as the indicated specific fuel consumption (ISFC) ratio to cancel the effect of the small variation in fuel flow rate on IMEP. The CA50 retard is defined as the difference between actual CA50 and MBT CA50 that is described by Eq. 3-2. As shown in Figure 6-20, the tested points fall onto the curve except for the over-advanced conditions. However, by definition, the knock-limited fuel efficiency loss at non-knock-limited conditions is zero (i.e., conditions with spark advanced past MBT timing to induce trace knock) so this small difference is not important.

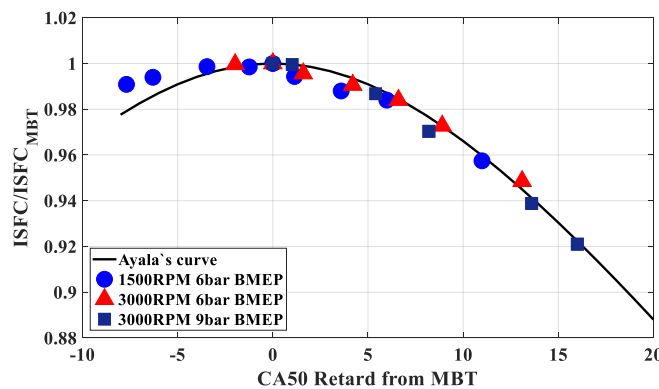


Figure 6-20 The correlation curve between CA50 retard from MBT and relative fuel efficiency from [18]. The correlation was validated with spark sweep tests in the present study (solid points).

The derivations for Eq. 6-5, which is used to calculate the knock-limited fuel loss due to enrichment (Step 3), are given in Appendix B.2. The experiments in the present study included both stoichiometric and rich operation. As already mentioned in Section 3.5, Section 5.2 and Section 5.3, at high-speed or high-load conditions, retarded spark timing caused increase in exhaust temperature and fuel enrichment was used to protect the turbine. Fuel efficiency deteriorated more at these enriched conditions, so the efficiency loss owing to fuel enrichment was also considered by including exhaust lambda in the equation of Step 3. The λ_i is the measured lambda of the exhaust when using the certification gasoline during the engine tests. It was used to include the effect of fuel enrichment induced by the knock limit on fuel efficiency loss. The $\lambda_{req,i}$ is the lambda requirement at MBT to ensure that the exhaust temperature

remains below 900°C. This factor must be considered because at high-speed condition, stoichiometric combustion was not always possible at MBT timing due to the turbine temperature limitations and this enrichment was not due to the knock. As shown in Figure 6-21, where the simulated exhaust temperatures at MBT CA50 for different conditions are plotted, the exhaust temperature can be higher than 900°C at some high-speed conditions. Therefore, the $\frac{\lambda_i}{\lambda_{req,i}}$ term of Eq. 6-5 was used to separate the fuel enrichment caused by retarded spark timing from the fuel enrichment necessary to protect the turbocharger at high engine speed and high load. For most conditions $\lambda_{req,i}$ is 1, and when the exhaust temperature is higher than 900°C for the conditions shown in Figure 6-21, $\lambda_{req,i}$ was calculated with the calibrated GT-Power model. The calculated map of $\lambda_{req,i}$ at normal temperature and high temperature conditions are given in Figure 6-22.

In Step 6, a single K value (K_w) for entire drive cycle was calculated. This K_w was weighted by KLFEL to quantify which K is most relevant to improving fuel efficiency.

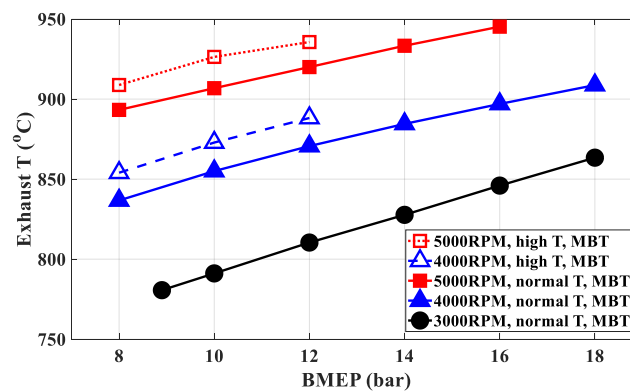
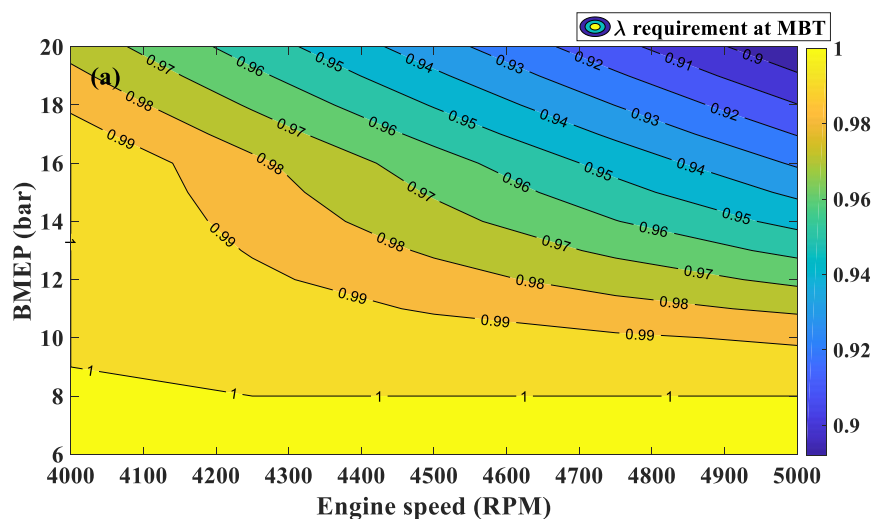


Figure 6-21 Simulated exhaust temperatures at high-speed, stoichiometric, MBT CA50 conditions.



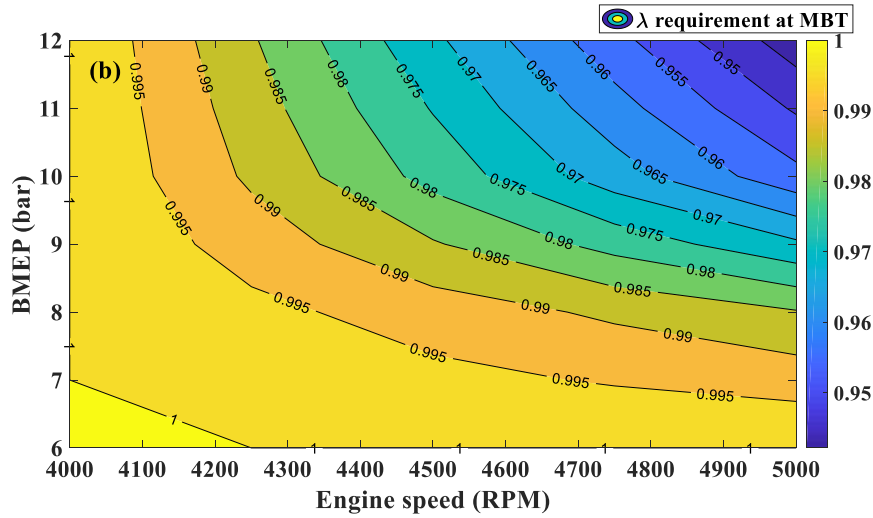


Figure 6-22 Lambda requirement (λ_{req}) map at MBT CA50 to ensure exhaust temperature below 900 °C. (a) is for normal-temperature conditions and (b) is for high-temperature conditions.

6.3.1.2 Quantify the Effect of RON and MON on Fuel Efficiency

The K-maps over the engine load and speed range were used to quantify the significance of RON and MON on improving fuel efficiency over a drive cycle. This was done by calculating the change in KLFEL due to the changes in RON and MON separately. This calculation method is introduced below:

1. Assume a 3 octane number change in RON and MON separately i.e. $\Delta RON = \pm 3$ and $\Delta MON = \pm 3$.
2. Calculate the change in OI with K values for the entire drive cycle with Eq. 6-9.

$$\Delta OI = [\Delta RON \ \Delta MON] \times \left(\frac{1-K}{K} \right) \quad \text{Eq. 6-9}$$

3. Calculate the knock-limited CA50 of the fuel after octane number change with Eq. 6-10 and Eq. 6-11. Eq. 6-10 is based on the correlation formulated in this study with literature data, as shown in Figure 6-23.

$$\Delta CA50 = 1.153 \cdot \Delta OI \quad \text{Eq. 6-10}$$

$$CA50_{new} = CA50_{cert} - \Delta CA50 \quad \text{Eq. 6-11}$$

4. Repeat the calculation of KEFEL for entire cycle with $CA50_{new}$ using the method introduced in Section 6.3.1.1

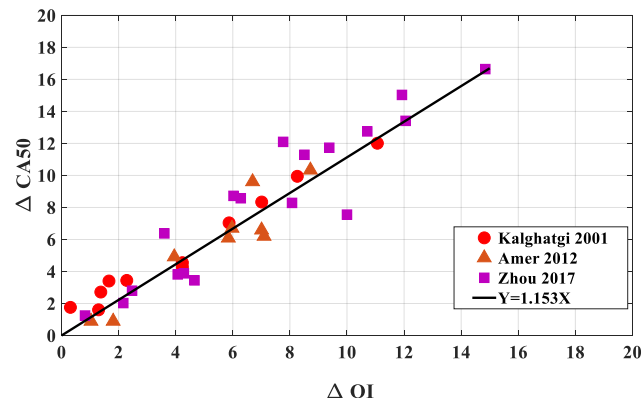


Figure 6-23 The correlation of ΔOI and $\Delta CA50$ based on literature data.

6.3.2 K-Distributions of Conventional Powertrain

6.3.2.1 UDDS and HWFET cycles

The engine operating conditions from vehicle test data on the UDDS and HWFET driving cycles are mostly at low-load and low-speed. Figure 6-24 shows the engine operating conditions of the conventional vehicle in UDDS and HWFET cycles superimposed on the normal temperature conditions K-map, which is relevant to these drive cycles. As seen, most conditions are at positive K for both cycles. Most low-load conditions are excluded from the K-map as K values at these conditions were not measured and the engine is not knock-limited at low-load with the tested certification fuel. Figure 6-25 shows the distributions of K based on KLFEL. The KLFEL for both cycles is minimal, suggesting engine knock is not a constraint on fuel efficiency for these drive cycles. Rather, fuel inefficiency at low-load conditions is attributed to other factors, particularly pumping loss due to significant throttling.

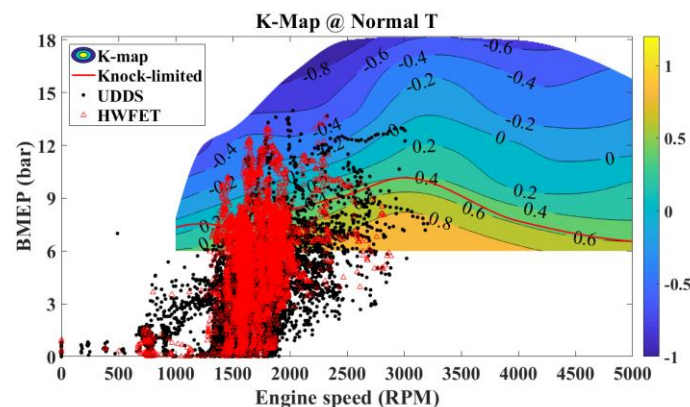


Figure 6-24 The engine operating conditions in UDDS and HWFET cycles spread over the normal-T K-map.

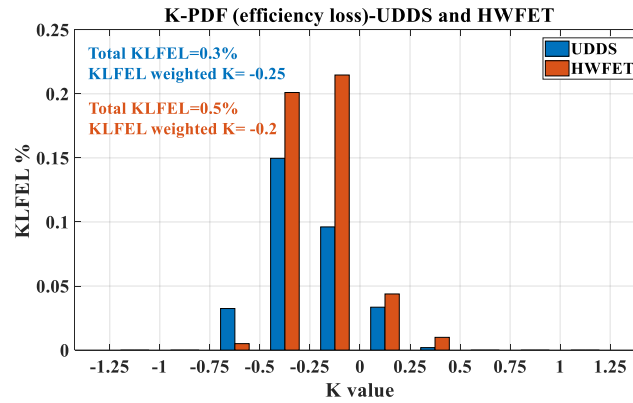


Figure 6-25 The distributions of knock-limited K based on KLFEL in the UDDS and HWFET drive cycles.

6.3.2.2 US06 cycle

In contrast to the UDDS and HWFET drive cycles, the US06 cycle features aggressive driving where the engine operates at higher load and more knock-limited conditions (Figure 6-26). Figure 6-27(a) and Figure 6-27(b) show the distributions of the knock-limited K (determined from the normal temperature conditions K-map) based on time and fuel consumption respectively. There is a significant amount of time and fuel consumption at knock-limited conditions (32% and 68% respectively). While the distributions of K based on a percent of drive cycle time and fuel consumption is through both positive and negative K (Figure 6-27a and Figure 6-27b), the overwhelming majority of KLFEL occurs at negative K (Figure 6-27c). As shown in Figure 6-27c, due to the knock limit, there is 6.3% fuel efficiency loss, suggesting that engine knock imposes a considerable penalty in fuel efficiency in the US06 cycle as compared to that of the UDDS and HWFET cycles. For a reference, increasing compression ratio by 1 improves engine thermal efficiency by $\sim 1\%$ [19, 120]. As seen in the distribution, the most KLFEL occurs at conditions of negative K, especially in the range of $-0.75 \sim -0.25$, resulting in a KLFEL-weighted $K = -0.44$.

Significance of RON and MON for Different Powertrains on Various Driving Cycles

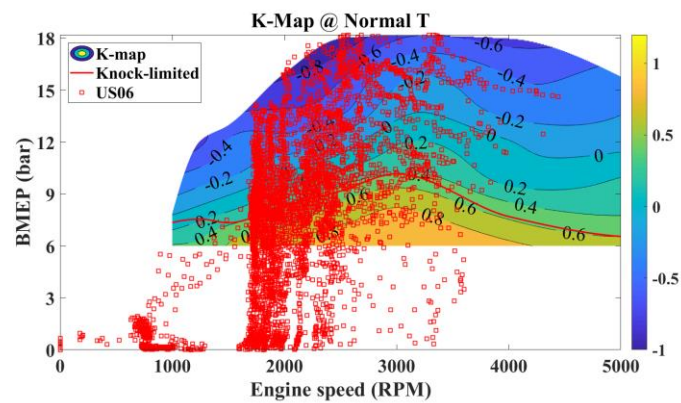


Figure 6-26 The engine operating conditions in US06 cycle spread over the normal-T K-map.

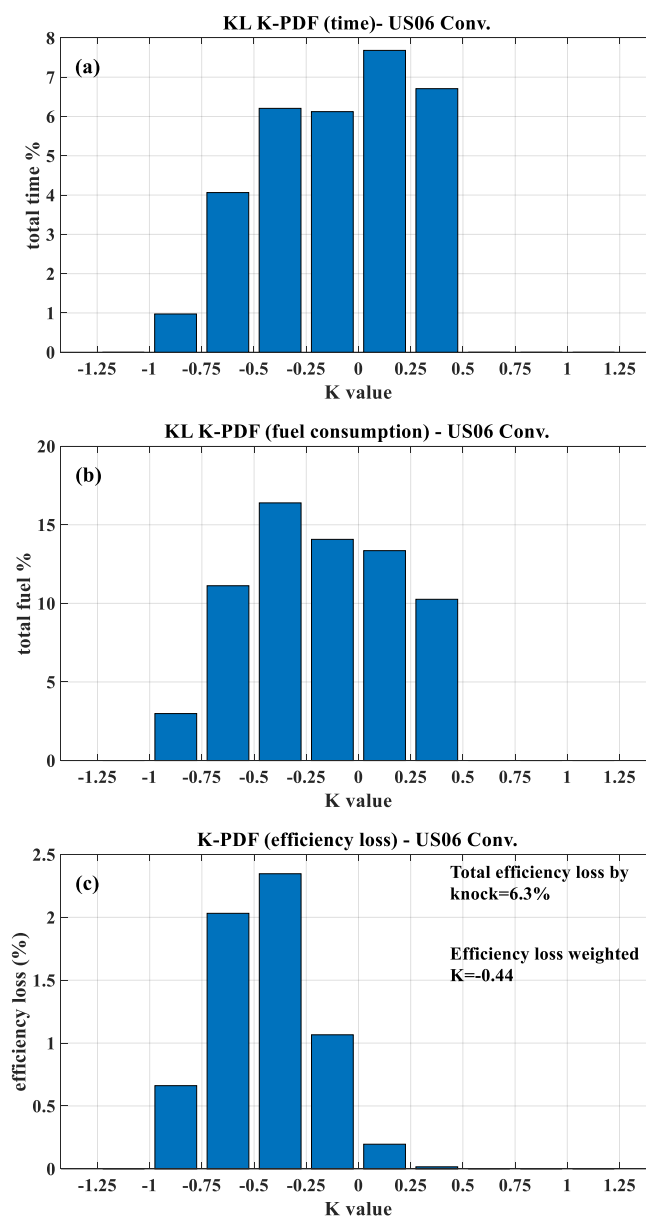


Figure 6-27 The distributions of knock-limited K based on (a) percent of entire drive cycle time, (b) fuel consumption and (c) KLFEL in US06 cycle.

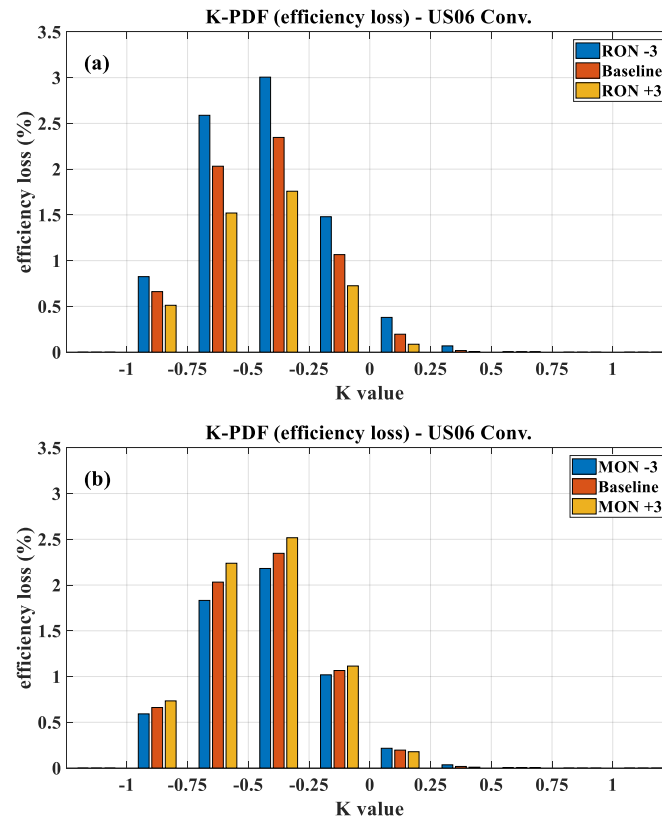


Figure 6-28 The effect of (a) RON and (b) MON the KLFEL-based distributions of K for US06 cycle.

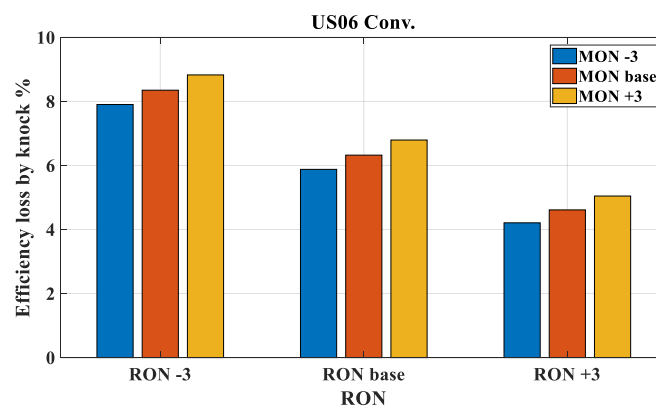


Figure 6-29 The effect of RON and MON on the overall KLFEL for US06 cycle.

Using the method introduced in Section 6.3.1 and the K distributions of fuel efficiency loss, the impact of RON and MON on KLFEL can now be investigated. Figure 6-28 shows the effect of RON and MON on the KLFEL-based distribution of K. Increasing RON reduces the KLFEL

for all conditions, but this effect is more pronounced when K is negative. In contrast, increasing the MON leads to more efficiency loss for conditions of negative K but less efficiency loss for conditions of positive K . Given that the majority of KLFEL occurs at negative K conditions, the overall KLFEL for entire drive cycle can be reduced by increasing RON or decreasing MON, as demonstrated by Figure 6-29. Also, increasing the RON has a more noticeable effect on efficiency improvement than decreasing the MON.

6.3.2.3 Davis Dam Towing

The distributions of K for the Davis Dam vehicle tests were calculated using the high-temperature K -map, as the laboratory engine experiments were conducted with high intake air and coolant temperatures, similar to the Davis Dam vehicle test conditions. The distributions of K based on fuel consumption at knock-limited conditions for two Davis Dam tests are given in Figure 6-30. Compared with the fuel consumption distribution of the US06 cycle, the Davis Dam distributions are shifted to more positive K . There is no fuel consumption at K lower than -0.5 but a significant amount of fuel consumed at K higher than 0.5 (11.6%). This is because the engine operates more at high-speed conditions (Figure 6-31), which tends to increase in-cylinder temperatures, therefore resulting in engine operation at high K .

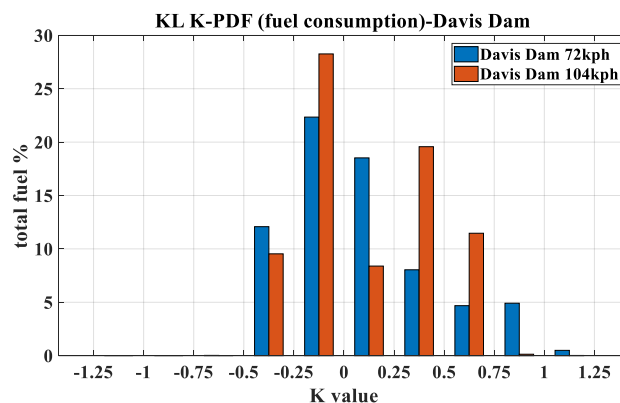


Figure 6-30 The distributions of K based on fuel consumption at the knock-limited conditions in the highway gradeability tests on Davis Dam Grade at 72 kph (45 mph) and 104 kph (65 mph).

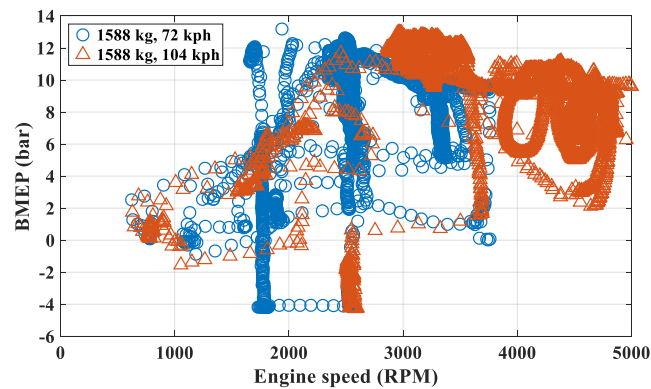


Figure 6-31 The engine operating conditions in the highway gradeability tests on Davis Dam Grade at 72 kph (45 mph) and 104 kph (65 mph). Note: the negative BMEP is due to the fuel cut-off during vehicle deceleration.

The KLFEL-based distributions of K are quite different for Davis Dam tests (Figure 6-32). For the lower speed test at 72 kph (45 mph), most KLFEL takes place at conditions of negative K and the KLFEL-weighted K for cycle is slightly negative ($K=-0.11$). In comparison, the KLFEL for the higher speed test at 104 kph (65 mph) dominantly occurs at conditions of positive K, and as a result, the KLFEL-weighted K is slightly positive ($K=+0.12$).

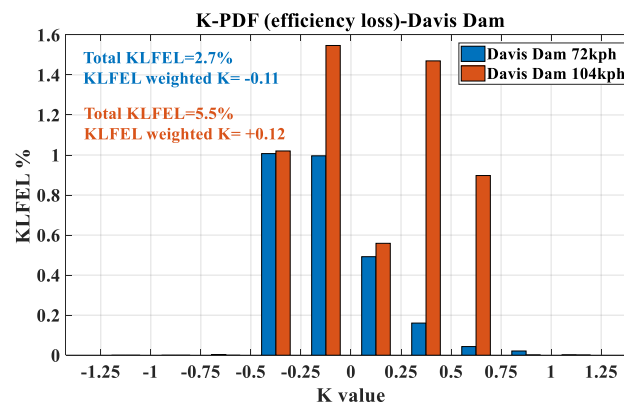


Figure 6-32 The distributions of K based on KLFEL in the highway gradeability tests on Davis Dam Grade at 72 kph (45 mph) and 104 kph (65 mph).

The KLFEL in the two Davis Dam vehicle tests are surprisingly lower than that of the US06 cycle. This is because the calculation method for KLFEL only accounts for fuel efficiency loss caused by spark retard from MBT timing and fuel enrichment related to knock mitigation. Because the engine is significantly knock-limited with the high intake and coolant temperatures in the Davis Dam tests, the transmission downshifts and the engine operates at different points than those found in the previous drive cycles to meet high power demands while avoiding excessive knock. This causes the engine to run at a higher speed and lower load, but still service the power demanded by the vehicle. The downshifting makes the engine run at conditions of

lower fuel efficiency (high-speed and part-load) than that found in the other drive cycles at normal temperature conditions for a given power demand. This can be explained by Figure 6-33, where the power demand in the Davis Dam tests is overall lower than that of the US06 cycle, but the engine speed is higher than the speed in US06. Fuel efficiency will decrease due to this downshifting induced by knock constraints. However, this fuel efficiency loss is not captured by the calculation method in this work.

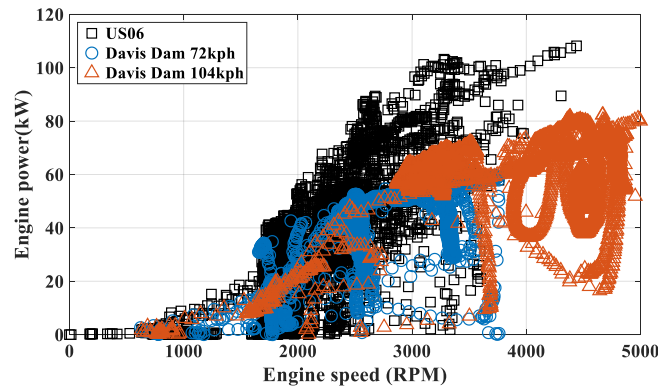


Figure 6-33 The engine speed and engine power in US06 cycle and Davis Dam tow rating.

The effect of RON and MON on the KLFEL for the Davis Dam vehicle tests (Figure 6-34) is different from the other drive cycles. Because of the significant KLFEL at positive K conditions, decreasing MON does not reduce the drive cycle fuel efficiency loss. Instead, increasing MON slightly improves the fuel efficiency for the test at 104 kph (Figure 6-34b) as indicated by the positive K_w (+0.12). The RON effect on KLFEL is more pronounced than the MON effect with 1% improvement in fuel efficiency by increasing RON by 3, but it is not as significant as it is on the US06 cycle where the K_w (= -0.44) is more negative.

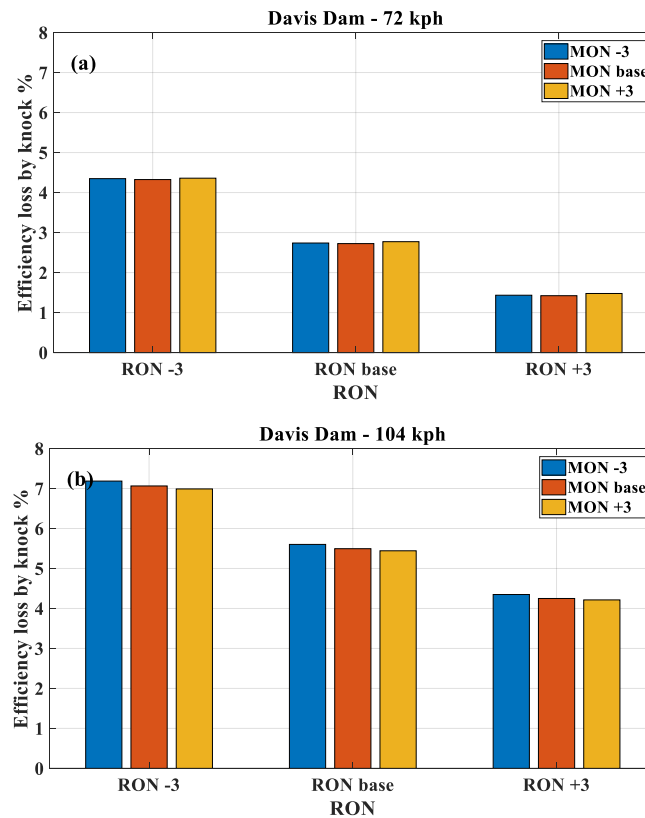


Figure 6-34 The effect of RON and MON on the overall KLFEL in the highway gradeability tests on Davis Dam Grade at (a) 72 kph and (b) 104 kph.

6.3.3 K-Distributions of Hybrid Powertrain

6.3.3.1 UDDS and HWFET cycles

The engine operation of HEV differs from that of the conventional powertrain as demonstrated by Figure 6-35. On the UDDS and HWFET cycles, the engine in the HEV configuration runs at higher loads and a narrower range of speed as compared to those of the conventional powertrain. This is because low-load conditions and transient operation is replaced by the electric motor and the engine often operates at higher load and conditions more similar to steady-state. Furthermore, given the assistance of the electrical drive system, the conventional powertrain engine is downsized for the hybrid powertrain, which also contributes to more operation in the high load range.

Significance of RON and MON for Different Powertrains on Various Driving Cycles

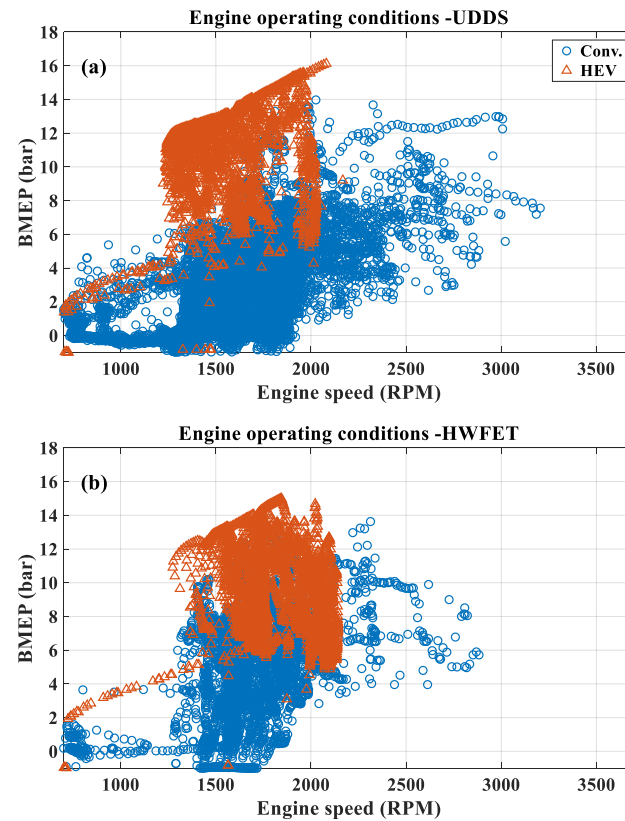
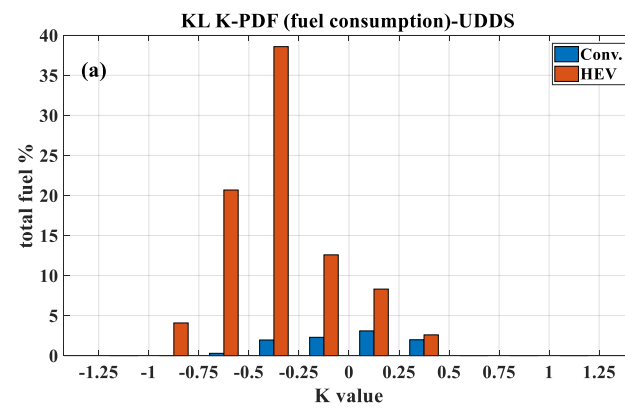


Figure 6-35 The comparison of engine operating conditions of the HEV and conventional vehicle in (a) UDDS cycle and (b) HWFET cycle.



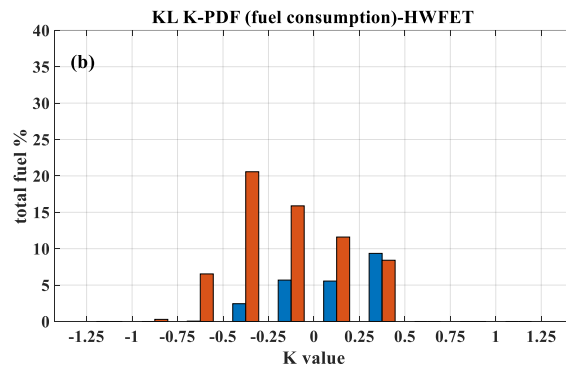


Figure 6-36 The distribution of knock-limited K based on fuel consumption of HEV vs. conventional powertrain in (a) UDDS cycle and (b) HWFET cycle.

The fuel consumption-based K distributions of the HEV in city and highway driving are given in Figure 6-36, showing that when being compared with conventional vehicle most fuel consumption of HEV occurs at conditions of negative K, especially in the range of -0.5 ~ -0.25. Comparing two drive cycles, the fuel consumption at the knock-limited condition on the UDDS cycle is more than that on the HWFET cycle. This is because the HWFET cycle is less dynamic than the UDDS cycle and engine works more at steady state with less involvement of the electric drive system.

The K value is more negative at higher load conditions where engine is under boosted operation and more knock-limited. As a result, there is more KLFEL at conditions of negative K, as demonstrated by Figure 6-37 where KLFEL primarily occurs at conditions of K from -0.75 to -0.25. Comparing the results in Figure 6-37 and in Figure 6-25, the engine is significantly more knock-limited for the HEV than for the conventional vehicle because the HEV configuration shifts the engine operation to a high load and low speed regime where knock is prevalent. The KLFEL for the conventional powertrain in UDDS and HWFET is less than 0.5%, while it increases to 8.1% in UDDS and 3.5% in HWFET for the HEV. Although the overall fuel consumption of the HEV was shown to be lower than that of the conventional vehicle by 38%, the 8.1% fuel efficiency loss suggests that further improvements to knock resistance have great capacity to increase drive cycle fuel efficiency for hybridized vehicles.

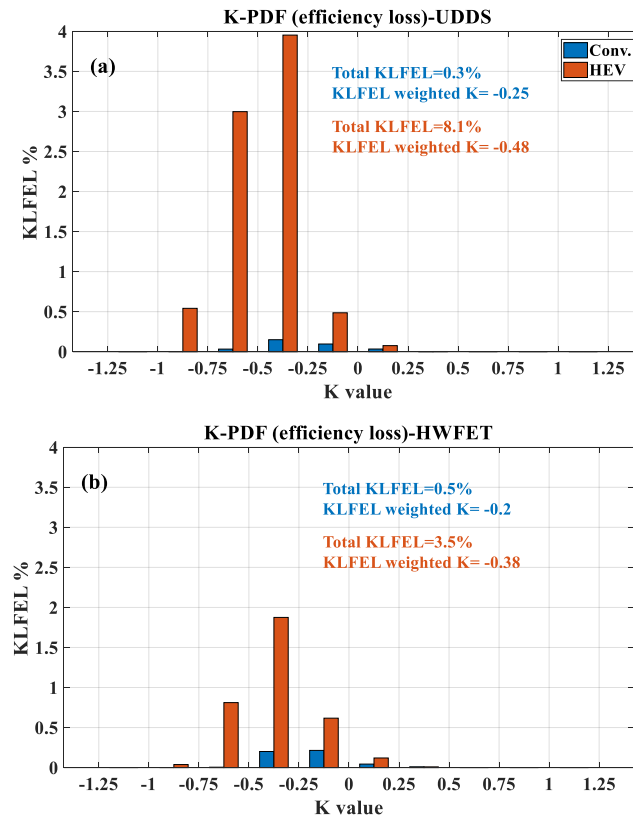


Figure 6-37 The KLFEL-based distributions of K of HEV vs. conventional powertrain in (a) the UDDS cycle and (b) in the HWFET cycle.

The effect of RON and MON on KLFEL is illustrated by Figure 6-38 for both the UDDS and HWFET cycles. On the UDDS cycle, it shows that increasing RON has the most dominant influence on fuel efficiency loss due to knock, with a 3% reduction in fuel inefficiency achieved when increasing RON by 3 and a 1% reduction in fuel inefficiency when decreasing MON by 3. This effect is consistent with the KLFEL-weighted K (K_w). When $K_w = -0.48$, the weighting factor of RON in the OI model is 1.48 and weighting factor of MON is -0.48, which means the contribution of increasing RON to fuel efficiency improvement is approximately three times that of the contribution of decreasing MON.

On the HWFET cycle, increasing RON also reduces KLFEL, but its effect is relatively weak as compared to the UDDS cycle, because the overall KLFEL is much lower in the HWFET than in the UDDS cycle. Decreasing MON reduces the fuel efficiency loss, but this effect is negligible, with less than 0.5% improvement for a 3 octane number change in MON.

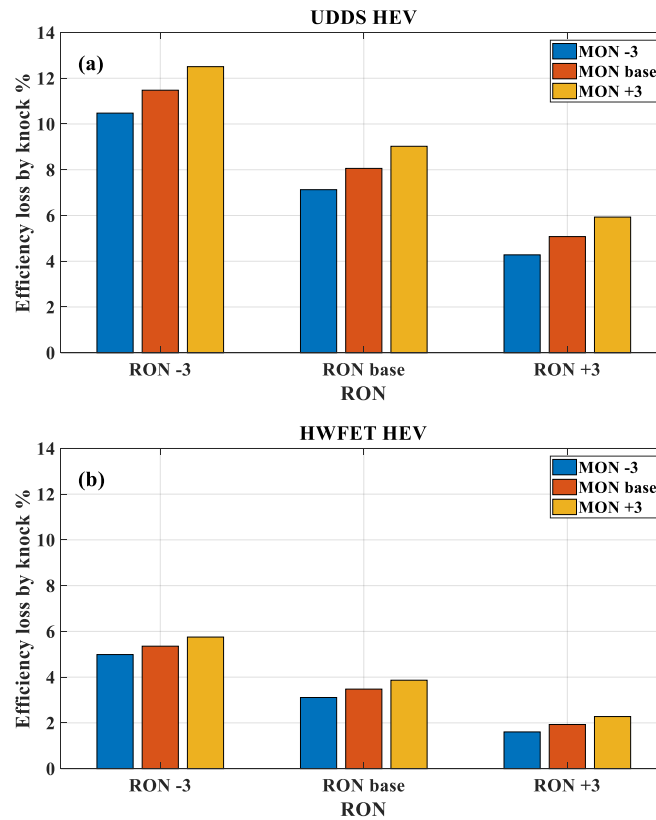


Figure 6-38 The effect of RON and MON on the overall KLFEL for HEV in (a) the UDDS cycle and (b) the HWFET cycle.

6.3.3.2 US06 cycle

The engine operating conditions of the HEV and conventional vehicle on the US06 cycle are compared in Figure 6-39. The high-load portion remains same for both powertrains, but the low-load range is nearly eliminated for the engine in the HEV due to the assistance of the electric motor. Also, the engine speed range is narrower for the HEV because the engine undergoes less transient operation when being assisted by electric motor.

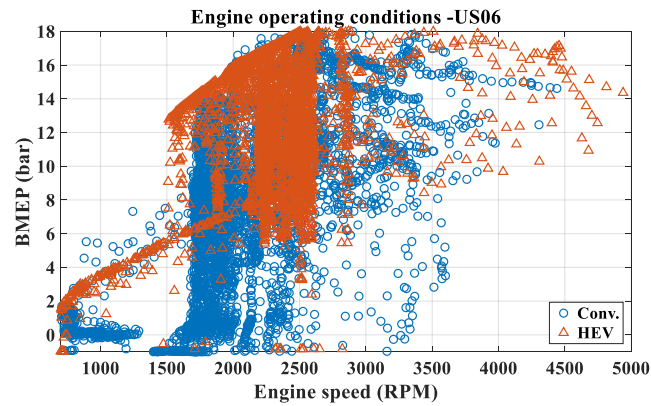


Figure 6-39 The comparison of engine operating conditions of the HEV and conventional vehicle through the US06 cycle.

The distributions of K based on percent of drive cycle time, fuel consumption and KLFEL on the US06 cycle are given in Figure 6-40, along with the comparison with those of the conventional powertrain. The engine of the HEV operates at negative K conditions for a larger portion of the total time than the engine of the conventional vehicle does. Similar to the conventional powertrain, fuel consumption at negative K is higher than that at positive K . The highest portion is at $-0.75 \sim -0.5$ for the HEV, which is more negative than that for the conventional powertrain. The KLFEL for the HEV in the US06 cycle is even higher, reaching 11% of the total fuel consumption. Also, the KLFEL occurs at K values more negative than those the conventional powertrain, as evidenced by the K_w of -0.61 for the HEV as compared to a K_w of -0.44 for the conventional vehicle. As predicted by the K_w and OI model, increasing RON by 3 ON reduces KLFEL by 3.4%, which is more three times the reduction of KLFEL when decreasing MON by 3 ON for the HEV on the US06 cycle. The effect of MON on KLFEL is more significant, with 1% improvement in KLFEL by decreasing MON by 3, which is higher than that of the conventional vehicle (0.5%).

Significance of RON and MON for Different Powertrains on Various Driving Cycles

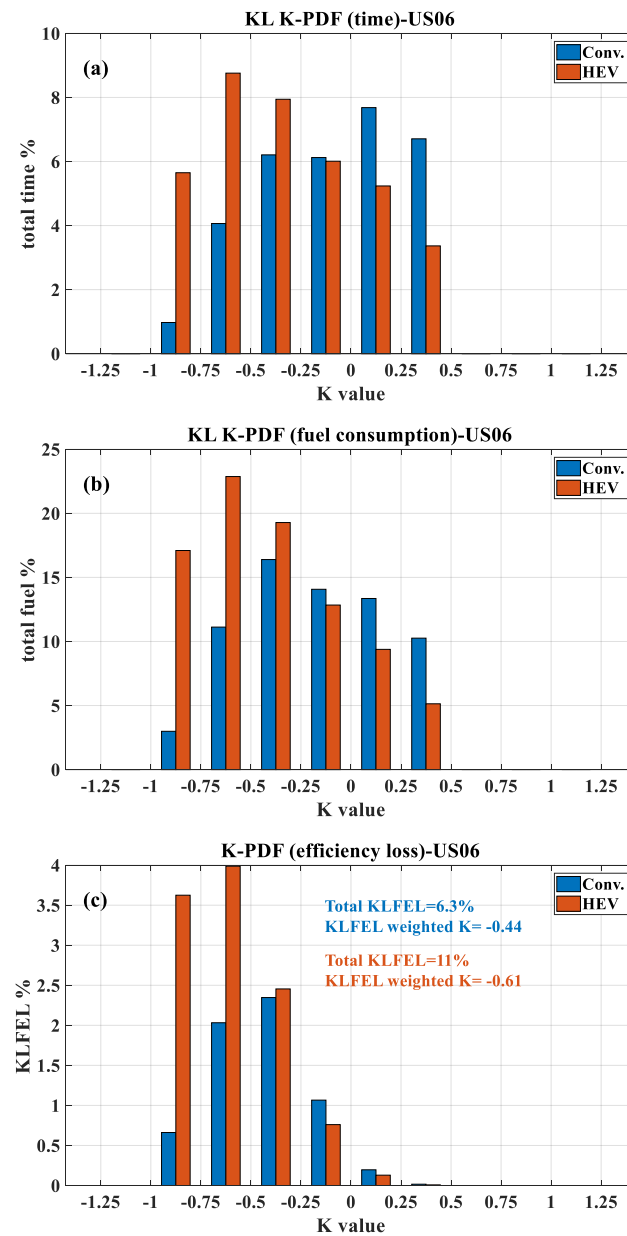


Figure 6-40 The distributions of knock-limited K of HEV vs. conventional powertrain based on (a) percent of drive cycle time, (b) fuel consumption and (c) KLFEL for the HEV through the US06 cycle.

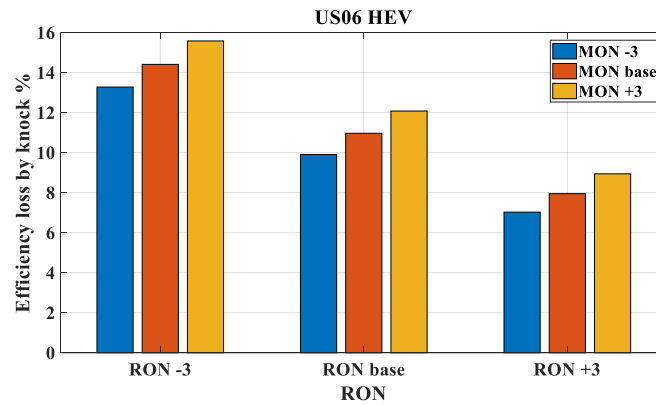


Figure 6-41 The effect of RON and MON on the overall KLFEL for the HEV through the US06 cycle.

6.3.4 K-Distributions of Plug-in Hybrid Powertrain

The PHEV64 has two modes: CD and CS. In the CD mode, electricity is the primary power source and the engine power is only used when the electric motor is unable to service the vehicle's power demand. The engine and electric motor usage in CD mode and CS mode on three drive cycles are listed in Table 6-11. On the UDDS and HWFET, the engine operation time in the CD mode is close to zero. While the engine is more involved in CD mode on the US06 cycle due to the high-power demand, the engine operating time and fuel consumption are still limited. In CS mode, PHEV64 works as a HEV where fuel is the primary energy source and the net electricity consumption is almost zero. Therefore, no K distributions are generated for the CD mode, as the engine operating is extremely limited.

Table 6-11 Electricity and fuel usage of PHEV64 in the CD mode and CS mode on three drive cycles.

	UDDS	HWFET	US06
Engine operating time (%) (CD/CS)	0.81 / 24.12	0 / 44.02	25.42 / 49.69
Fuel consumption (L/100km) (CD/CS)	0.14 / 5.13	0 / 5.90	4.58 / 8.5
Electricity Consumption (Wh/km) (CD/CS)	199.8 / 3	246.4 / 4.8	172.4 / 5.2

6.3.4.1 UDDS and HWFET cycles in the CS mode

For the PHEV, engine operates at higher load as compared to HEV and conventional vehicle, as indicated by the distribution of fuel consumption (Figure 6-42) where more fuel is consumed

at more negative K conditions. The KLFEL-based distributions of K in CS mode on the UDDS and HWFET cycles are given in Figure 6-43. In both cycles, the most KLFEL occurs at negative K conditions with most of the loss in the range $K = -0.75 \sim -0.5$. The KLFEL of the PHEV64 in both cycles are higher than those of the HEV, especially in the HWFET cycle (7.9% for the PHEV64 versus 3.5% for the HEV). The reason for this difference in the HWFET cycle is that in the CS mode, the battery works as an energy buffer, and the relatively larger battery of the PHEV allows higher charging and discharging power. This permits more freedom of the optimization of engine operation. As shown in Figure 6-44, in the discharging stage, the motor of the PHEV provides higher power for a longer time than that of HEV does, and consequently, the PHEV allows the engine to charge the battery at a higher power for a longer time in order to maintain the battery SOC at a constant level. As a result, the average engine output of the PHEV is in a more knock-limited regime than that of the HEV engine.

Significance of RON and MON for Different Powertrains on Various Driving Cycles

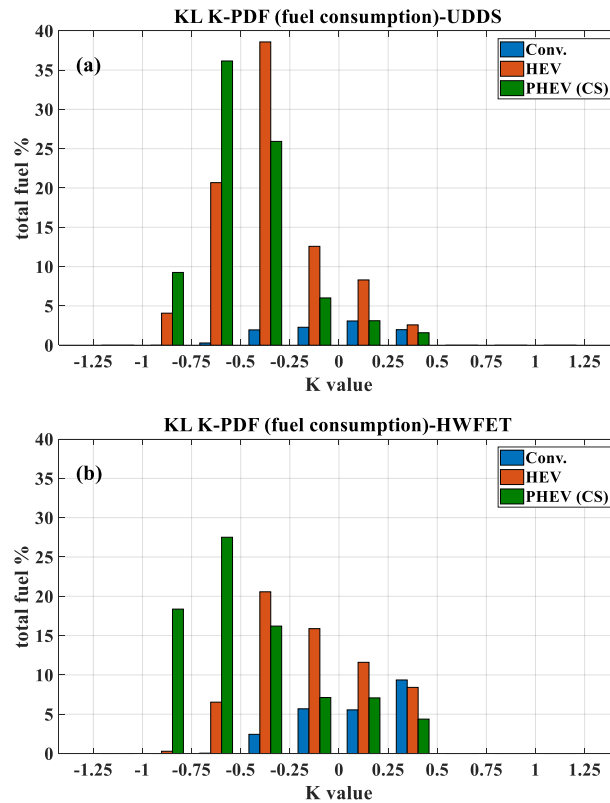


Figure 6-42 The distributions of knock-limited K based on fuel consumption for the PHEV64 vs. the other two powertrains in CS mode through the (a) the UDDS and (b) HWFET cycle.

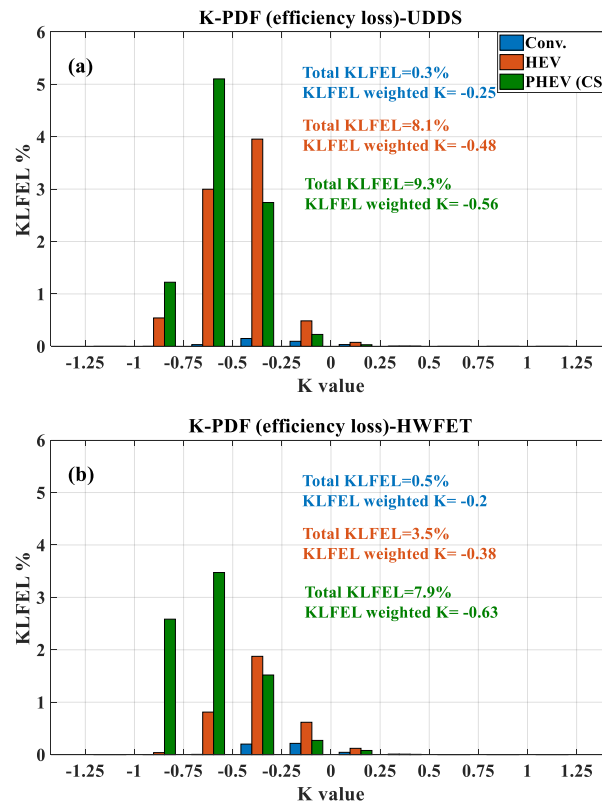


Figure 6-43 The KLFEL-based distributions of K for the PHEV64 vs. the other two powertrains in CS mode through the (a) the UDDS and (b) HWFET cycle.

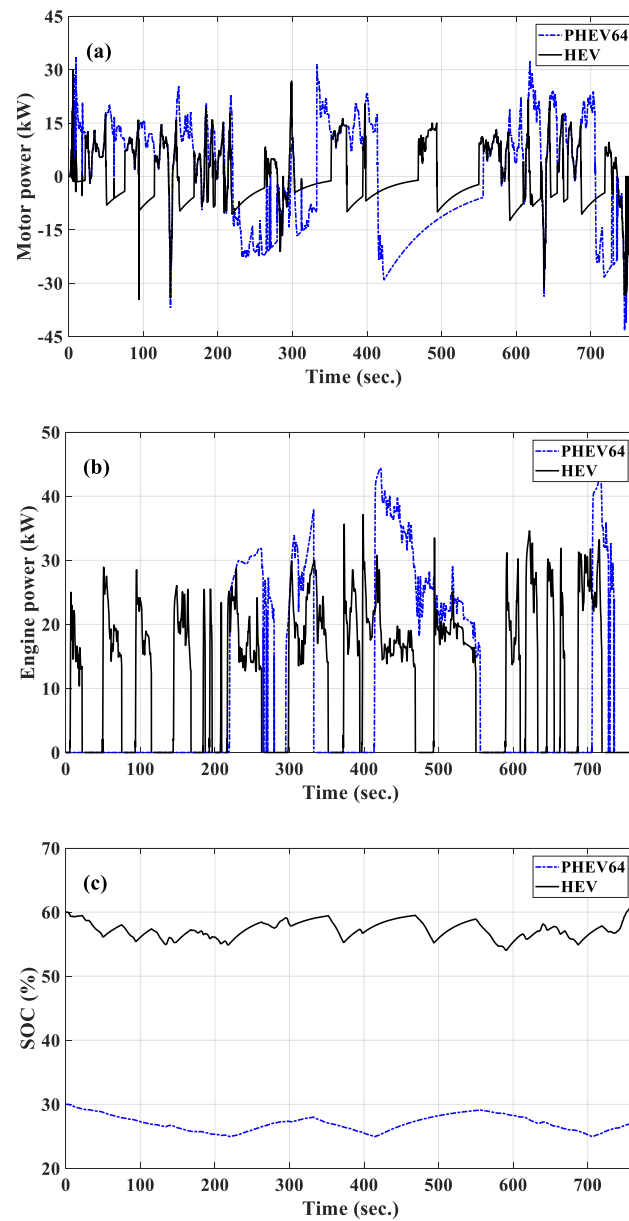


Figure 6-44 The (a) motor power, (b) engine power and (c) battery SOC in CS mode of PHEV64 vs. HEV in HWFET cycle.

The effect of RON and MON of KLFEL is demonstrated by Figure 6-45 for UDDS and HWFET cycles. The effects for both cycles are identical. Increasing RON by 3 reduces 3.4% fuel loss and decreasing MON by 3 reduces only 1.2% fuel loss, which are higher than those for HEV.

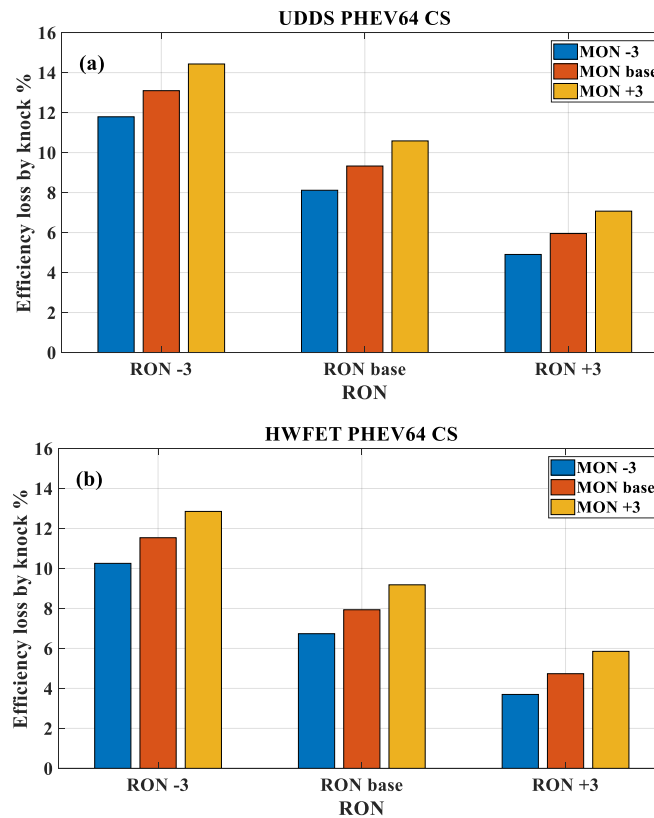


Figure 6-45 The effect of RON and MON on the overall KLFEL of PHEV64 in CS mode over (a) the UDDS cycle and (b) the HWFET cycle.

6.3.4.2 US06 cycle in the CS mode

The PHEV64 is similar to the other vehicle configurations in that the engine is still the most knock-limited through the US06 cycle. Engine operates at more negative K conditions with a significant amount of fuel consumed at $K < -0.75$ (Figure 6-46a). As shown in Figure 6-46b, there is a substantial knock-limited fuel efficiency loss through the drive cycle (14.6%). Nearly all the KLFEL happens at negative K, and the loss happens largely in the K range from -1 to -0.75. The total KLFEL in CS mode is much higher than that of HEV and conventional vehicle and accordingly the K_w is the most negative for the PHEV than for the other two. The effect of RON and MON on KLFEL for the PHEV64 through the US06 cycle is shown in Figure 6-47. RON has a significant effect on KLFEL, improving 4.3% fuel efficiency in CS mode when RON is increased by 3 ON. The effect of MON on fuel efficiency is relatively weaker, with 1.5% fuel efficiency improvement when decreasing the MON by 3 ON.

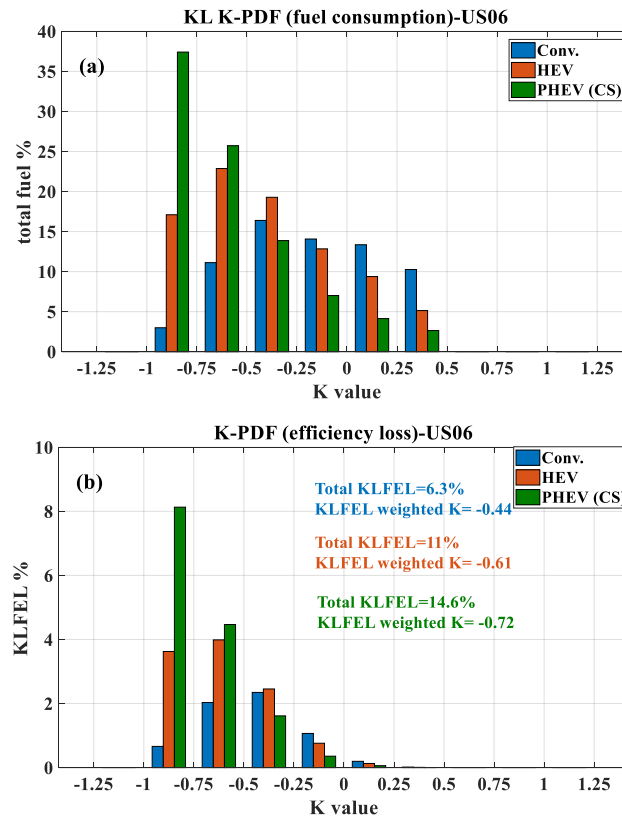


Figure 6-46 The distributions of K based on (a) fuel consumption and (b) KLFEL for the PHEV64 vs the other two powertrains in the US06 cycle.

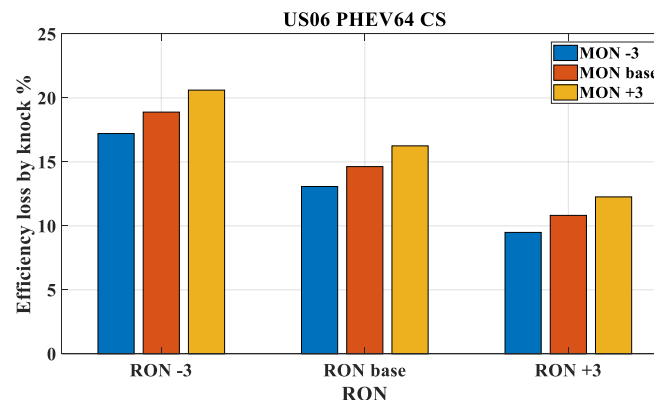


Figure 6-47 The effects of RON and MON the total KLFEL of the PHEV64 through the US06 cycle in the CS mode.

6.4 Discussion

With increasing penetration of hybrid vehicles in future, a question of interest is how the significance of RON and MON changes with the degree of powertrain hybridization. This can be speculated by comparing the engine operation of HEV and PHEV64 in the CS mode as the PHEV in the CS mode essentially works as a full hybrid with larger battery pack and more

powerful motor i.e. deeper degree of hybridization. With deeper degree of electrification, the engine has more freedom to operate within a smaller region. From the comparison in Figure 6-48, the majority of engine work of the PHEV is produced in a small region along the wide-open-throttle (WOT) curve where the engine is more knock-limited, whereas engine work is more evenly distributed over a wider region for the HEV. In addition, as shown in Table 6-12, the fuel efficiency loss due to the knock limit of the PHEV (CS mode) is much higher than that of the HEV, and as shown by the figures above, for a give change in octane numbers, the fuel efficiency can be improved more for the PHEV than for the HEV. This indicates that with deeper degree of electrification (or hybridization), knock becomes a more significant constraint in improving fuel efficiency and fuel octane numbers plays a more important role in reducing fuel consumption. Furthermore, when powertrain hybridization is combined with other engine technologies such as high compression ratio or downsizing, fuel efficiency improvement will also be more limited by knock and the significance of fuel RON and MON will be more profound.

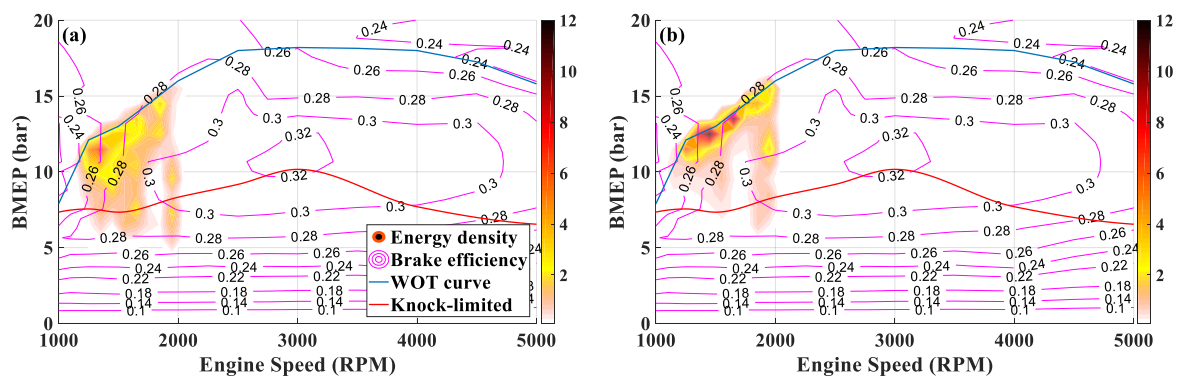


Figure 6-48 The fuel energy distributions of (a) HEV and (b) PHEV64 in the CS mode over the UDDS cycle (the energy density cloud was calculated with grids of 100 RPM and 1 bar BMEP).

The knock limit in the present study is for the engine of compression of 9.3:1 which is relatively low compared with the newest GTDI engines on the market. Future engine will be using even higher compression ratio to improve fuel efficiency, in which case engine may become knock-limited at lower load where the knock-limited K is higher. Reducing the MON may make the knock a potential burden for these high compression engines. Considering the very moderate effect of decreasing MON on improving fuel efficiency in some drive cycles, reducing MON may not be a good option in terms of improving fuel efficiency. Therefore, instead of decreasing MON, increasing RON should be a better method to improve fuel efficiency.

6.5 Summary

Table 6-12 Summary of KLFEL and K_w of different powertrains.

Cycle KLFEL (%) / K_w Powertrain	UDDS	HWFET	US06	Davis Dam (45 mph)	Davis Dam (65 mph)
Conventional	0.3 / -0.25	0.5 / -0.2	6.3 / -0.44	2.7 / -0.11	5.5 / +0.12
Full HEV	8.1 / -0.48	3.5 / -0.28	11 / -0.61	N/A	
PHEV64 (CD)	N/A	N/A	12.8 / -0.68		
PHEV64 (CS)	9.3 / -0.56	7.9 / -0.63	14.6 / -0.72		

This work investigated the significance of RON and MON to conventional, full hybrid and plug-in hybrid powertrains in different driving conditions using the Octane Index model. The distributions of K based on fuel consumption and KLFEL were calculated, with which the effects of RON and MON on fuel efficiency was quantified. The summary of the KLFEL and K_w for all three powertrains over different drive cycles is given in Table 6-12.

For the conventional powertrain, the engine is not knock-limited on the UDDS and HWFET cycles but is more knock-limited on the US06 and Davis Dam cycles where up to 6% fuel efficiency loss is resulted by the knock limit. Although there is a significant fraction of the total time and fuel consumption at conditions of positive K but the KLFEL primarily occurs at conditions of near-zero or slightly negative K. As a result, fuel efficiency can be effectively improved by increasing RON. Increasing MON has minor promoting or neutral effect on the fuel efficiency.

For the full hybrid, the low-load condition is replaced by the electric motor and engine operates at higher load. Therefore, the engine is significantly more knock-limited than the conventional powertrain for all three drive cycles where up to 11% fuel efficiency loss is resulted. Both the fuel consumption and the knock-limited fuel efficiency loss occur at conditions of more negative K where increasing RON by 3 improves the fuel efficiency by 3% while decreasing MON by 3 only reduces 1% fuel efficiency loss.

For the plug-in hybrid, because of the more powerful motor and larger battery, the average engine load is even higher than that of HEV. Therefore, the engine is even more knock-limited than the engine of HEV with up to 14.6% fuel efficiency loss resulted. The distribution of K

shifts to more negative K where increasing RON by 3 reduces 4% fuel loss. Decreasing MON has less effect on improving fuel efficiency with 1.5% fuel efficiency improvement by decreasing MON by 3.

By comparing the engine operating conditions and the knock-limited fuel efficiency loss of HEV and PHEV in the CS mode, it can be concluded that with deeper degree of powertrain hybridization, knock will be a more limiting factor for fuel efficiency improvement to which fuel octane numbers will be more significant.

7 Conclusions and Recommendations for Future Study

7.1 Conclusions

With respect to the research questions proposed for the thesis, following conclusions have been made.

Development of a rigorous method for the experimental measurement of Octane Index and K over a wide range of engine operating conditions.

This work investigated four methods for determining K and OI, including two regression methods and two PRF methods, using the experimental data from the literature. Although all four methods produced consistent results of K, the PRF methods that match the knock resistance of the test fuel with a PRF were more rigorous and yielded the most accurate results. The regression methods, on the other hand, required a pre-defined relationship between OI and knock-limited engine performance (i.e. KLSA) and specially formulated fuel sets of uncorrelated RON and MON in order to work. Given the accuracy and simplicity of the fuel requirement, the PRF method via direct comparison was deemed to be the most suitable method for the experimental measurement of OI and K. This work then developed a novel fuel blending system to use this method to determine K over a wide range of engine operating conditions. This was an important contribution to the methodology of fuel octane research.

K maps of a modern, production GTDI engine.

Conclusions and Recommendations for Future Study

This work comprehensively determined K values over the operation map of a 4-cylinder 2L production engine representing modern SI engine technologies. This work covered nearly all conditions where the engine operation could be potentially knock-limited, substantially expanding the previous efforts where only high-load conditions were studied. A decreasing trend of K with increasing load was observed throughout the conditions studied. The effect of other engine operation parameters on K, such as engine speed and charge temperature, were less consistent, partially because the engine was controlled with the factory ECU settings instead of varying one parameter a time. The obtained K-maps are therefore more realistic in terms of practical engine operation.

With the large dataset of K, this work further investigated the correlation between K and end-gas states in the 2L GTDI engine and a CFR engine. It was found that K correlated strongly with the cylinder pressure at the spark timing since this was the initial pressure of the flame compression which later triggered autoignition. K correlated even more closely with the end gas temperature at later stage of combustion, i.e. CA60 – CA80 where autoignition was primarily driven by temperature. These findings suggested that K is physically meaningful as it is strongly correlated to the state of the end-gas.

The significance of a fuel's RON and MON to drive cycle fuel efficiency in conventional, hybrid and plug-in hybrid powertrains.

This work finally investigated the significance of RON and MON to knock-limited, fuel efficiency loss over several drive cycles. The investigation was conducted using the determined K-maps and considering the engine used in different powertrain configurations. The results showed that a conventional vehicle was not knock-limited on the UDDS and HWFET cycles, but it was more knock-limited on the US06 cycle and Davis Dam towing tests where the driving conditions were more aggressive. The HEV and PHEV64 were noticeably more knock-limited across all drive cycles, as the engine operation was shifted to knock-prone high load and low speed conditions. Although there was significant drive cycle time and fuel consumption at conditions of positive K, the KLFEL mostly occurred at negative K conditions, and this trend was more obvious for the HEV and PHEV64. The analysis showed that increasing the RON of the gasoline reduced KLFEL for all powertrains in all drive cycles. But decreasing the MON had only a minor promoting or no effect on KLFEL for most drive cycles. The effect of RON on KLFEL was much stronger for the HEV and PHEV than for the conventional vehicle, as the KLFEL-weighted K was more negative for HEV and PHEV. Given the significant fuel

consumption and time occurring at the knock-limited conditions of positive K and the moderate effect of decreasing MON on fuel efficiency improvement, it was suggested that increasing RON without aggressively decreasing MON be an optimal solution to improving the fuel efficiency of future SI engines.

7.2 Recommendations

7.2.1 *Effect of fuel composition on K*

The K values were measured using a single certification gasoline (91.6 RON) in this work. Although the OI model has been found to be a good indicator of fuels' knock resistance, the model assumes that K is independent of fuel properties, which has not been proven. Most studies on this topic used the regression methods to determine OI and K with a series of fuels of uncorrelated RON and MON. Such a methodology relies on the assumption that fuel properties are independent of K. The K measurement method developed in this work could be used to test this assumption by using several different sensitive fuels, and in particular, a set of fuels with the same RON and MON, but different composition (i.e. variation of aromatics, olefins, paraffins, etc.). This would enable a rigorous determination of the fundamental role of fuel properties in the OI model.

7.2.2 *Octane Index Model and Detailed Chemical Kinetics*

The current study modelled end-gas conditions using GT-Power that did not incorporate the chemical kinetics of the fuel. The end-gas thermodynamic state and chemical kinetics are strongly coupled. For example, the LTHR may start during the flame-induced compression under boosted conditions. However, the amplitude of LTHR is small compared with the HRR of the premixed flame, making itself undetectable from the in-cylinder pressure trace. Recent studies [50, 53-55, 59, 89] have found some connections between LTHR and K. A comprehensive study on this topic has not been performed in literature. A future topic of interest, therefore, is to calculate the end-gas condition with experimental data using the method similar to ref.[121] and exploring the fundamental relationship between end-gas conditions and K values. It should be noted that the fuels used for this experiment should be those having the available chemical mechanisms validated for engine conditions.

7.2.3 Relationship between Octane Index on Knock-Limited Engine Performance

It is well established that fuels of higher OI have stronger knock resistance. However, the functional form of the relationship between OI and the knock-limited performance is not clear. The correlation used in the present study (Figure 6-23) was based on a simple linear relation with the limited data available. A more accurate function for describing this relationship will enable more accurate quantification of how the knock limit affects engine performance and fuel efficiency. This work can be done by benchmarking the knock-limited performance of a series of PRFs ranging from low octane number to high octane number.

7.2.4 Significance of RON and MON for High Compression Ratio Engines

The engine used in this study has the compression ratio of 9.3:1, which is relatively low compared to newer engines in the market. The results in Section 4.3.2.4 of this study showed K was insensitive to the compression ratio, but the threshold of knock-limited operation could be different should the compression ratio change. At a given BMEP and RPM, the CA50 at trace knock will be more retarded when compression ratio is higher, therefore a condition that is not knock-limited for a lower compression ratio can become knock-limited for the engine of higher compression ratio. The most positive K values measured at part-load in this study were not knock-limited (Section 5.2), but those K values will become knock-limited if an engine of higher compression ratio is used. This would shift the KLFEL-based distribution of K and the impact of the RON and MON on drive cycle fuel efficiency loss due to knock would also be affected. An interesting future study would repeat much of the methodology used in this thesis on a higher compression ratio engine by mapping K and quantifying KLFEL using vehicle analysis.

A. References

- [1] B.E. Economics, BP Energy Outlook 2018 Edition, 2018.
- [2] T. Johnson, A. Joshi, Review of Vehicle Engine Efficiency and Emissions, SAE International, 2018.
- [3] G. Kalghatgi, Is it really the end of internal combustion engines and petroleum in transport?, *Applied Energy* 225 (2018) 965-974.
- [4] P. Najt, A Pragmatic Approach to Reducing the CO₂ Footprint of The Internal Combustion Engine, 2017.
- [5] E. Kasseris, J.B. Heywood, Charge Cooling Effects on Knock Limits in SI DI Engines Using Gasoline/Ethanol Blends: Part 1-Quantifying Charge Cooling, SAE International, 2012.
- [6] J.B. Heywood, *Internal Combustion Engine Fundamentals*, McGraw-Hill, New York, 1988.
- [7] C.D. Miller, Roles of Detonation Waves and Autoignition in Spark - Ignition Engine Knock as Shown by Photographs Taken at 40,000 and 200,000 Frames Per Sec, SAE International, 1947.
- [8] M.J. Pilling, *Low-temperature combustion and autoignition*, Elsevier 1997.
- [9] I. Glassman, R.A. Yetter, N.G. Glumac, *Combustion* (Fifth Edition), in: I.G.A.Y.G. Glumac (Ed.), *Combustion* (Fifth Edition), Academic Press, Boston, 2015, pp. xv.
- [10] J.F. Griffiths, C. Mohamed, Chapter 6 Experimental and numerical studies of oxidation chemistry and spontaneous ignition phenomena, in: M.J. Pilling (Ed.), *Comprehensive Chemical Kinetics*, Elsevier 1997, pp. 545-660.
- [11] C.K. Westbrook, Chemical kinetics of hydrocarbon ignition in practical combustion systems, *Proceedings of the Combustion Institute* 28 (2000) 1563-1577.
- [12] R.J. Nates, A.D.B. Yates, Knock Damage Mechanisms in Spark-Ignition Engines, SAE International, 1994.
- [13] J. Fitton, R. Nates, Knock Erosion in Spark-Ignition Engines, SAE International, 1996.
- [14] D. Bradley, C. Morley, Chapter 7 Autoignition in spark-ignition engines, in: M.J. Pilling (Ed.), *Comprehensive Chemical Kinetics*, Elsevier 1997, pp. 661-760.
- [15] R.C. Costa, J.R. Sodré, Compression ratio effects on an ethanol/gasoline fuelled engine performance, *Applied Thermal Engineering* 31 (2011) 278-283.
- [16] S.M. Shahed, K.-H. Bauer, Parametric Studies of the Impact of Turbocharging on Gasoline Engine Downsizing, doi:10.4271/2009-01-1472(2009).
- [17] A. Hula, A. Bunker, A. Maguire, J. Alson, Light-Duty Automotive Technology, Carbon Dioxide Emissions, and Fuel Economy Trends: 1975 Through 2017, 2017.
- [18] F.A. Ayala, M.D. Gerty, J.B. Heywood, Effects of Combustion Phasing, Relative Air-fuel Ratio, Compression Ratio, and Load on SI Engine Efficiency, SAE International, 2006.
- [19] T.G. Leone, J.E. Anderson, R.S. Davis, A. Iqbal, R.A. Reese, M.H. Shelby, W.M. Studzinski, The Effect of Compression Ratio, Fuel Octane Rating, and Ethanol Content on Spark-Ignition Engine Efficiency, *Environmental Science & Technology* 49 (2015) 10778-10789.
- [20] H.H. Jung, T.G. Leone, M.H. Shelby, J.E. Anderson, T. Collings, Fuel Economy and CO₂ Emissions of Ethanol-Gasoline Blends in a Turbocharged DI Engine, *SAE Int. J. Engines* 6 (2013) 422-434.
- [21] F.L. Dryer, Chemical kinetic and combustion characteristics of transportation fuels, *Proceedings of the Combustion Institute* 35 (2015) 117-144.
- [22] G. Kalghatgi, *Fuel/Engine Interactions*, SAE International 2013.
- [23] Standard Test Method for Research Octane Number of Spark-Ignition Engine Fuel, ASTM International, West Conshohocken, PA, 2011.
- [24] Standard Test Method for Motor Octane Number of Spark-Ignition Engine Fuel, ASTM International, West Conshohocken, PA, 2011.
- [25] V. Mittal, J.B. Heywood, W.H. Green, The Underlying Physics and Chemistry behind Fuel Sensitivity, *SAE Int. J. Fuels Lubr.* 3 (2010) 256-265.

References

- [26] A. Prakash, C. Wang, A. Janssen, A. Aradi, R. Cracknell, Impact of Fuel Sensitivity (RON-MON) on Engine Efficiency, (2017).
- [27] W.R. Leppard, The chemical origin of fuel octane sensitivity, SAE Technical Paper, 1990.
- [28] M. Mehl, T. Faravelli, F. Giavazzi, E. Ranzi, P. Scorletti, A. Tardani, D. Terna, Detailed Chemistry Promotes Understanding of Octane Numbers and Gasoline Sensitivity, *Energy & Fuels* 20 (2006) 2391-2398.
- [29] C.K. Westbrook, M. Mehl, W.J. Pitz, M. Sjöberg, Chemical kinetics of octane sensitivity in a spark-ignition engine, *Combustion and Flame* 175 (2017) 2-15.
- [30] T.M. Foong, K.J. Morganti, M.J. Brear, G. da Silva, Y. Yang, F.L. Dryer, The Effect of Charge Cooling on the RON of Ethanol/Gasoline Blends, *SAE Int. J. Fuels Lubr.* 6 (2013) 34-43.
- [31] C.S. Sluder, J.P. Szybist, R.L. McCormick, M.A. Ratcliff, B.T. Zigler, Exploring the Relationship Between Octane Sensitivity and Heat-of-Vaporization, *SAE Int. J. Fuels Lubr.* 9 (2016) 80-90.
- [32] C.S. Sluder, Estimation of the Fuel Efficiency Potential of Six Gasoline Blendstocks Identified by the U.S. Department of Energy's Co-Optimization of Fuels and Engines Program, SAE International, 2019.
- [33] D. Bradley, C. Morley, H.L. Walmsley, Relevance of Research and Motor Octane Numbers to the Prediction of Engine Autoignition, SAE International, 2004.
- [34] T. Davies, R. Cracknell, G. Lovett, L. Cruff, J. Fowler, Fuel Effects in a Boosted DISI Engine, SAE International, 2011.
- [35] A. Prakash, R. Cracknell, V. Natarajan, D. Doyle, A. Jones, Y.S. Jo, M. Hinojosa, P. Lobato, Understanding the Octane Appetite of Modern Vehicles, *SAE Int. J. Fuels Lubr.* 9 (2016).
- [36] G.T. Kalghatgi, Fuel Anti-Knock Quality- Part II. Vehicle Studies - How Relevant is Motor Octane Number (MON) in Modern Engines?, SAE International, 2001.
- [37] G.T. Kalghatgi, Fuel Anti-Knock Quality - Part I. Engine Studies, SAE International, 2001.
- [38] G.T. Kalghatgi, Auto-Ignition Quality of Practical Fuels and Implications for Fuel Requirements of Future SI and HCCI Engines, SAE International, 2005.
- [39] G.T. Kalghatgi, K. Nakata, K. Mogi, Octane Appetite Studies in Direct Injection Spark Ignition (DISI) Engines, SAE International, 2005.
- [40] V. Mittal, J.B. Heywood, The Relevance of Fuel RON and MON to Knock Onset in Modern SI Engines, SAE International, 2008.
- [41] A. Amer, H. Babiker, J. Chang, G. Kalghatgi, P. Adomeit, A. Brassat, M. Günther, Fuel Effects on Knock in a Highly Boosted Direct Injection Spark Ignition Engine, *SAE International Journal of Fuels and Lubricants* 5 (2012) 1048-1065.
- [42] C.N. Orlebar, A. Joedicke, W. Studzinski, The Effects of Octane, Sensitivity and K on the Performance and Fuel Economy of a Direct Injection Spark Ignition Vehicle, SAE International, 2014.
- [43] S. Remmert, S. Campbell, R. Cracknell, A. Schuetze, A. Lewis, K. Giles, S. Akehurst, J. Turner, A. Popplewell, R. Patel, Octane Appetite: The Relevance of a Lower Limit to the MON Specification in a Downsized, Highly Boosted DISI Engine, *SAE Int. J. Fuels Lubr.* 7 (2014) 743-755.
- [44] J.W.G. Turner, A. Popplewell, R. Patel, T.R. Johnson, N.J. Darnton, S. Richardson, S.W. Bredda, R.J. Tudor, C.I. Bithell, R. Jackson, S.M. Remmert, R.F. Cracknell, J.X. Fernandes, A.G.J. Lewis, S. Akehurst, C.J. Brace, C. Copeland, R. Martinez-Botas, A. Romagnoli, A.A. Burluka, Ultra Boost for Economy: Extending the Limits of Extreme Engine Downsizing, *SAE Int. J. Engines* 7 (2014) 387-417.
- [45] Y.S. Jo, L. Bromberg, J. Heywood, Octane Requirement of a Turbocharged Spark Ignition Engine in Various Driving Cycles, SAE International, 2016.
- [46] C. Wang, A. Prakash, A. Aradi, R. Cracknell, H. Xu, Significance of RON and MON to a modern DISI engine, *Fuel* 209 (2017) 172-183.
- [47] T.J. Davies, R.F. Cracknell, B. Head, K. Hobbs, T. Riley, A new method to simulate the octane appetite of any spark ignition engine, SAE International, 2011.
- [48] J.C. Livengood, P.C. Wu, Correlation of autoignition phenomena in internal combustion engines and rapid compression machines, *Symposium (International) on Combustion* 5 (1955) 347-356.
- [49] Z. Zhou, Y. Yang, M. Brear, J. Lacey, T.G. Leone, J.E. Anderson, M.H. Shelby, A Comparison of Four Methods for Determining the Octane Index and K on a Modern Engine with Upstream, Port or Direct Injection, SAE International, 2017.
- [50] M. Kassai, C. Aksu, T. Shiraishi, R. Cracknell, M. Shibuya, Mechanism Analysis on the Effect of Fuel Properties on Knocking Performance at Boosted Conditions, SAE International, 2019.

References

- [51] M.D. Gerty, J.B. Heywood, An Investigation of Gasoline Engine Knock Limited Performance and the Effects of Hydrogen Enhancement, SAE International, 2006.
- [52] G.T. Kalghatgi, R.A. Head, The Available and Required Autoignition Quality of Gasoline - Like Fuels in HCCI Engines at High Temperatures, SAE International, 2004.
- [53] J.P. Szybist, D.A. Splitter, Understanding chemistry-specific fuel differences at a constant RON in a boosted SI engine, *Fuel* 217 (2018) 370-381.
- [54] J.P. Szybist, D.A. Splitter, Pressure and temperature effects on fuels with varying octane sensitivity at high load in SI engines, *Combustion and Flame* 177 (2017) 49-66.
- [55] D. Vuilleumier, M. Sjöberg, Significance of RON, MON, and LTHR for Knock Limits of Compositionally Dissimilar Gasoline Fuels in a DISI Engine, (2017).
- [56] D. Vuilleumier, X. Huan, T. Casey, M. Sjöberg, Uncertainty Assessment of Octane Index Framework for Stoichiometric Knock Limits of Co-Optima Gasoline Fuel Blends, SAE International, 2018.
- [57] E.P. Kasseris, J.B. Heywood, Comparative Analysis of Automotive Powertrain Choices for the Next 25 Years, SAE International, 2007.
- [58] L. Lemazurier, N. Shidore, N. Kim, A. Moawad, A. Rousseau, P. Bonkoski, J. Delhom, Impact of Advanced Engine and Powertrain Technologies on Engine Operation and Fuel Consumption for Future Vehicles, SAE International, 2015.
- [59] K.P. Somers, R.F. Cracknell, H.J. Curran, A chemical kinetic interpretation of the octane appetite of modern gasoline engines, *Proceedings of the Combustion Institute* 37 (2019) 4857-4864.
- [60] A. Emadi, *Advanced electric drive vehicles*, Boca Raton : CRC Press, [2015]2015.
- [61] M. Kuypers, Application of 48 Volt for Mild Hybrid Vehicles and High Power Loads, SAE International, 2014.
- [62] A. Moawad, A. Rousseau, Impact of Electric Drive Vehicle Technologies on Fuel Efficiency to Support 2017-2025 CAFE Regulations, *SAE International Journal of Alternative Powertrains* 3 (2014) 163-175.
- [63] M. Ehsani, G. Yimin, K.L. Butler, Application of electrically peaking hybrid (ELPH) propulsion system to a full-size passenger car with simulated design verification, *IEEE Transactions on Vehicular Technology* 48 (1999) 1779-1787.
- [64] Downloadable Dynamometer Database Advanced Mobility Technology Laboratory (AMTL) at Argonne National Laboratory
- [65] M. Ehsani, Y. Gao, J.M. Miller, Hybrid Electric Vehicles: Architecture and Motor Drives, *Proceedings of the IEEE* 95 (2007) 719-728.
- [66]
- N. Jalil, N.A. Kheir, M. Salman. A rule-based energy management strategy for a series hybrid vehicle. In: editor^editors. *Proceedings of the 1997 American Control Conference* (Cat. No.97CH36041); 6-6 June 1997 1997. p. 689-693 vol.681.
- [67] G. Pistoia, 22. Automakers' Powertrain Options for Hybrid and Electric Vehicles, *Electric and Hybrid Vehicles - Power Sources, Models, Sustainability, Infrastructure and the Market*, Elsevier.
- [68] M. Menne, J. Reinert, R. De Doncker, Energy-efficiency evaluation of traction drives for electric vehicles, *EVS-15*, (1998).
- [69] O. Bitsche, G. Gutmann, Systems for hybrid cars, *Journal of Power Sources* 127 (2004) 8-15.
- [70] A. Emadi, K. Rajashekara, S.S. Williamson, S.M. Lukic, Topological overview of hybrid electric and fuel cell vehicular power system architectures and configurations, *IEEE Transactions on Vehicular Technology* 54 (2005) 763-770.
- [71] J. German, Hybrid vehicles: Technology development and cost reduction, *ICCT technical Brief*, (2015).
- [72] A. Nagasaka, M. Nada, H. Hamada, S. Hiramatsu, Y. Kikuchi, H. Kato, Development of the Hybrid/Battery ECU for the Toyota Hybrid System, SAE International, 1998.
- [73] J. Kapadia, D. Kok, M. Jennings, M. Kuang, B. Masterson, R. Isaacs, A. Dona, C. Wagner, T. Gee, Powersplit or Parallel - Selecting the Right Hybrid Architecture, doi:10.4271/2017-01-1154(2017).
- [74] S. Delprat, J. Lauber, T.M. Guerra, J. Rimaux, Control of a parallel hybrid powertrain: optimal control, *IEEE Transactions on Vehicular Technology* 53 (2004) 872-881.

References

- [75] C. Cubito, L. Rolando, F. Millo, B. Ciuffo, S. Serra, G. Trentadue, M. Garcia Otura, G. Fontaras, Energy Management Analysis under Different Operating Modes for a Euro-6 Plug-in Hybrid Passenger Car, SAE International, 2017.
- [76] G.T. Inc., GT-SUITE 2018 Software Package. www.gtisoft.com.
- [77] A.N. Lab, Autonomie. <https://www.autonomie.net/expertise/Autonomie.html>.
- [78] T. Feese, C.L. Hill. Prevention Of Torsional Vibration Problems In Reciprocating Machinery. In: editor^editors. Proceedings of the 38th turbomachinery symposium; 2009: Texas A&M University. Turbomachinery Laboratories. p.
- [79] J. Yi, S. Wooldridge, G. Coulson, J. Hilditch, C.O. Iyer, P. Moilanen, G. Papaioannou, D. Reiche, M. Shelby, B. VanDerWege, C. Weaver, Z. Xu, G. Davis, B. Hinds, A. Schamel, Development and Optimization of the Ford 3.5L V6 EcoBoost Combustion System, SAE International Journal of Engines 2 (2009) 1388-1407.
- [80] F. Millo, C.V. Ferraro, Knock in S.I. Engines: A Comparison between Different Techniques for Detection and Control, SAE International, 1998.
- [81] C.S. Draper, Pressure waves accompanying detonation in the internal combustion engine, Journal of the Aeronautical Sciences 5 (1938) 219-226.
- [82] A.J. Shahlari, J. Ghandhi, Pressure-Based Knock Measurement Issues, SAE International, 2017.
- [83] K. Takeda, S. Takashi, Y. Yoshida, Z. Lin, A. Iijima, H. Shoji, A Study on the Knocking Characteristics of an SI-HCCI Engine by Using In-Cylinder Visualization, SAE International, 2016.
- [84] V. De Bellis, L. Teodosio, D. Siano, F. Minarelli, D. Cacciatore, Knock and Cycle by Cycle Analysis of a High Performance V12 Spark Ignition Engine. Part 1: Experimental Data and Correlations Assessment, SAE International Journal of Engines, SAE International, 2015, pp. 1993-2001.
- [85] K. Reif, Gasoline engine management : systems and components, Wiesbaden : Springer Gabler, 2014.2014.
- [86] J.S. Chickos, W.E. Acree Jr, Enthalpies of vaporization of organic and organometallic compounds, 1880–2002, Journal of Physical and Chemical Reference Data 32 (2003) 519-878.
- [87] T.G. Leone, E.D. Olin, J.E. Anderson, H.H. Jung, M.H. Shelby, R.A. Stein, Effects of Fuel Octane Rating and Ethanol Content on Knock, Fuel Economy, and CO₂ for a Turbocharged DI Engine, SAE Int. J. Fuels Lubr. 7 (2014) 9-28.
- [88] Performance Requirements for Determining Tow-Vehicle Gross Combination Weight Rating and Trailer Weight Rating, SAE International, 2016.
- [89] R.F. Cracknell, A. Prakash, K.P. Somers, C. Wang, Impact of Detailed Fuel Chemistry on Knocking Behaviour in Engines, in: M. Günther, M. Sens (Eds.), Knocking in Gasoline Engines: 5th International Conference, December 12-13, 2017, Berlin, Germany, Springer International Publishing, Cham, 2018, pp. 245-254.
- [90] R.A. Stein, D. Polovina, K. Roth, M. Foster, M. Lynskey, T. Whiting, J.E. Anderson, M.H. Shelby, T.G. Leone, S. VanderGriend, Effect of Heat of Vaporization, Chemical Octane, and Sensitivity on Knock Limit for Ethanol - Gasoline Blends, SAE Int. J. Fuels Lubr. 5 (2012) 823-843.
- [91] S. Mamikoglu, J. Andric, P. Dahlander, Impact of Conventional and Electrified Powertrains on Fuel Economy in Various Driving Cycles, SAE International, 2017.
- [92] G.M. Rassweiler, L. Withrow, Motion Pictures of Engine Flames Correlated with Pressure Cards, SAE International, 1938.
- [93] S. Cheng, Y. Yang, M.J. Brear, M. Frenklach, Quantifying uncertainty in kinetic simulation of engine autoignition, Combustion and Flame 216 (2020) 174-184.
- [94] S. Halbach, P. Sharer, S. Pagerit, A.P. Rousseau, C. Folkerts, Model Architecture, Methods, and Interfaces for Efficient Math-Based Design and Simulation of Automotive Control Systems, SAE International, 2010.
- [95] N. Kim, A. Rousseau, H. Lohse-Busch, Advanced Automatic Transmission Model Validation Using Dynamometer Test Data, SAE International, 2014.
- [96] J.E. Anderson, T.G. Leone, M.H. Shelby, T.J. Wallington, J.J. Bizub, M. Foster, M.G. Lynskey, D. Polovina, Octane Numbers of Ethanol-Gasoline Blends: Measurements and Novel Estimation Method from Molar Composition, SAE International, 2012.

References

- [97] V. Mittal, J.B. Heywood, The Shift in Relevance of Fuel RON and MON to Knock Onset in Modern SI Engines Over the Last 70 Years, *SAE Int. J. Engines* 2 (2009) 1-10.
- [98] T. Han, G. Lavoie, M. Wooldridge, A. Boehman, Dual Fuel Injection (DI + PFI) for Knock and EGR Dilution Limit Extension in a Boosted SI Engine, *SAE International*, 2018.
- [99] A. Joshi, Review of Vehicle Engine Efficiency and Emissions, *SAE International*, 2020.
- [100] I.Z. Syed, A. Mukherjee, J. Naber, Numerical Simulation of Autoignition of Gasoline-Ethanol/Air Mixtures under Different Conditions of Pressure, Temperature, Dilution, and Equivalence Ratio, *SAE International*, 2011.
- [101] Y. Chen, R. Raine, A study on the influence of burning rate on engine knock from empirical data and simulation, *Combustion and Flame* 162 (2015) 2108-2118.
- [102] M. Rothe, T. Heidenreich, U. Spicher, A. Schubert, Knock Behavior of SI-Engines: Thermodynamic Analysis of Knock Onset Locations and Knock Intensities, *SAE Transactions* 115 (2006) 165-176.
- [103] G. Xiaofeng, R. Stone, C. Hudson, I. Bradbury, The Detection and Quantification of Knock in Spark Ignition Engines, *SAE International*, 1993.
- [104] R. Cracknell, M. Kassai, T. Shiraishi, A. Festa, S. Gail, A. Aradi, M. Shibuya, Is the "K Value" of an Engine Truly Fuel Independent?, *SAE International*, 2020.
- [105] S. Gopujkar, J. Worm, J. Duncan, W. Hansley, Determination of Octane Index and K in a 2.0L, 4-Cylinder Turbocharged SI Engine Using the Primary Reference Fuel (PRF) Method, *SAE International*, 2020.
- [106] F. Battin-Leclerc, Detailed chemical kinetic models for the low-temperature combustion of hydrocarbons with application to gasoline and diesel fuel surrogates, *Progress in Energy and Combustion Science* 34 (2008) 440-498.
- [107] J.E. Dec, Y. Yang, Boosted HCCI for High Power without Engine Knock and with Ultra-Low NO_x Emissions - using Conventional Gasoline, *SAE Int. J. Engines* 3 (2010) 750-767.
- [108] M. Mehl, W. Pitz, M. Sarathy, Y. Yang, J.E. Dec, Detailed Kinetic Modeling of Conventional Gasoline at Highly Boosted Conditions and the Associated Intermediate Temperature Heat Release, *SAE International*, 2012.
- [109] G. Kalghatgi, P. Risberg, H.-E. Ångström, A Method of Defining Ignition Quality of Fuels in HCCI Engines, *SAE International*, 2003.
- [110] Y. Yang, J.E. Dec, M. Sjöberg, C. Ji, Understanding fuel anti-knock performances in modern SI engines using fundamental HCCI experiments, *Combustion and Flame* 162 (2015) 4008-4015.
- [111] H.J. Curran, P. Gaffuri, W.J. Pitz, C.K. Westbrook, A Comprehensive Modeling Study of n-Heptane Oxidation, *Combustion and Flame* 114 (1998) 149-177.
- [112] H.J. Curran, P. Gaffuri, W.J. Pitz, C.K. Westbrook, A comprehensive modeling study of iso-octane oxidation, *Combustion and Flame* 129 (2002) 253-280.
- [113] automobile-catalog, Ford Edge 2.0L EcoBoost FWD (aut. 8) (2019) full detailed specifications listing and photo gallery. https://www.automobile-catalog.com/auta_details1.php.
- [114] A. Moawad, N. Kim, N. Shidore, A. Rousseau, Assessment of vehicle sizing, energy consumption and cost through large scale simulation of advanced vehicle technologies, Argonne National Lab.(ANL), Argonne, IL (United States), 2016.
- [115] N.R. Council, Transitions to Alternative Transportation Technologies—" Plug-in Hybrid Electric Vehicles, National Academies Press 2010.
- [116] Z.J. Sroka, M.J.J.o.K. Cieślak, An impact of engine downsizing on change of engine weight, 22 (2015).
- [117] V. Freyermuth, E. Fallas, A. Rousseau, Comparison of Powertrain Configuration for Plug-in HEVs from a Fuel Economy Perspective, *SAE International Journal of Engines* 1 (2008) 392-398.
- [118] Recommended Practice for Measuring the Exhaust Emissions and Fuel Economy of Hybrid-Electric Vehicles, Including Plug-in Hybrid Vehicles, *SAE International*, 2010.
- [119] P. Sharer, A. Rousseau, S. Pagerit, P. Nelson, Midsize and SUV Vehicle Simulation Results for Plug-In HEV Component Requirements, *SAE International*, 2007.
- [120] P. Smith, J. Heywood, W. Cheng, Effects of Compression Ratio on Spark-Ignited Engine Efficiency, *SAE International*, 2014.

References

[121] T.M. Foong, M.J. Brear, K.J. Morganti, G. da Silva, Y. Yang, F.L. Dryer, Modeling End-Gas Autoignition of Ethanol/Gasoline Surrogate Blends in the Cooperative Fuel Research Engine, *Energy & Fuels*, doi:10.1021/acs.energyfuels.6b02380(2016).

B. Appendix

B.1. Interpolation Methods

When generating the K-maps and calculating the K values for a drive cycle, the interpolation of K was needed as K values were measured at the scattered conditions. The interpolation was conducted with the respect of RPM and BMEP. Four common interpolation methods were investigated, including linear interpolation, cubic spline, thin-plate harmonic (TPH) spline and biharmonic spline. The effect of the interpolation method on the distribution of K is demonstrated by Figure 7-1 and Figure 7-2. The distribution in Figure 7-1 is for all conditions that can be covered by the K-map (including some over-advanced conditions) while Figure 7-2 is only for the knock-limited conditions. The difference caused by the interpolation method is noticeable for the positive K region especially for $K=0.4 \sim 0.8$. This difference is not significant for the knock-limited case as most positive K are not for knock-limited conditions. In the present study, the distributions are only for the knock-limited conditions, so using different interpolation methods does not cause much difference in the results.

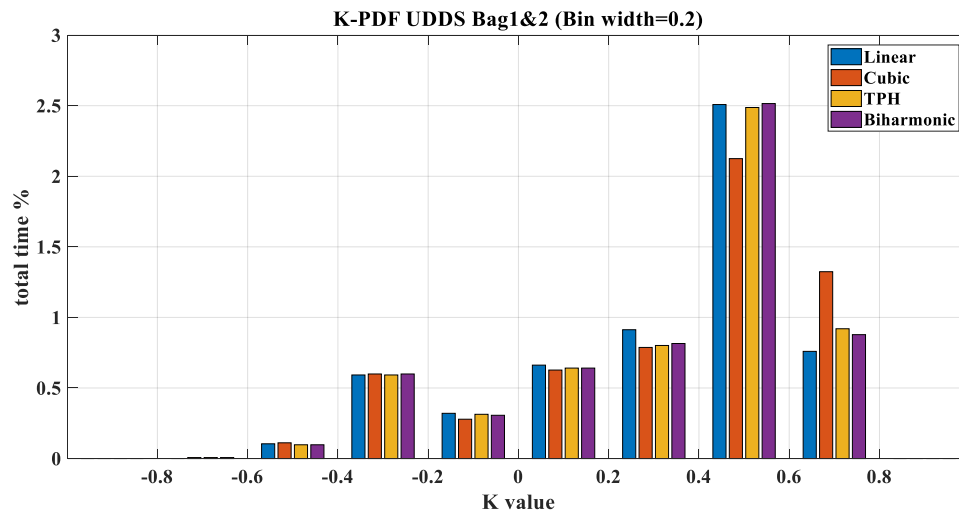


Figure 7-1 The effect of interpolation method on the distribution of K including both over-advanced and knock-limited conditions.

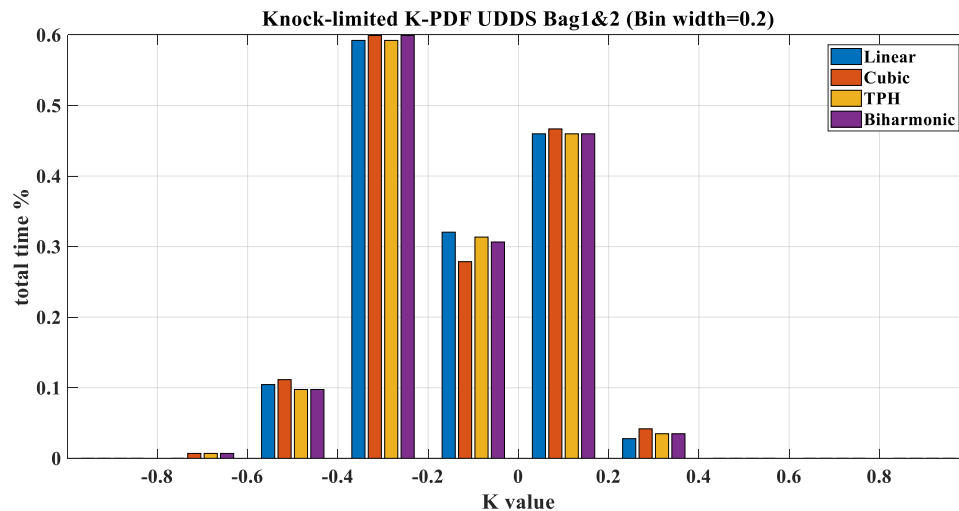


Figure 7-2 The effect of interpolation method on the distribution of K including only knock-limited conditions.

However, to make the results more accurate, these methods were compared in more details. The interpolated K values using different methods for load sweep at several engine speeds are shown by Figure 7-3. The biharmonic method is not included as it always produces the same method as the TPH. As can be seen, at 1250 RPM and 2000 RPM, three methods produce identical results, and this is the case for most conditions as well. But at 1500 RPM and 3000 RPM, a small hook appears at low-load condition for the linear and cubic methods, which means K increases with engine load. This is not sensible as K should be decreasing with engine load at a given engine speed. Due to this difference, only the TPH method was used for the interpolation of K, although the effect of interpolation method on the knock-limited K distribution is rather weak.

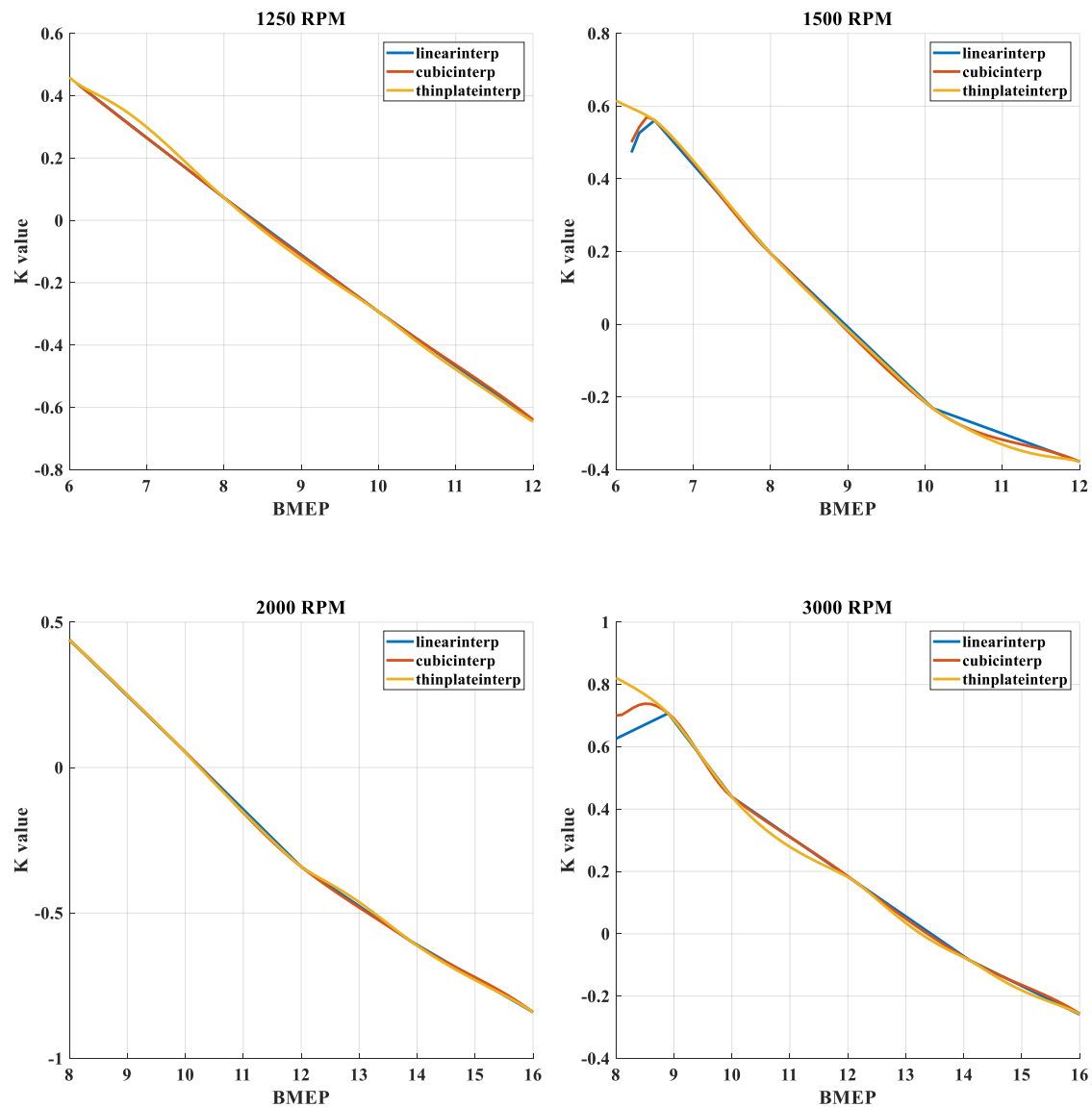


Figure 7-3 The comparison of interpolation methods at several different conditions.

B.2. Determination of Knock-Limited Fuel Efficiency Loss

Assumption:

At a given CA50 and given NMEP, within a small change in lambda, fuel consumption is inverse of lambda. This is confirmed with the GT-Power simulation of lambda sweep at various engine operating conditions at the constant CA50 and engine load (Figure 7-4).

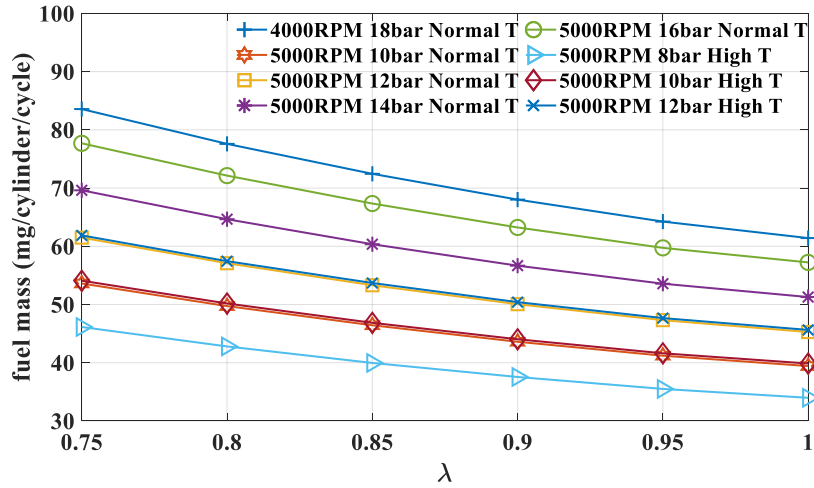


Figure 7-4 The simulated fuel consumption for lambda sweep at constant CA50=MBT and constant load.

Definitions and denotations:

$\eta_x = 1 - 0.168 \left[\sqrt{(1 + 4.443 \cdot 10^{-3} \cdot x^2)} - 1 \right]$ is the correlation developed in [18] and is used to characterize the effect of CA50 retard on the fuel efficiency relative to that at $CA50_{MBT}$.

$x = CA50 - CA50_{MBT}$ is the CA50 retarded from $CA50_{MBT}$.

λ is the exhaust lambda at the test condition.

λ_{req} is the maximum lambda required to lower exhaust temperature below 900°C at MBT CA50 condition.

$\dot{m}_{rtd}$ is the fuel flow rate at a condition with CA50 retarded from $CA50_{MBT}$.

$\dot{m}_{MBT}$ is the fuel flow rate at a condition with $CA50=CA50_{MBT}$.

Deviation:

At a given lambda λ , the relation between fuel flow consumption rates at retarded CA50 and that at MBT CA50 can be expressed by Eq. 7-1.

$$\dot{m}_{rtd} \cdot \eta_x = \dot{m}_{MBT} \quad \text{Eq. 7-1}$$

Based on the assumption, at a given CA50, the relation between fuel flow rates at different enrichment is given by Eq. 7-2.

Appendix

$$\dot{m}_1 \cdot \lambda_1 = \dot{m}_2 \cdot \lambda_2 \quad \text{Eq. 7-2}$$

At a given engine output (IMEP), the optimal fuel consumption rate is achieved with $CA50=CA50_{MBT}$ and λ_{req} , and with Eq. 7-2 it can be expressed by Eq. 7-3.

$$\dot{m}_{opt} \cdot \lambda_{req} = \dot{m}_{MBT} \cdot \lambda \quad \text{Eq. 7-3}$$

Combining Eq. 7-1 and Eq. 7-3, the optimal fuel consumption rate can be expressed by Eq. 7-4.

$$\dot{m}_{opt} = \dot{m}_{rtd} \cdot \eta_x \cdot \frac{\lambda}{\lambda_{req}} \quad \text{Eq. 7-4}$$

The knock-limited fuel loss is defined as the difference between actual fuel flow rate at a knock-limited condition and the optimal fuel flow rate at a knock-free condition, and is given by Eq. 7-5

$$\dot{m}_{loss} = \dot{m}_{rtd} - \dot{m}_{opt} = \dot{m}_{rtd} \cdot \left(1 - \eta_x \cdot \frac{\lambda}{\lambda_{req}}\right) \quad \text{Eq. 7-5}$$

Therefore, for any engine operating condition, the knock-limited fuel efficiency loss (KLFEL) can be expressed as Eq. 7-6.

$$KLFEL = 1 - \eta_x \cdot \frac{\lambda}{\lambda_{req}} \quad \text{Eq. 7-6}$$

C. Abbreviations

AER	All electric range
aBDC	After bottom dead center
AKI	Anti-knock index
aTDC	After top dead center
bBDC	Before bottom dead center
BEV	Battery electric vehicle
BISG	Belt integrated starter generator
BMEP	Brake mean effective pressure
BP	Backpressure
bTDC	Before top dead center
BTE	Brake thermal efficiency
CA	Crank angle
CA50	Crank angle at 50% of the total heat release
CAD	Crank angle degree
CAFE	Corporate Average Fuel Economy
CD	Charge-depleting
CFR	Cooperative fuel research
CISG	Crank integrated starter-generator
CR	Compression ratio
CS	Charge-sustaining
CVT	Continuously variable transmission
DCT	Dual clutch transmission
DI	Direct injection
DISI	Direct-injection spark-ignition
EGM	Electric motor/generator
EPA	Environmental protection agency
ESS	Energy storage system
EVC	Intake valve closing
EVO	Exhaust valve opening
FC	Fuel consumption
FCV	Fuel cell vehicle
FE	Fuel economy
FMEP	Friction mean effective pressure
GCWR	Gross Combination Weight Rating
GIMEP	Gross indicated mean effective pressure
GTDI	Gasoline turbocharged direct-injection engine
HEV	Hybrid electric vehicle
HoV	Heat of vaporization
HWFET	Highway Fuel Economy Test
IAT	Intake air temperature
ICE	Internal combustion engine

Abbreviations

IMEP	Indicated mean effective pressure
ISFC	Indicated specific fuel consumption
ITHR	Intermediate-temperature heat release
IVC	Intake valve closing
IVO	Intake valve opening
KLFEL	Knock-limited fuel efficiency loss
KLSA	Knock-limited spark advance
kph	kms per hour
LDV	Light-duty vehicle
LTHR	Low-temperature heat release
LUT	Look-up table
MAP	manifold air pressure
MBT	Maximum brake torque
MFB	mass fraction burned
MFC	Mass flow controller
MON	Motor octane number
MPG	Miles per US gallon
mph	Miles per hour
MY	Model year
NMEP	Net mean effective pressure
NRMSE	Normalized mean root square error
NTC	Negative temperature coefficient
OI	Octane index
ON	Octane number
PFI	Port fuel injection
PHEV	Plug-in hybrid electric vehicle
PRF	Primary reference fuel
PSD	Power-spectral-density
RON	Research octane number
RPM	Revolution per minute
S	Octane sensitivity
SI	Spark-ignition
SOC	State of charge
T_{comp15}	Unburned gas temperature at 15 bar compression pressure
TDC	Top dead center
TEL	tetraethyllead
Ti-VCT	Twin independent variable cam timing
TPH	Thin-plate harmonic spline interpolation
TRF	Toluene reference fuel
UDDS	Urban Dynamometer Driving Schedule
UFI	Upstream fuel injection
VVT	Variable valve timing