### Contents

| Contents  | i    |
|---|------|
| List of Figures   | viii |
| List of Tables  | xiii |
| List of Equations   | xiv  |
| Nomenclature  | xvii |
| Chapter 1 – Introduction  | 1    |
| 1. The imperative for transitioning to sustainable transportation: low carbon fuels as a solution for reducing transport sector emissions | 2    |
| 2. Alternatives for addressing carbon emissions in the transportation sector  | 3    |
| 3. Challenges and concerns related to tailpipe emissions from internal combustion engine vehicles using low carbon fuels                  | 6    |
| 4. Document content and structure   | 7    |
| 5. References   | 10   |
| Chapter 2 – A Comprehensive Review of Low Carbon Fuels for Diesel Engines   | 15   |
| 1. Introduction   | 16   |
| 2. Types of low carbon fuels for compression ignition engines   | 17   |
| 2.1. Biofuels: from the first generation to the state-of-the-art  | 18   |
| 2.1.1. Fatty Acid Methyl Ester and Rapeseed Methyl Ester  | 19   |
| 2.1.2. Hydrotreated vegetable oil   | 25   |
| 2.2. Synthetic fuels: recycling existing carbon   | 30   |

| 2.2.1. Fischer-Tropsch Diesel   | 31   |
|---|--|
| 2.2.2. OMEx   | 35   |
| 3. Low carbon fuel blends: achieving specific fuel characteristics  | 41   |
| 3.1. Multi-fuel blends  | 41   |
| 3.2. Additives  | 48   |
| 4. Optimizing the vehicle for low carbon fuels  | 51   |
| 4.1. Aftertreatment systems with low carbon fuels   | 51   |
| 4.2. Re-designing the engine for low carbon fuels   | 54   |
| 5. Challenges and barriers for low carbon fuels   | 55   |
| 6. Motivation of the study  | 57   |
| 7. Objectives of the study  | 58   |
| 8. References   | 60   |
|   |  |
| Chapter 3 – Tools and Methodology   | 75   |
| Chapter 3 – Tools and Methodology   | <b>75</b><br>77  |
|   |  |
| 1. Introduction   | 77   |
| 1. Introduction.         2. Experimental facilities.  | 77<br>78   |
| 1. Introduction.         2. Experimental facilities.         2.1. Multicylinder engine description.   | 77<br>78<br>78   |
| 1. Introduction.         2. Experimental facilities.         2.1. Multicylinder engine description.         2.1.1. Engine description.  | 77<br>78<br>78<br>78   |
| 1. Introduction.         2. Experimental facilities.         2.1. Multicylinder engine description.         2.1.1. Engine description.         2.1.2. Fuel injection system.  | 77<br>78<br>78<br>78<br>78<br>79   |
| 1. Introduction.         2. Experimental facilities.         2.1. Multicylinder engine description.         2.1.1. Engine description.         2.1.2. Fuel injection system.         2.1.3. Air management and exhaust gas recirculation systems.   | 77<br>78<br>78<br>78<br>78<br>79<br>80   |
| 1. Introduction.         2. Experimental facilities.         2.1. Multicylinder engine description.         2.1.1. Engine description.         2.1.2. Fuel injection system.         2.1.3. Air management and exhaust gas recirculation systems.         2.1.4. Engine control system.   | 77<br>78<br>78<br>78<br>78<br>79<br>80<br>80   |
| 1. Introduction.         2. Experimental facilities.         2.1. Multicylinder engine description.         2.1.1. Engine description.         2.1.2. Fuel injection system.         2.1.3. Air management and exhaust gas recirculation systems.         2.1.4. Engine control system.         2.2. Test cell characteristics. | <ul> <li>77</li> <li>78</li> <li>78</li> <li>78</li> <li>79</li> <li>80</li> <li>80</li> <li>81</li> </ul> |

| 2.2.4. Mass flow measurement           | 83  |
|--|-----|
| 2.2.5. Emissions measurement           | 84  |
| 2.2.6. Soot measurement                | 86  |
| 2.2.7. Data acquisition systems        | 87  |
| 3. Fuel properties and characteristics | 88  |
| 4. Theoretical tools                   | 94  |
| 4.1. Combustion diagnosis model        | 94  |
| 4.1.1. Mean effective pressure         | 95  |
| 4.1.2. Combustion efficiency           | 96  |
| 4.2. Equivalent fuel consumption       | 97  |
| 5. Testing methodologies               | 97  |
| 5.1. Stationary operation              | 97  |
| 5.2. Calibration types and test matrix | 99  |
| 5.2.1. Drop-in calibration             | 99  |
| 5.2.2. Calibration optimization        | 100 |
| 6. Statistical modelling approach      | 101 |
| 6.1. Design of Experiments (DOE)       | 101 |
| 6.1.1. Screening                       | 103 |
| 6.1.2. Factorial tests                 | 106 |
| 6.1.3. Combined data                   | 107 |
| 6.2. Modelling                         | 108 |
| 6.3. Optimization                      | 110 |
| 6.4. Validation                        | 111 |
| 7. Summary and conclusions             | 114 |

| 8. References | 16 |
|---------------|----|
|---------------|----|

| Chapter 4 – Drop-in use of low carbon fuel blends in compression ignition engines  | 121   |
|--|---|
| 1. Introduction  | 122   |
| 2. Combustion, performance and emissions   | 123   |
| 2.1. Engine settings: reaching drop-in operation   | 123   |
| 2.2. Combustion under drop-in calibration settings   | 129   |
| 2.3. Performance and emissions of drop-in fuel operation   | 133   |
| 2.3.1. Fuel energy utilization   | 133   |
| 2.3.2. Criteria pollutant evaluation   | 136   |
| 3. Unmeasured effects of the use of drop-in fuels  | 139   |
| 4. Summary and conclusions   | 142   |
| 5. References  | 144   |
|  |   |
| Chapter 5 – Optimization of low carbon fuel blends calibration in compression ignition engines   | 147   |
|  | 147<br>149  |
| engines  |   |
| engines 1. Introduction  | 149   |
| engines         1. Introduction  | 149<br>151  |
| engines         1. Introduction.         2. Engine responses with DOE modelling.         2.1. Low-to-medium-load engine performance.   | 149<br>151<br>155   |
| engines         1. Introduction.         2. Engine responses with DOE modelling.         2.1. Low-to-medium-load engine performance.         2.2. High-load engine performance.  | 149<br>151<br>155<br>159  |
| engines         1. Introduction.         2. Engine responses with DOE modelling.         2.1. Low-to-medium-load engine performance.         2.2. High-load engine performance.         3. Fixed combustion phasing analysis.  | 149<br>151<br>155<br>159<br>161   |
| engines         1. Introduction.         2. Engine responses with DOE modelling.         2.1. Low-to-medium-load engine performance.         2.2. High-load engine performance.         3. Fixed combustion phasing analysis.         3.1. Fuel consumption impact.  | <ol> <li>149</li> <li>151</li> <li>155</li> <li>159</li> <li>161</li> <li>162</li> </ol>              |
| engines         1. Introduction.         2. Engine responses with DOE modelling.         2.1. Low-to-medium-load engine performance.         2.2. High-load engine performance.         3. Fixed combustion phasing analysis.         3.1. Fuel consumption impact.         3.2. NOx emissions impact.                                     | <ol> <li>149</li> <li>151</li> <li>155</li> <li>159</li> <li>161</li> <li>162</li> <li>164</li> </ol> |
| engines         1. Introduction.         2. Engine responses with DOE modelling.         2.1. Low-to-medium-load engine performance.         2.2. High-load engine performance.         3. Fixed combustion phasing analysis.         3.1. Fuel consumption impact.         3.2. NOx emissions impact.         3.3. Soot emissions impact. | 149<br>151<br>155<br>159<br>161<br>162<br>164<br>166  |

| 4.3. NOx emissions impact   | 176   |
|---|---|
| 4.4. Soot emissions impact  | 180   |
| 5. Experimental optimized responses analysis  | 184   |
| 6. Summary and conclusions  | 188   |
| 6.1. Low-to-medium load and high load performance   | 188   |
| 6.2. Fixed combustion phasing   | 189   |
| 6.3. Fixed calibration settings   | 190   |
| 6.4. Optimized calibration  | 191   |
| 7. References   | 192   |
| 8. Appendix   | 194   |
| 8.1. Optimization calibration settings  | 194   |
|   |   |
| Chapter 6 – Life Cycle Analysis of Low Carbon Fuels for Light-Duty Combustion<br>Engine Vehicles  | 197   |
| Engine Vehicles   | <b>197</b><br>199   |
|   |   |
| Engine Vehicles   | 199   |
| Engine Vehicles   | 199<br>200  |
| Engine Vehicles   | 199<br>200<br>201   |
| Engine Vehicles.         1. Introduction.         1.1. Life cycle analysis: fundamentals and conventions for evaluating the impact of road vehicles.         1.1.1. Goal and scope definition.         1.1.2. Lifecycle inventory (LCI)   | <ol> <li>199</li> <li>200</li> <li>201</li> <li>202</li> </ol>  |
| Engine Vehicles.         1. Introduction.         1.1. Life cycle analysis: fundamentals and conventions for evaluating the impact of road vehicles.         1.1.1. Goal and scope definition.         1.1.2. Lifecycle inventory (LCI)         1.1.3. Lifecycle impact assessment (LCIA)   | <ol> <li>199</li> <li>200</li> <li>201</li> <li>202</li> <li>203</li> </ol>                           |
| Engine Vehicles.         1. Introduction.         1.1. Life cycle analysis: fundamentals and conventions for evaluating the impact of road vehicles.         1.1.1. Goal and scope definition.         1.1.2. Lifecycle inventory (LCI)         1.1.3. Lifecycle impact assessment (LCIA)         1.1.4. Interpretation, reporting and review.  | <ol> <li>199</li> <li>200</li> <li>201</li> <li>202</li> <li>203</li> <li>205</li> </ol>              |
| Engine Vehicles.         1. Introduction.         1.1. Life cycle analysis: fundamentals and conventions for evaluating the impact of road vehicles.         1.1.1. Goal and scope definition.         1.1.2. Lifecycle inventory (LCI)         1.1.3. Lifecycle impact assessment (LCIA)         1.1.4. Interpretation, reporting and review.         1.2. Study contributions, novelty, and implications. | <ol> <li>199</li> <li>200</li> <li>201</li> <li>202</li> <li>203</li> <li>205</li> <li>206</li> </ol> |

| 2.1.2. Cradle-to-road methodology   | 208 |
|---|-----|
| 2.1.3. Functional unit, energy flow and system boundaries   | 208 |
| 2.1.4. Impact categories  | 211 |
| 2.2. Life cycle inventory   | 212 |
| 2.2.1. Vehicle manufacturing  | 212 |
| 2.2.2. Vehicle maintenance  | 215 |
| 2.2.3. Energy production and distribution   | 216 |
| 2.2.4. Vehicle operation: WTT, TTW & WTW  | 217 |
| 3. Impact assessment of low carbon fuel use in light-duty vehicles  | 229 |
| 3.1. Stationary assessment  | 229 |
| 3.2. Driving cycle assessment   | 233 |
| 3.3. Cradle-to-road impact assessment   | 236 |
| 4. Summary and conclusions  | 245 |
| 4.1. Global Warming Potential – GWP   | 245 |
| 4.2. Terrestrial acidification – TAP; fine particle matter formation – PMFP & human health ozone formation – HOFP | 246 |
| 4.3. Water consumption – WCP  | 246 |
| 5. References   | 247 |
| 6. Appendix   | 257 |
| 6.1. Life cycle inventory for the vehicle manufacturing   | 257 |
| 6.1.1. Glider   | 257 |
| 6.1.2. Drivetrain   | 259 |
| Chapter 7 – Conclusions and suggestions for future work   | 263 |
| 1. Introduction   | 264 |

| Bibliography  | 273 |
|---|-----|
| 3.2. Powertrain hybridization   | 270 |
| 3.1. Aftertreatment system evaluation and vehicle tests                                 | 270 |
| 3. Suggestions for future work  | 269 |
| 2.3. Life Cycle Analysis of Low Carbon Fuels for Light-Duty Combustion Engine Vehicles  | 269 |
| 2.2. Optimization of low carbon fuel blends calibration in compression ignition engines | 267 |
| 2.1. Drop-in use of low carbon fuel blends in compression ignition engines              | 266 |
| 2. Summary and conclusions  | 264 |

## **List of Figures**

#### Chapter 1 - Introduction

| Figure 1. GHG emissions by sector for Europe and the World                             | 2  |
|--|----|
| Figure 2. Different alternatives to solving the GHG dilemma in the transport sector    | 5  |
| Figure 3. Main challenges on the emissions of ICEVs                                    | 6  |
| Figure 4. Graphical representation of the argument line followed in the investigation  | 9  |
| Chapter 2 – A Comprehensive Review of Low Carbon Fuels for Diesel Engines              |    |
| Figure 1. Classification of fuels by different criteria                                | 18 |
| Figure 2. FAME production pathways   | 21 |
| Figure 3. NOx-soot tradeoff compared to diesel across different studies with FAME      | 24 |
| Figure 4. HC-CO tradeoff compared to diesel across different studies with FAME         | 25 |
| Figure 5. HVO production pathways  | 27 |
| Figure 6. NOx-soot tradeoff compared to diesel across different studies with HVO       | 29 |
| Figure 7. HC-CO tradeoff compared to diesel across different studies with HVO          | 29 |
| Figure 8. Synthetic diesel production pathways   | 31 |
| Figure 9. NOx-soot tradeoff compared to diesel across different studies with FT-Diesel | 35 |
| Figure 10. NOx-soot tradeoff compared to diesel across different studies with OMEx     | 37 |
| Figure 11. HC-CO tradeoff compared to diesel across different studies with OMEx        | 39 |
| Chapter 3 – Tools and methodology  |    |
| Figure 1. Piston bowl profile  | 79 |
| Figure 2. Test cell schematic  | 81 |
| Figure 3. Low Carbon Fuel (LCF) blends volumetric composition                          | 88 |
| Figure 4. Bivariate correlation between relevant fuel properties                       | 91 |
| Figure 5. Balance of fuel properties for the studied LCF blends                        | 93 |
|  |    |

| Figure 6. Schematic description of the drop-in calibration methodology  | 100                      |
|---|--------------------------|
| Figure 7. Three-dimensional Box-Behnken design representation   | 102                      |
| Figure 8. Three-dimensional and two-dimensional screening design representation   | 103                      |
| Figure 9. One-dimensional representation of the "one at a time" screening methodology for a single calibration parameter  | 104                      |
| Figure 10. Representation of the effect sizing evaluation for the reduction of parameters from 8 to 6 for responses BSNOx, soot and BSFC with the combined normalized effect (CNR)  | 104                      |
| Figure 11. Three-dimensional and two-dimensional 2-k factorial design representation  | 106                      |
| Figure 12. Three-dimensional and two-dimensional representation of the combined screening and 2-k factorial design  | 107                      |
| Figure 13. Example of fitted vs. experimental values and residuals vs. experimental values for the linear model   | 109                      |
| Figure 14. Soot, BSNOx and BSFC map from the linear regression models   | 111                      |
| Figure 15. Fitted vs. experimental values for BSFC, BSNOx and BSSoot in the validation dataset outside of the calibration data for the models   | 113                      |
|   |                          |
| Chapter 4 – Drop-in use of low carbon fuel blends in compression ignition engines   |                          |
| Chapter 4 – Drop-in use of low carbon fuel blends in compression ignition engines<br>Figure 1. Pedal requirement for the different LCF blends at the tested operating conditions  | 124                      |
|   | 124<br>125               |
| Figure 1. Pedal requirement for the different LCF blends at the tested operating conditions   |                          |
| Figure 1. Pedal requirement for the different LCF blends at the tested operating conditions<br>Figure 2. Achieved load for the different LCF blends at 3750 rpm and 100% pedal  | 125                      |
| Figure 1. Pedal requirement for the different LCF blends at the tested operating conditions<br>Figure 2. Achieved load for the different LCF blends at 3750 rpm and 100% pedal<br>Figure 3. Injection settings for the different LCF blends under the drop-in calibration<br>Figure 4. Charge renovation settings for the different LCF blends under the drop-in  | 125<br>126               |
| <ul> <li>Figure 1. Pedal requirement for the different LCF blends at the tested operating conditions</li> <li>Figure 2. Achieved load for the different LCF blends at 3750 rpm and 100% pedal</li> <li>Figure 3. Injection settings for the different LCF blends under the drop-in calibration</li> <li>Figure 4. Charge renovation settings for the different LCF blends under the drop-in calibration</li> <li>Figure 5. Peak pressure of Ref. Diesel compared with LCD100, LCD66 and LCD33;</li> </ul>   | 125<br>126<br>128        |
| <ul> <li>Figure 1. Pedal requirement for the different LCF blends at the tested operating conditions</li> <li>Figure 2. Achieved load for the different LCF blends at 3750 rpm and 100% pedal</li> <li>Figure 3. Injection settings for the different LCF blends under the drop-in calibration</li> <li>Figure 4. Charge renovation settings for the different LCF blends under the drop-in calibration</li> <li>Figure 5. Peak pressure of Ref. Diesel compared with LCD100, LCD66 and LCD33; MaxOME66 and MaxOME33; RE100 and R33</li> <li>Figure 6. Comparison of the Heat Release Rate (HRR) of Ref. Diesel with LCD100, LCD66</li> </ul> | 125<br>126<br>128<br>130 |

| Figure 9. Brake-specific fuel consumption (BSFC) and equivalent BSFC (BSFCeq) for the different LCF blends under the drop-in calibration  | 133                             |
|---|---------------------------------|
| Figure 10. Energy distribution for Ref. Diesel under the drop-in calibration at the tested operating conditions   | 134                             |
| Figure 11. Gross brake efficiency (GBE); combustion inefficiency; and exhaust energy loss for the different LCF blends under the drop-in calibration  | 135                             |
| Figure 12. Brake-specific NOx emissions (BSNOx) for the different LCF blends under the drop-in calibration  | 137                             |
| Figure 13. Brake-specific soot emissions (BSSoot) for the different LCF blends under the drop-in calibration  | 138                             |
| Figure 14. Brake-specific HC emissions (BSHC) and Brake-specific CO emissions (BSHC) for the different LCF blends under the drop-in calibration   | 139                             |
| Figure 15. Injector usage summary including the operation time and the fuels used before breakage   | 140                             |
| Figure 16. Relation between the wear scar diameter, the oxygen content, the water content and the viscosity of the fuels  | 141                             |
|   |                                 |
| Chapter 5 – Optimization of low carbon fuel blends calibration in compression ignition  |                                 |
| Chapter 5 – Optimization of low carbon fuel blends calibration in compression ignition engines<br>Figure 1. Schematic of the analysis approach of the chapter   | 150                             |
| engines   | 150<br>155                      |
| engines<br>Figure 1. Schematic of the analysis approach of the chapter<br>Figure 2. Correlation matrix of the optimization space for the BSFC, BSNOx, Soot and CA50   |                                 |
| <ul> <li>engines</li> <li>Figure 1. Schematic of the analysis approach of the chapter</li> <li>Figure 2. Correlation matrix of the optimization space for the BSFC, BSNOx, Soot and CA50 for the LCD100, LCD66 and LCD33 fuels at the operating condition 2000 rpm @ 8 bar</li> <li>Figure 3. Correlation matrix of the optimization space for the BSFC, BSNOx, Soot and CA50</li> </ul>  | 155                             |
| engines<br>Figure 1. Schematic of the analysis approach of the chapter<br>Figure 2. Correlation matrix of the optimization space for the BSFC, BSNOx, Soot and CA50<br>for the LCD100, LCD66 and LCD33 fuels at the operating condition 2000 rpm @ 8 bar<br>Figure 3. Correlation matrix of the optimization space for the BSFC, BSNOx, Soot and CA50<br>for the MaxOME66 and MaxOME33 fuels at the operating condition 2000 rpm @ 8 bar<br>Figure 4. Correlation matrix of the optimization space for the BSFC, BSNOx, Soot and CA50   | 155<br>157                      |
| <ul> <li>engines</li> <li>Figure 1. Schematic of the analysis approach of the chapter</li> <li>Figure 2. Correlation matrix of the optimization space for the BSFC, BSNOx, Soot and CA50 for the LCD100, LCD66 and LCD33 fuels at the operating condition 2000 rpm @ 8 bar</li> <li>Figure 3. Correlation matrix of the optimization space for the BSFC, BSNOx, Soot and CA50 for the MaxOME66 and MaxOME33 fuels at the operating condition 2000 rpm @ 8 bar</li> <li>Figure 4. Correlation matrix of the optimization space for the BSFC, BSNOx, Soot and CA50 for the R33 and RE100 fuels at the operating condition 2000 rpm @ 8 bar</li> <li>Figure 5. Correlation matrix of the optimization space for the BSFC, BSNOx, Soot and CA50</li> </ul>  | 155<br>157<br>158               |
| engines<br>Figure 1. Schematic of the analysis approach of the chapter<br>Figure 2. Correlation matrix of the optimization space for the BSFC, BSNOx, Soot and CA50<br>for the LCD100, LCD66 and LCD33 fuels at the operating condition 2000 rpm @ 8 bar<br>Figure 3. Correlation matrix of the optimization space for the BSFC, BSNOx, Soot and CA50<br>for the MaxOME66 and MaxOME33 fuels at the operating condition 2000 rpm @ 8 bar<br>Figure 4. Correlation matrix of the optimization space for the BSFC, BSNOx, Soot and CA50<br>for the R33 and RE100 fuels at the operating condition 2000 rpm @ 8 bar<br>Figure 5. Correlation matrix of the optimization space for the BSFC, BSNOx, Soot and CA50<br>at the operating condition 3750 rpm @ max. load  | 155<br>157<br>158<br>160        |
| <ul> <li>engines</li> <li>Figure 1. Schematic of the analysis approach of the chapter</li> <li>Figure 2. Correlation matrix of the optimization space for the BSFC, BSNOx, Soot and CA50 for the LCD100, LCD66 and LCD33 fuels at the operating condition 2000 rpm @ 8 bar</li> <li>Figure 3. Correlation matrix of the optimization space for the BSFC, BSNOx, Soot and CA50 for the MaxOME66 and MaxOME33 fuels at the operating condition 2000 rpm @ 8 bar</li> <li>Figure 4. Correlation matrix of the optimization space for the BSFC, BSNOx, Soot and CA50 for the R33 and RE100 fuels at the operating condition 2000 rpm @ 8 bar</li> <li>Figure 5. Correlation matrix of the optimization space for the BSFC, BSNOx, Soot and CA50 at the operating condition 3750 rpm @ max. load</li> <li>Figure 6. BSFC at different loads under fixed CA50 values</li> </ul> | 155<br>157<br>158<br>160<br>163 |

| Figure 10. Effect of fuel blend properties over the normalized required fuel mass at different engine conditions                    | 170 |
|---|-----|
| Figure 11. Effect of fuel blend properties over the BSFC at different engine conditions for cases with equal settings               | 172 |
| Figure 12. BSFC at different engine conditions with equal engine settings   | 175 |
| Figure 13. Effect of fuel blend properties over the BSNOx at different engine conditions for cases with equal settings              | 178 |
| Figure 14. BSNOx at different engine conditions with equal engine settings  | 179 |
| Figure 15. Effect of fuel blend properties over the BSSoot at different engine conditions for cases with equal settings             | 180 |
| Figure 16. BSSoot at different engine conditions with equal engine settings   | 183 |
| Figure 17. BSFC comparison for the optimized vs. drop-in calibration  | 185 |
| Figure 18. BSNOx (top) and BSSoot (bottom) comparison for the optimized vs. drop-in calibration                                     | 186 |
| Figure 19. BSHC (top) and BSCO (bottom) comparison for the optimized vs. drop-in calibration  | 187 |
| Chapter 6 – Life Cycle Analysis of Low Carbon Fuels for Light-Duty Combustion Engine Vehicles                                       |     |
| Figure 1. Overview of the impact categories that are covered in the ReCiPe2016 method and their relation to the areas of protection | 205 |
| Figure 2. Vehicle system boundaries and elementary flows during the cradle-to-road process  | 209 |
| Figure 3. Schematic for the LCF production assuming renewable sources of energy and raw components                                  | 210 |
| Figure 4. GWP distribution for the vehicle manufacturing material stage (without assembly energy)                                   | 213 |
| Figure 5. Speed profile for the class 3b WLTC   | 219 |
| Figure 6. Engine map discretization schematic   | 221 |
| Figure 7. BSFC difference between the complete and simplified engine maps for the   | 222 |

Figure 7. BSFC difference between the complete and simplified engine maps for the 222 reference diesel fuel

| Figure 8. Difference in the BSNOx between the complete and simplified engine maps for the reference diesel fuel            | 224 |
|--|-----|
| Figure 9. GT-Power vehicle model schematic   | 225 |
| Figure 10. Distribution of the engine operating conditions during the WLTP cycle for different vehicle segments            | 226 |
| Figure 11. Cycle fuel consumption comparison between the complete and simplified engine map                                | 227 |
| Figure 12. Cycle NOx and soot emissions comparison between the complete and simplified engine map                          | 228 |
| Figure 13. TTW CO2 emissions for the stationary operating conditions   | 231 |
| Figure 14. WTW CO2 emissions for the stationary operating conditions   | 232 |
| Figure 15. Vehicle operation fuel consumption in liters per 100 km   | 233 |
| Figure 16. Vehicle operation CO <sub>2</sub> emissions per km. The dashed lines represent the reference diesel result      | 234 |
| Figure 17. Vehicle operation NOx emissions per km. The dashed lines represent the reference diesel result                  | 235 |
| Figure 18. Vehicle operation soot emissions per km. The dashed lines represent the reference diesel result                 | 236 |
| Figure 19. Life cycle GWP for three vehicle segments manufactured in 2023 using LCFs for 10 years or 120000 km             | 238 |
| Figure 20. Summarized life cycle GWP for three vehicle segments manufactured in 2023 using LCFs for 10 years or 120000 km  | 239 |
| Figure 21. Summarized life cycle TAP for three vehicle segments manufactured in 2023 using LCFs for 10 years or 120000 km  | 241 |
| Figure 22. Summarized life cycle PMPF for three vehicle segments manufactured in 2023 using LCFs for 10 years or 120000 km | 242 |
| Figure 23. Summarized life cycle HOFP for three vehicle segments manufactured in 2023 using LCFs for 10 years or 120000 km | 243 |
| Figure 24. Summarized life cycle WCP for three vehicle segments manufactured in 2023 using LCFs for 10 years or 120000 km  | 244 |
|  |     |

#### **List of Tables**

| Chapter 2 – A Comprehensive Review of Low Carbon Fuels for Diesel Engines   |     |  |  |
|---|-----|--|--|
| Table 1. Chemical and physical properties of different pure fuels   | 46  |  |  |
| Table 2. Chemical and physical properties of different fuel blends  | 47  |  |  |
| Chapter 3 – Tools and methodology   |     |  |  |
| Table 1. Engine characteristics   | 78  |  |  |
| Table 2. Injection system characteristics   | 79  |  |  |
| Table 3. Test cell instrumentation summary  | 82  |  |  |
| Table 4. Horiba MEXA 7100 D-EGR components, measurement principles range, and associated uncertainty                          | 84  |  |  |
| Table 5. Main fuel properties at standard conditions  | 90  |  |  |
| Table 6. Minimum targets for the LCF calibration optimization   | 101 |  |  |
| Chapter 5 – Optimization of low carbon fuel blends calibration in compression ignition engines                                |     |  |  |
| Table 1. Calibration ranges for the different fuels at the tested operating conditions  | 152 |  |  |
| Table 2. Selected CA50 range for each operating condition   | 161 |  |  |
| Table 3. Iso-setting calibration setting levels   |     |  |  |
| Chapter 6 – Life Cycle Analysis of Low Carbon Fuels for Light-Duty Combustion Engine Vehicles                                 |     |  |  |
| Table 1. Vehicle and driving strategy characteristics   | 207 |  |  |
| Table 2. Impact categories overview   | 211 |  |  |
| Table 3. Summarized inventory data for the vehicle manufacture  | 214 |  |  |
| Table 4. Vehicle manufacture GWP in kg CO <sub>2</sub> -eq/kg vehicle from selected literature                                | 215 |  |  |
| Table 5. Summarized inventory data for the vehicle maintenance  | 216 |  |  |
| Table 6. Well-to-tank carbon intensity for the different fuels assuming completely renewable energy sources and raw materials |     |  |  |

Table 7. Tank-to-wheel carbon intensity for the different fuels assuming complete 218 combustion

 Table 8. Emission correction coefficients for the WLTP cycle using simplified engine maps
 229

#### List of equations

Chapter 3 – Tools and methodology

Equation 1

$$c_{wet} = k_w \cdot c_{dry} \tag{85}$$

Equation 2  

$$k_{w} = \left(\frac{1}{1 + \alpha \times 0.005 \times (c_{CO_{2}} + c_{CO}) - \frac{1.608 \times H_{a}}{1000 + 1.608 \times H_{a}}}\right) \times 1.008$$
85

Equation 3 
$$\dot{m}_{emission} = \left(x_i \cdot \frac{MW_{emission}}{MW_{exh}}\right) \cdot \dot{m}_{exh}$$
 86

Equation 4 
$$SX = \frac{\dot{m}_{emission}}{P}$$
 86

Equation 5 
$$EGR \ [\%] = \frac{CO_{2intake-dry} - CO_{2ambient}}{CO_{2exhaust-dry} - CO_{2ambient}} \times 100$$

Equation 6 soot 
$$[mg/m^3] = \frac{1}{0.405} \cdot 4.95 \cdot FSN \cdot e^{(0.38 \cdot FSN)}$$
 87

Equation 7  

$$r = \frac{\sum(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum(x_i - \bar{x})^2 \sum(y_i - \bar{y})^2}}$$
89

Equation 8 
$$\Delta HRL = m_{cyl} \cdot \Delta u_{cyl} + \Delta Q_w + p \cdot \Delta V - (h_{f,inj} - u_{f,g}) \cdot \Delta m_{f,evap} + R_{cyl} \quad 94$$
$$\cdot T_{cyl} \cdot \Delta m_{bb}$$

Equation 9  

$$IMEP = \frac{\int_{-360}^{360} p dV}{V_{sweep}}$$
95

Equation 10  $COV_{IMEP} = \frac{\sigma_{IMEP_i}}{\overline{IMEP}} = \frac{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(IMEP_i - \overline{IMEP})^2}}{\overline{IMEP}}$ 96

Equation 11 
$$BTE = \frac{P_{brake}}{Q_{fuel}}$$
 96

Equation 12  

$$\eta_{comb} = \frac{(\dot{m}_{air} + \dot{m}_{fuel})(LHV_{CO}X_{CO} + LHV_{HC}X_{HC})}{Q_{fuel}}$$
96

Equation 13  

$$\eta_{exh} = \frac{(\dot{m}_{air} + \dot{m}_{fuel})(h_{exh @ T exhaust} - h_{exh @ T amb})}{Q_{fuel}}$$
97

Equation 14 
$$\eta_{cool} = 1 - BTE - \eta_{exh} - \eta_{comb} - \eta_{mech}$$
 97

Equation 15  

$$BSFC_{eq} = \frac{LHV_{LCF} \cdot \dot{m}_{LCF}}{LHV_{diesel} \cdot P}$$
97

Equation 16 
$$SE_i = \frac{\sigma_i}{\sqrt{n}}$$
 105

Equation 17  

$$SR_{i} = \frac{\frac{y_{2} - y_{1}}{x_{2} - x_{1}}}{SE_{i}}$$
105

Equation 18  

$$NR_i = \frac{|SR_i - \min(|SR|)|}{\max(|SR|) - \min(|SR|)}$$
105

Equation 19  

$$CNR_i = \sum_{response} NR_{iresponse}$$
105

xvi

Equation 20 
$$Y = b_0 + \sum b_i X_i + \sum b_{ij} X_i X_j$$
 108

Equation 21 
$$Z = c_1 x_1 + c_2 x_2 + \dots + c_n x_n$$
 110

Equation 22 
$$a_{m1}x_1 + a_{m2}x_2 + \dots + a_{mn}x_n \le b_m$$
 110

Equation 23 
$$x_1, x_2, ..., x_n \ge 0$$
 110

# Chapter 6 – Life Cycle Analysis of Low Carbon Fuels for Light-Duty Combustion Engine Vehicles

Equation 1 
$$k_{CO_2} = y_{C_{fuel}} \cdot \left(\frac{M_C + M_{O_2}}{M_C}\right)$$
 217

Equation 2 
$$m_{CO_2} = k_{CO_2} \cdot m_{fuel}$$
 218

Equation 3 
$$BSE_{diff.} = BSE_{simp.\ map} - BSE_{comp.\ map}$$
 222

Equation 4 
$$E_{cycle} = c_{correction} \cdot E_{simplified map}$$
 229

#### Nomenclature

#### Acronyms

| AFR         | Air-to-Fuel Ratio  |
|-------------|--|
| AP          | Acidification Potential  |
| ATS         | Aftertreatment System  |
| BMEP        | Brake Mean Effective Pressure  |
| BSEC        | Brake Specific Energy Consumption  |
| BSFC        | Brake Specific Fuel Consumption  |
| BSFCeq      | Equivalent Brake Specific Fuel Consumption   |
| BTE         | Brake Thermal Efficiency   |
| BTL<br>CA50 | Biomass-to-Liquid<br>Combustion Phasing/Crank Angle at which 50 % of the heat from combustion has<br>been released |
| CC          | Catalytic Converter  |
| CCS         | Carbon Capture and Storage   |
| CCU         | Carbon Capture and Utilization   |
| CDPF        | Catalyzed Diesel Particulate Filter  |
| CED         | Cumulative Energy Demand   |
| CFCs        | Chlorofluorocarbons  |
| CFPP        | Cold Filter Plugging Point   |
| CH4         | Methane  |
| CI          | Compression Ignition   |
| CN          | Cetane Number  |
| CNR         | Combined Normalized Response   |
| CO          | Carbon Monoxide  |
| CO2         | Carbon Dioxide   |
| COME        | Castor Oil Methyl Ester  |
| СР          | Cloud Point  |
| CR          | Compression Ratio  |
| DAC         | Direct Air Capture   |
| DI          | Direct Injection   |
| DICI        | Direct Injection Compression Ignition  |
| DMF         | Dimethyl Furan   |
| DNPE        | Di-n-pentyl Ether  |
| DOC         | Diesel Oxidation Catalyst  |

| DOE   | Design of Experiments  |
|-------|--|
| DPF   | Diesel Particulate Filter  |
| ECU   | Engine Control Unit  |
| EEPS  | Engine Exhaust Particle Sizer  |
| EF    | Environmental Footprint  |
| EGR   | Exhaust Gas Recirculation  |
| EGT   | Exhaust Gas Temperature  |
| EOC   | End of Combustion  |
| EOL   | End of Life  |
| EP    | Euthrophication Potential  |
| ET    | Energizing Time  |
| EV    | Electric Vehicle   |
| EVO   | Exhaust Valve Opening  |
| FAME  | Fatty Acid Methyl Ester  |
| FFA   | Free Fatty Acid  |
| FID   | Flame Ionization Detector  |
| FIS   | Fuel Injection System  |
| FSN   | Filter Smoke Number  |
| FT    | Fischer-Tropsch  |
| FTIR  | Fourier-transform infrared spectroscopy                              |
| FU    | Functional Unit  |
| GBE   | Gross Brake Efficiency   |
| GHG   | Greenhouse Gas   |
| GM    | General Motors   |
| GREET | Greenhouse Gases, Regulated Emissions and Energy Use in Technologies |
| GTL   | Gas-to-Liquid  |
| GWP   | Global Warming Potential   |
| HC    | Hydrocarbons   |
| HCLD  | Heated Chemiluminescence Detector                                    |
| HHV   | Higher Heating Value   |
| HOFP  | Human Ozone Formation Potential                                      |
| HPA   | Heteropoly Acids   |
| HRL   | Total Heat Released  |
| HRR   | Heat Release Rates   |
| HTP   | Human Toxicity Potential   |
| HVO   | Hydrotreated Vegetable Oil   |
| ICE   | Internal Combustion Engine   |
|       |  |

| ICEV  | Internal Combustion Engine Vehicle                    |
|-------|---|
| IDID  | Internal Diesel Injector Deposits                     |
| IDT   | Ignition Delay Time                                   |
| IMEP  | Indicated Mean Effective Pressure                     |
| IP    | Injection Pressure                                    |
| IQR   | Interquartile Range                                   |
| ISCC  | International Sustainability and Carbon Certification |
| ISFC  | Indicated Specific Fuel Consumption                   |
| ITE   | Indicated Thermal Efficiency                          |
| IVC   | Inlet Valve Closing                                   |
| LCA   | Life Cycle Assessment                                 |
| LCF   | Low Carbon Fuel                                       |
| LCI   | Life Cycle Inventory                                  |
| LCIA  | Life Cycle Impact Assessment                          |
| LHV   | Lower Heating Value                                   |
| LNT   | Lean-Nox Trap   |
| LO    | Lemon Oil   |
| LTHR  | Low Temperature Heat Release                          |
| MFB   | Mass Fraction Burned                                  |
| MPD   | Magneto-Pneumatic Detector                            |
| N2O   | Nitrous Oxide   |
| NDIR  | Non-Dispersive InfraRed                               |
| NG    | Natural Gas   |
| NMVOC | Non-Methane Volatile Organic Compound                 |
| NO    | Nitrogen Monoxide                                     |
| NO2   | Nitrogen Dioxide                                      |
| NOx   | Nitrogen Oxides                                       |
| NP    | Nanoparticles   |
| NR    | Normalized Response                                   |
| NVH   | Noise Vibration and Harshness                         |
| ODP   | Ozone Depletion Potential                             |
| OEF   | Organization Environmental Footprint                  |
| OESI  | Oxygen Extended Sooting Index                         |
| OMEx  | Oxymethylene Dimethyl Ethers                          |
| PAHs  | Polycyclic Aromatic Hydrocarbons                      |
| PCS   | Post-combustion Capture System                        |
| PEF   | Product Environmental Footprint                       |
|       |   |

| 5.00 <i>(</i> 5 |  |
|-----------------|--|
| PKME            | Pistacia Khinjuk Methyl Ester                  |
| PM              | Particulate Matter                             |
| PMFP            | Particle Matter Formation Potential            |
| PODEs           | Polyoxymethylene Ethers                        |
| POME            | Palm Oil Methyl Ester                          |
| PRR             | Pressure Rise Rates                            |
| PSO-NS          | Particle Swarm Optimization-Novelty Search     |
| PSZ             | Partially Stabilized Zirconia                  |
| PTG             | Power-to-Gas                                   |
| PTL             | Power-to-Liquid                                |
| PY              | Pyrogallol                                     |
| RDE             | Real Driving Emissions                         |
| RME             | Rapeseed Methyl Ester                          |
| RSB             | Roundtable of Sustainable Biofuels             |
| RSM             | Response Surface Methodology                   |
| SCR             | Selective Catalytic Reducer                    |
| SI              | Spark Ignition                                 |
| SO2             | Sulfur Dioxide                                 |
| SOC             | Start of Combustion/State of Charge            |
| SOI             | Start of Injection                             |
| SR              | Standardized Response                          |
| SX              | Specific Emissions                             |
| TDC             | Top Dead Center                                |
| THC             | Total Hydrocarbon                              |
| TTW             | Tank-to-Wheel                                  |
| TWC             | Three-way Catalyst                             |
| VGT             | Variable Geometry Turbine                      |
| WCP             | Water Consumption Potential                    |
| WLTC            | Worldwide harmonized Light vehicles Test Cycle |
| WPO             | Waste Plastic Oil                              |
| WSD             | Wear Scar Diameter                             |
| WTT             | Well-to-Tank                                   |
| WTT CI          | Well-to-Tank Carbon Intensity                  |
| WTW             | Well-to-Wheel                                  |
|                 |  |