Contents

Contents **i**

List of Figures **v**

List of Tables **xv**

Nomenclature **xvii**

1 Introduction **1**
1.1 Motivation 1
1.2 Context 6
1.3 Thesis Objective 8
1.4 Thesis outline 9
References 10

2 Fundamentals and literature review **15**
2.1 Introduction 15
2.2 Diesel-like spray combustion 16
2.2.1 Atomization 17
2.2.2 Evaporation and fuel-air mixing 21
2.2.3 Autoignition 24
2.2.4 Mixing-controlled combustion 26
2.3 OMEn-type fuels 29
2.3.1 Characterization 31
2.3.2 Use of OMEn-type fuels in ICEs. 36
2.3.3 Reference spray flames of OMEn-type fuels 44
2.4 Summary 48
References 50

3 Tools and methodology **65**
3.1 Introduction 65
3.2 Physical properties 67

3.3 Chemical mechanism 69
3.4 Chemiluminescence 72
3.5 Canonical combustion configurations 75
3.5.1 Closed homogeneous reactor 75
3.5.2 Laminar flamelets 77
3.6 CFD model implementation 82
3.6.1 Description of the numerical model 82
3.6.2 Equations of fluid motion 88
3.6.3 Turbulence modelling 89
3.6.4 Turbulence chemistry interaction 99
3.7 Fluid Age 109
3.8 Summary 113
References 113

Appendix **123**
3.A Reaction mechanism and thermodynamic properties of chemiluminescence species 123

4 Canonical configuration results **127**
4.1 Introduction 127
4.2 Closed homogeneous reactor 130
4.3 Laminar flamelets 133
4.4 Chemiluminescence species 138
4.5 A comparison of chemical mechanism and OMEn chain length . 140
4.6 Summary and conclusions 149
References 151

Appendix **155**
4.A Yc definition influence 155

5 Analysis of fuel effects for Spray A within a RANS framework 157
5.1 Introduction 157
5.2 Simulation methodology 158
5.3 Inert spray mixing characteristics 161
5.4 Global combustion parameters 164
5.5 Spray autoignition sequence 167
5.6 Flame structure at quasi-steady state 173
5.7 Summary and conclusions 176
References 178

6 Analysis of fuel and nozzle effects within a LES framework 181

6.1 Introduction . . . 181
6.2 Simulation methodology . . . 182
6.3 Inert spray mixing characteristics . . . 184
6.4 Global combustion parameters validation . . . 191
6.5 Validation of CFD spray combustion evolution by means of experimental diagnostics . . . 196
6.6 Spray autoignition sequence . . . 206
6.7 Analysis of lift-off length stabilization . . . 214
6.8 Analysis of low temperature conditions . . . 224
6.9 Summary and conclusions . . . 231
References . . . 233

Appendix **237**
6.A Particularities of OME1 ignition - SA vs SD . . . 237

7 Conclusions and future works **241**
7.1 Introduction . . . 241
7.2 Conclusions . . . 242
7.3 Future works . . . 247

Global Bibliography **249**