

Contents

	Page
Abstract	III
Nomenclature	VIII
1 Introduction	1
1.1 Background	1
1.2 Simulations in the Development of Diesel Engines	2
1.2.1 Modelling of Combustion Processes	2
1.2.2 PDF-Based Engine Simulations	3
1.2.3 Kinetic Models for Diesel Fuel Surrogates	7
1.3 Motivation and Objectives	8
1.4 Outline of the Work	9
2 Combustion in Diesel Engines	11
2.1 Introduction	11
2.2 Diesel Fuels	11
2.3 Combustion Process Characterisation	12
2.3.1 Fuel Injection and Mixture Formation	13
2.3.2 Ignition and Combustion	14
2.4 Pollutant Formation	17
2.4.1 Exhaust Gas Composition	17
2.4.2 Common Diesel Pollutants	18
2.5 Heat Release by Combustion	21
2.5.1 Thermodynamic Model	22
2.5.2 Characteristic Parameters	23
3 Stochastic Modelling of Diesel Engines	25
3.1 Introduction	25
3.2 Turbulent Reactive Flows	25
3.2.1 Relevance in the Context of Diesel Engines	25
3.2.2 Statistical Modelling and Closure Problem	27
3.3 Probability Density Function (PDF) Modelling	29
3.3.1 Background	29
3.3.2 Statistical Description	30
3.3.3 Composition Joint PDF Transport Equation	35
3.3.4 Monte Carlo Simulations	36

III

3.4	Chemical Kinetics	37
3.4.1	Reaction Kinetics	37
3.4.2	Analysis of Reaction Mechanisms	39
3.4.3	Soot Modelling	40
3.5	Direct Injection Stochastic Reactor Model (DI-SRM)	43
3.5.1	Background	43
3.5.2	Overall Formulation	44
3.5.3	MDF Transport Equation	45
3.5.4	Diesel In-Cylinder Processes	46
3.5.5	Mixing Modelling	49
3.5.6	Numerical Solution	51
4	DI-SRM Tailor-Made for Diesel Engines	53
4.1	Introduction	53
4.2	Mixing Time for the DI-SRM	53
4.3	Direct Fuel Injection and Vaporisation	55
4.4	Model Parameter Studies	59
4.4.1	Design Parameters	59
4.4.2	Accuracy of the Results	61
4.5	Aspects of Chemical Complexity	65
4.5.1	n-Heptane as Diesel Surrogate	66
4.5.2	Reaction Mechanism Effects	66
5	Mixing Time Modelling in the DI-SRM Context	71
5.1	Introduction	71
5.2	Turbulence and Mixing	71
5.2.1	Time and Length Scales	71
5.2.2	Mixing Time Effects	73
5.2.3	Mixing in the DI-SRM	74
5.3	Representative Mixing Time Model	75
5.3.1	Modelling Concept and Assumptions	75
5.3.2	Mixing Time Based on 3D CFD Data	77
5.3.3	Parametrised Mixing Time	79
5.4	Application to Engines with Single Fuel Injection	82
5.4.1	Methodology	82
5.4.2	Validation of the Method	84
5.4.3	Mixing Time Constant	85
5.4.4	Model Performance	87
5.5	Application to Engines with Double Fuel Injection	92
5.5.1	Overall Assumptions	93
5.5.2	Simulation Results	93
5.5.3	Practical Aspects of Simulations	95

6 Engine Simulation Framework for the DI-SRM	99
6.1 Introduction	99
6.2 Simulation Process	99
6.3 Automated Method of Mixing Time Determination	101
6.3.1 Self-Calibration Procedure	101
6.3.2 DI-SRM and Genetic Algorithm	103
6.3.3 Validation of the Method	105
6.3.4 Computations	111
6.4 Parametrised DI-SRM for Engine Performance Studies	111
6.4.1 Overall Concept	112
6.4.2 Computational Setup	113
6.4.3 Mixing Time Tabulation	115
6.4.4 Performance of the Method	118
7 Simulation of Emission Formation and Fuel Effects	125
7.1 Introduction	125
7.2 Fuel Effects Under Diesel Conditions	125
7.2.1 Simulation Method and Surrogate Fuels	126
7.2.2 Chemical Effects of Fuel Composition	128
7.2.3 Engine Performance for Various Fuels	130
7.3 Kinetic Effects in Simulating NO _x Formation	131
7.3.1 Baseline Results	132
7.3.2 Temporary Evolution of NO _x	132
7.3.3 Local Results in ϕ -T Space	134
7.4 Aspects of Simulating Soot for Diesel Engines	135
7.4.1 Locality of Soot Formation	136
7.4.2 Practical Aspects of Soot Modelling	139
8 Summary and Concluding Remarks	141
8.1 General Findings	141
8.2 Conclusions	142
8.3 Recommendations for Future Work	146
References	147
Appendices	159
A Test Engines	159
B Engine Operating Points	160