

Contents

ACKNOWLEDGEMENTS.....
ABSTRACT
ZUSAMMENFASSUNG.....
CONTENTS.....
1 INTRODUCTION.....	1
1.1 Motivation.....	1
1.2 Objective of this study	2
1.3 Structure of the thesis	2
2 LITERATURE REVIEW.....	3
2.1 Turbulent combustion modeling.....	3
2.1.1 Chemistry model.....	5
2.1.2 Turbulence-chemistry interaction.....	6
2.2 Soot modeling.....	9
2.2.1 Soot phenomenology	10
2.2.2 Semi-empirical models	12
2.2.3 Detailed models	14
3 METHODOLOGY.....	19
3.1 Overview CMC activities	19
3.2 CMC related governing equations	20
3.2.1 CMC equations	20
3.2.2 CMC sub-models	22
3.2.3 Soot model	24

Contents

3.2.4	CMC solver and boundary conditions	27
3.3	CFD related governing equations	27
3.3.1	Gas phase	27
3.3.2	CFD-CMC interfacing	30
3.3.3	Spray model	30
4	RESULTS I: SANDIA CONSTANT-VOLUME CHAMBER.....	37
4.1	Experimental test facility	37
4.2	Numerical considerations	40
4.3	Validation of soot model for steady n-heptane sprays	41
4.3.1	Ignition delay and lift-off length.....	41
4.3.2	Flame structure.....	43
4.3.2.1	Unconditional averages	43
4.3.2.2	Conditional averages	45
4.3.3	Soot formation	47
4.3.3.1	Soot reference case A1.....	47
4.3.3.2	Soot model sensitivity analysis.....	48
4.3.3.3	Unconditional quantities.....	49
4.3.3.4	Conditional quantities.....	52
4.3.3.5	Unconditional soot terms.....	55
4.3.4	Comparison with conceptual model	57
4.4	Influence of combustion model	60
4.4.1	Flame structure.....	60
4.4.2	Ignition delay and lift-off length.....	63
4.4.2.1	Discussion on ignition delay.....	64
4.4.2.2	Discussion on lift-off length	69
4.4.3	Soot formation	73
4.4.3.1	Soot averages.....	73
4.4.3.2	Soot source terms.....	75
4.4.4	Short injection case.....	80

5	RESULTS II: WÄRTSILÄ MARINE SPRAY COMBUSTION CHAMBER	85
5.1	Experimental test facility	85
5.2	Numerical considerations	88
5.3	Non-reactive conditions	90
5.4	Reactive conditions	92
5.4.1	Ignition process	92
5.4.2	Lift-off length.....	95
5.4.3	Flame structure.....	96
6	RESULTS III: SANDIA HEAVY-DUTY DIESEL ENGINE	99
6.1	Experimental test facility	99
6.2	Numerical considerations	102
6.3	Validation soot model for reference cases	104
6.3.1	Mixture formation.....	104
6.3.2	Pressure traces and AHRR.....	105
6.3.2.1	HTC cases	105
6.3.2.2	LTC cases.....	107
6.3.2.3	Double injection.....	107
6.3.3	Flame structure.....	108
6.3.3.1	HTC case.....	110
6.3.3.2	LTC case	112
6.3.4	Soot formation	114
6.3.4.1	Sensitivity soot model constants.....	114
6.3.4.2	Algorithm for line-of-sight soot natural luminosity ...	116
6.3.4.3	HTC cases	119
6.3.4.4	LTC cases.....	122
6.3.4.5	Double injection.....	126
6.3.5	Soot structure and discussion.....	128
6.3.5.1	Soot structure	128
6.3.5.2	n-Heptane hypothesis	131
6.3.5.3	Soot oxidation.....	133

Contents

7	CONCLUSIONS	135
7.1	Conclusions.....	135
7.2	Suggestions for future work.....	139
	REFERENCES	141
	APPENDIX	157
	CURRICULUM VITAE	165