

Contents

List of Figures	vi
List of Tables	vii
Nomenclature	ix
1 Introduction	1
1.1 Motivation	1
1.2 Applied methods	2
2 Fundamentals on Hydrogen Combustion Engines	3
2.1 Properties of hydrogen as an engine fuel	3
2.2 Mixture formation strategies for hydrogen engines	4
2.3 Hydrogen research engines investigated	7
3 Modelling Turbulent Flow and Combustion	9
3.1 Governing equations	9
3.1.1 Equations of State	9
3.1.2 Reynolds averaged Navier Stokes equations (RANS)	10
3.2 Classification of turbulent flow and combustion	12
3.2.1 Characteristic numbers for turbulent flow	12
3.2.2 Characteristic numbers for combustion theory	14
3.3 Turbulence models	15
3.3.1 $k - \epsilon$ model	16
3.3.2 $k - \epsilon$ RNG model	17
3.3.3 $k - \omega$ model	17
3.3.4 Shear Stress Transport model	18
3.3.5 Reynolds stress models	18
3.4 Investigated combustion models	19
3.4.1 Species transport vs mixture fraction approach	19
3.4.2 Eddy-Break-Up Model	21
3.4.3 Turbulent Flame Speed Closure with Laminar Flamelet Model	21
3.4.4 Extended Coherent Flame Model	22
4 1D and Quasi-Dimensional Simulation of In-Cylinder Flow	25
4.1 1D hydrogen engine simulations with GTPower	25
4.1.1 Analysis of engine losses	26
4.1.2 Computation of wall temperatures by FSI	28
4.2 Quasi-dimensional combustion simulations with Gasdyn	29
4.2.1 Basics on the fractal combustion model	30

4.2.2	Validation of the combustion simulations	31
4.3	Discussion of the results: Possibilities and limits of 1D engine simulations	31
5	3D CFD Simulation of Cryogenic Mixture Formation	33
5.1	Generation of moving engine meshes	34
5.1.1	General settings	34
5.1.2	Minimum valve lift	34
5.1.3	Local mesh refinement	35
5.1.4	Applied meshing algorithms	36
5.2	Advanced models for cryogenic mixture formation	36
5.2.1	Differential diffusion model	36
5.2.2	Real gas model	37
5.2.3	Recommended models for engine simulations	41
5.3	Simulation setup for mixture formation simulations	41
5.3.1	Solver settings	41
5.3.2	Fluid boundary conditions	42
5.3.3	Wall temperatures	42
5.3.4	Initialisation	43
5.4	Mixture formation simulation in the thermodynamical engine	43
5.4.1	Standard simulation	43
5.4.2	Ideal gas with variable heat capacity	45
5.4.3	Influence of CFD wall temperatures	46
5.4.4	Summary of the thermodynamical engine simulations	47
5.5	Mixture formation simulation in the optical engine	49
5.5.1	Mesh study for mixture formation simulations	50
5.5.2	Study on turbulence models	50
5.5.3	Comparison of the compression pressure traces	51
5.5.4	Comparison to LIF measurements	52
5.5.5	Turbulent kinetic energy during compression	54
5.6	Discussion of the results: 3D CFD mixture formation simulations	55
6	3D CFD Simulation of Premixed Hydrogen Combustion	57
6.1	Strategy for combustion simulations	57
6.1.1	Simulation setup	58
6.1.2	Initialisation of the combustion simulations	58
6.1.3	Ignition modelling	58
6.2	Survey on the applied combustion models	59
6.2.1	Eddy-Break-Up model	59
6.2.2	Turbulent Flame Speed Closure with Laminar Flamelet Model	60
6.2.3	Extended Coherent Flame Model	63
6.3	Combustion simulation in the thermodynamical engine	64
6.3.1	Mesh study for combustion simulations	64
6.3.2	Portability of the model settings to various engine operating points	67
6.3.3	Validation of the computed wall heat flux	68
6.3.4	Summary of the thermodynamical engine simulations	71
6.4	Combustion simulation in the optical engine	72
6.4.1	Modelled optical operating point with combustion	72

6.4.2	Corrective measures for the computed pressure trace	73
6.4.3	Comparison of in-cylinder pressure and burn rate	75
6.4.4	Comparison of computed flame propagation to LIF measurements	76
6.4.5	Summary of the optical engine simulations	77
6.5	Discussion of the results: 3D CFD engine combustion simulations	77
7	Modelling Frost Formation within a Commercial CFD Code	79
7.1	Fundamentals on modelling the formation of frost	79
7.2	Description of the applied model	81
7.2.1	Modelling desublimation of water vapour at a cold surface	81
7.2.2	Computation of the frost surface temperature	84
7.2.3	Modelling the growth of the frost layer	85
7.3	Quantitative validation using a basic test case	86
7.3.1	Experimental boundary conditions	87
7.3.2	Simulation setup	88
7.3.3	Comparison to experimental data	88
7.4	Qualitative validation at a cryogenic hydrogen injection test rig	91
7.4.1	Experimental boundary conditions	91
7.4.2	Simulation setup	91
7.4.3	Comparison to experimentally observed frost growth	92
7.5	Discussion of the results: Coupling of a frosting model to a CFD solver	93
7.5.1	Accuracy of the model	93
7.5.2	Prospect of future improvements of the frost formation model	95
7.5.3	Suitability of the frosting model for engine applications	96
8	Application of the Frost Formation Model	99
8.1	Description of the simulation setup	100
8.1.1	Transient fluid simulation	100
8.1.2	Steady state temperature simulation	102
8.1.3	Necessary simplification of the model geometry	103
8.2	Validation of the FSI model	103
8.2.1	Experimental measurements for the validation of the FSI model	105
8.2.2	Comparison of computed temperatures to experimental data	105
8.3	Simulation of frost formation within the mixture formation unit	106
8.4	How to avoid frost formation	109
8.5	Discussion of the results	111
9	Summary and Outlook	113
9.1	Results achieved	113
9.2	Suggestions for future improvements	114
9.3	Conclusions	115
A	Additional Figures	117
A.1	Figures Chapter 5	117
A.2	Figures Chapter 6	131
A.3	Figures Chapter 7	149

B CFX and ICEM Scripts	150
B.1 ICEM Script for the Delaunay Mesher	150
B.2 CFX solver settings ensuring mass conservation	151
B.3 c_p - Tables	152
B.3.1 Normal- and Para - Hydrogen	152
B.3.2 Nitrogen and Oxygen	153
C Bibliography	154