

Contents

List of Figures	xxi
List of Tables	xxv
Nomenclature	xxvii
1 Introduction	1
1.1 Hydrogen as a Fuel for Internal Combustion Engines	1
1.1.1 Combustion Characteristics of Hydrogen	2
1.1.2 Mixture Formation Strategies for Hydrogen Engines	4
1.1.2.1 External Mixture Formation	4
1.1.2.2 Internal Mixture Formation	5
1.2 Review of Research Activities	7
1.2.1 State-of-the-Art: Hydrogen Engine Technology . . .	8
1.2.1.1 BMW Group, Germany	9
1.2.1.2 MAN Nutzfahrzeuge Group, Germany . . .	10
1.2.1.3 Ford Motor Company, USA	10
1.2.1.4 Technical University of Graz, Austria	10
1.2.1.5 Argonne and Sandia National Laboratories, USA	11
1.2.1.6 University of Ghent, Belgium	12
1.2.1.7 Hydrogen Research Institute, Canada . . .	12

1.2.2	State-of-the-Art: Hydrogen Turbulent Combustion Modelling	12
1.2.2.1	University of Armed Forces Munich, Germany	13
1.2.2.2	Institut Francais du Petrole (IFP), France	14
1.2.2.3	Los Alamos National Laboratories, USA	14
1.2.2.4	University of Leeds, GB	15
1.3	Motivation and Objectives of the Present Work	16
2	Subject of Investigation	19
2.1	Description of Hydrogen Research Engines	19
2.1.1	Thermodynamic Research Engine	19
2.1.1.1	Engine Specifications	19
2.1.1.2	Thermodynamic Engine Operating Points for CFD Validation	21
2.1.2	Transparent Research Engine	22
2.1.2.1	Engine Specifications	22
2.1.2.2	Transparent Engine Operating Points for CFD Validation	24
2.2	Thermodynamic Research Engine Measurements	25
2.2.1	Nitric Oxides Formation	25
2.2.2	Unburned Hydrogen in the Exhaust	27
2.2.3	Indicated Efficiency	28
3	Computational Model	31
3.1	Conservation Equations for Reacting Flows	31
3.1.1	Navier-Stokes Equations	32
3.1.2	Species Transport and Energy Equation	33
3.2	Turbulence Modelling and Wall Treatment	35

3.2.1	Eddy Viscosity Turbulence Models	36
3.2.1.1	The Standard $k-\epsilon$ Model	36
3.2.1.2	The RNG $k-\epsilon$ Model	37
3.2.1.3	The Shear Stress Transport Model	37
3.2.2	The Reynolds Stress Turbulence Model	38
3.3	Initial and Boundary Conditions	39
3.4	Computational Mesh	40
3.4.1	Gas Exchange Phase	41
3.4.2	Hydrogen Injection Phase	42
3.4.3	Compression and Expansion Stroke	43
3.5	Numerical Settings	43
4	Turbulent Combustion Modelling	45
4.1	Classification of Hydrogen Engine Combustion Regimes	45
4.2	The Laminar Flamelet Model	47
4.3	Turbulent Flame Speed Closure Approach	50
4.3.1	The Zimont Model	51
4.3.2	The Bradley Model	53
4.4	Flame Surface Density Approach	56
4.4.1	The Extended Coherent Flame Model	56
4.4.2	Modelling of Turbulent Strain Rate	59
4.5	Ignition Model	60
5	Hydrogen Burning Velocities	61
5.1	Basic Considerations	62
5.1.1	Flame Propagation Relations	62
5.1.1.1	Laminar Flame Front Velocities S_n and S_l	62
5.1.1.2	Laminar Burning Velocities u_n and u_l	63

5.1.1.3	Turbulent Flame Speed U_t	64
5.1.2	Sensitivity on Thermochemical Conditions of the Mixture	64
5.1.2.1	Dependency on Equivalence Ratio	65
5.1.2.2	Dependency on Temperature and Pressure	66
5.1.3	Flame Instabilities of Premixed Hydrogen Combustion	67
5.1.3.1	Thermodiffusive Instabilities	68
5.1.3.2	Hydrodynamic Instabilities	68
5.2	Review of Flame Speed Measurements	69
5.2.1	Investigations of Milton & Keck	69
5.2.2	Investigations of Iijima & Takeno	70
5.2.3	Investigations of C. K. Law et al.	70
5.2.4	Investigations of Verhelst and Bradley et al.	71
5.2.4.1	Experimental Investigations	71
5.2.4.2	Instability Correction of Burning Velocities	72
5.3	Computations with Detailed Chemical Kinetic Model	73
5.3.1	Validation by Experimental Data	73
5.3.2	Laminar Flame Speed at Engine-Relevant Conditions	75
5.4	Measurements on ETH-LAV Compression Machine	77
5.4.1	Investigated Conditions	77
5.4.2	Experimental Setup	78
5.4.3	Estimation of Mixture Homogenisation and Turbulence Intensity	80
5.4.4	Measuring Methods	83
5.4.4.1	Optical Analysis of OH-Chemiluminescence	83
5.4.4.2	Thermodynamic Analysis of Pressure Traces	86
5.4.5	Determination of Laminar Burning Velocities	86

5.4.6	Comparison of Unstable and Stable Flames	88
5.4.6.1	Estimation of the Magnitude of Instability	89
5.4.6.2	Correction of Flame Front Instabilities	90
5.5	Derivation of Laminar Flame Speed Correlations	93
5.5.1	Reaction Mechanism Correlation	94
5.5.2	Extension of Leeds Database	94
5.5.3	ETH-LAV Experimental Correlation (2007)	96
5.5.4	Comparison of Correlations	97
5.6	Summary of Results	102
6	Simulation of Mixture Formation	103
6.1	Transparent Engine Mixture Formation	103
6.1.1	Validation of H ₂ -Injection by LIF Measurements	104
6.1.1.1	Operating Point O1: $\lambda = 2.4$, SOI = -120° CA	104
6.1.1.2	Operating Point O2: $\lambda = 2.4$, SOI = -45° CA	108
6.1.2	Mixture and Turbulence Kinetic Energy Spatial Distribution	109
6.1.2.1	Operating Point O1: $\lambda = 2.4$, SOI = -120° CA	110
6.1.2.2	Operating Point O2: $\lambda = 2.4$, SOI = -45° CA	114
6.2	Thermodynamic Engine Mixture Formation	115
6.2.1	Operating Point D1: $\lambda = 1.0$, SOI = -120° CA	116
6.2.2	Operating Point D2: $\lambda = 1.0$, SOI = -60° CA	117
6.2.3	Operating Point D3: $\lambda = 1.0$, SOI = -25° CA	117
6.2.4	Operating Point D4: $\lambda = 2.4$, SOI = -120° CA	120
6.3	Summary of Results	122
7	Simulation of Heat Release	123
7.1	Sensitivity on Variable Enthalpy and Pressure	124

7.2	Port Fuel Injection Operation	126
7.2.1	The Zimont Model	127
7.2.2	The Bradley Model	130
7.2.3	The Extended Coherent Flame Model	132
7.3	Homogeneous and Stratified DI Operation	135
7.3.1	The Zimont Model	136
7.3.1.1	Pressure Traces and Heat Release Rate . . .	136
7.3.1.2	Characteristic Combustion Properties . . .	139
7.3.1.3	Propagation of Flame Front	141
7.3.1.4	Comparison with Reaction Mechanism Correlation	143
7.3.1.5	Comparison with ETH-LAV Experimental Correlation	145
7.3.1.6	Global Quantities	147
7.3.2	The Bradley Model	149
7.3.2.1	Pressure Traces and Heat Release Rate . . .	149
7.3.2.2	Global Quantities	152
7.3.3	The Extended Coherent Flame Model	154
7.3.3.1	Pressure Traces and Heat Release Rate . . .	154
7.3.3.2	Global Quantities	156
7.4	Multi-Injection Operation	158
7.4.1	Pressure Traces and Heat Release Rate	159
7.4.2	Propagation of Flame Front	161
7.5	Summary of Results	161
8	Conclusions and Outlook	165
8.1	Computational Model	165
8.2	Hydrogen Burning Velocities	167

8.3 Consequences for Engine Combustion Design	169
A Model Coefficients	171
A.1 Turbulence Models	171
A.1.1 The Standard k - ε Model	171
A.1.2 The RNG k - ε Model	171
A.1.3 The Shear Stress Transport Model	172
A.1.4 The Reynolds Stress Turbulence Model	172
A.2 Combustion Models	173
A.2.1 The Zimont Model	173
A.2.2 The Bradley Model	173
A.2.3 The Extended Coherent Flame Model	173
B Hydrogen laminar flame speed correlations	175
B.1 ETH-LAV Experimental Correlation (2007)	175
B.2 Reaction Mechanism Correlation	176
B.3 Extended Leeds Database	177
C Computational Mesh	179
D Hydrogen/Oxygen Reaction Mechanism	181
Bibliography	183
Curriculum Vitae	197