# Contents

**Contents** **i**

**List of Figures** **vii**

**List of Tables** **xiv**

**Nomenclature** **xvii**

**1 Introduction** **1**
1.1 General Context . . . . . 1
1.2 Objectives and Methodology . . . . . 6
1.3 Thesis Outline . . . . . 8
References . . . . . 9

**2 Fundamentals of SCR systems and UWS sprays** **15**
2.1 Introduction . . . . . 15
2.2 $NO_x$ formation mechanisms . . . . . 16
2.2.1 Generation of NO . . . . . 16
2.2.1.1 Thermal mechanism . . . . . 17
2.2.1.2 Prompt mechanism . . . . . 17
2.2.1.3 Fuel mechanism . . . . . 17
2.2.2 Generation of $NO_2$ . . . . . 18
2.3 $NO_x$ limitations, EURO norms . . . . . 19
2.4 $NO_x$ reduction methods . . . . . 21
2.4.1 Pre-combustion methods . . . . . 21
2.4.2 Post-combustion methods . . . . . 21
2.4.2.1 Exhaust Gas Recirculation . . . . . 21

2.4.2.2 $NO_x$ Storage Catalyst . . . 21
2.4.2.3 Selective Catalytic Reduction . . . 22
2.5 Selective Catalytic Reduction . . . 22
2.5.1 UWS dosing units . . . 25
2.5.2 Hydraulic characterization . . . 25
2.5.3 Spray characterization . . . 28
2.5.3.1 Primary Atomization . . . 28
2.5.3.2 Secondary Atomization . . . 31
2.5.3.3 Microscopic spray characteristics . . . 33
2.5.3.4 Macroscopic spray characteristics . . . 38
2.5.3.5 Droplet evaporation . . . 41
2.5.3.6 Droplet impingement . . . 43
References . . . 44

**3 Literature review** **53**
3.1 Introduction . . . 53
3.2 Experimental studies . . . 54
3.3 Computational studies . . . 61
3.3.1 UWS evaporation . . . 62
3.3.2 Spray/wall interaction models . . . 64
3.3.3 Treatment of the spray . . . 65
References . . . 68

**4 Computational Methodology** **77**
4.1 Introduction . . . 77
4.2 Computational Fluid Dynamics Modeling . . . 78
4.2.1 Navier-Stokes equations . . . 79
4.2.2 Turbulence modeling . . . 80
4.2.2.1 Reynolds-Averaged Navier-Stokes . . . 81
4.2.2.2 Large Eddy Simulation . . . 84
4.2.3 Liquid phase representation . . . 86
4.2.3.1 Eulerian-Eulerian treatment . . . 86
4.2.3.2 Eulerian-Lagrangian treatment . . . 89
4.2.4 Numerical methods . . . 97
4.3 Pre-processing . . . 100
4.3.1 Internal flow campaign . . . 101
4.3.1.1 *Generation 1* . . . 102
4.3.1.2 *Generation 2* . . . 105
4.3.1.3 Boundary conditions . . . 105
4.3.1.4 Initial conditions . . . 107

4.3.2 External flow campaign . . . 107
4.3.2.1 Reproduction of the experimental test rig . . . 108
4.3.2.2 Boundary conditions . . . 108
4.3.2.3 Initial conditions . . . 109
4.3.3 Reproduction of a close-coupled SCR system . . . 110
4.3.3.1 Boundary conditions . . . 111
4.3.3.2 Initial conditions . . . 112
4.3.4 Meshing . . . 112
4.3.4.1 Internal flow simulations . . . 114
4.3.4.2 External flow simulations . . . 115
4.4 Solver . . . 118
4.4.1 Mixture Model simulations . . . 118
4.4.2 Volume-Of-Fluid simulations . . . 118
4.4.3 DDM approach of the test rig . . . 119
4.5 Post-processing . . . 122
4.5.1 Internal Flow characterization . . . 122
4.5.1.1 Index based on viscosity . . . 122
4.5.1.2 Index based on TKE . . . 122
4.5.1.3 Index of quality for droplet characterization . 123
4.5.1.4 Hydraulic characteristics . . . 123
4.5.2 Droplet detection and characterization . . . 124
4.5.3 Spray tip penetration and spray angle . . . 125
4.5.4 Breakup Length . . . 126
4.5.5 Chemistry . . . 127
4.5.5.1 Uniformity Index . . . 127
4.5.5.2 Conversion Efficiency . . . 127
References . . . 127

**5 Analysis of the UWS near-field spray 135**
5.1 Introduction . . . 135
5.2 Mixture Model simulations . . . 135
5.2.1 RANS mesh sensitivity study . . . 136
5.2.2 LES quality study . . . 136
5.2.3 Hydraulic characterization . . . 138
5.2.4 Flow morphology . . . 139
5.2.5 Breakup length . . . 144
5.2.6 Effect on the rotation of the geometry on the LES results 146
5.3 Volume-Of-Fluid simulations . . . 149
5.3.1 Introduction of the AMR technique . . . 149
5.3.1.1 Hydraulic validation . . . 150

5.3.1.2 Flow morphology . . . 151
5.3.1.3 VOF Index of quality . . . 152
5.3.2 Performance of *Generation 2* geometry . . . 152
5.3.3 Macroscopic characteristics . . . 155
5.3.3.1 Near-field spray morphology . . . 155
5.3.3.2 Spray penetration . . . 157
5.3.3.3 Spray angle . . . 158
5.3.3.4 Plume interaction . . . 159
5.3.4 Microscopic characteristics . . . 160
5.3.4.1 Determination of the steady-state behavior . . . 160
5.3.4.2 Droplet characterization . . . 162
5.3.5 Coupling with DDM simulations . . . 170
5.4 Conclusions . . . 172
5.4.1 Mixture Model approach . . . 172
5.4.2 Volume-Of-Fluid approach . . . 173
References . . . 174

**6 Analysis of the UWS far-field spray 177**
6.1 Introduction . . . 177
6.2 Validation of the chemical model . . . 178
6.3 Spray characteristics under cross-flow conditions . . . 180
6.3.1 Effect of the injection pressure . . . 182
6.3.2 Effect of the cross-flow velocity . . . 186
6.4 Droplet evaporation dynamics . . . 187
6.4.1 Effect of the injection pressure . . . 188
6.4.2 Effect of the spray injection angle . . . 189
6.5 Conclusions . . . 196
References . . . 197

**7 Characterization of a CC-SCR 199**
7.1 Introduction . . . 199
7.2 LES Index of quality . . . 200
7.3 Analysis of the droplet size PDF . . . 201
7.3.1 Effect of the injection pressure . . . 202
7.3.2 Effect of the exhaust temperature . . . 203
7.3.3 Effect of the number of swirler blades . . . 204
7.4 Analysis of the ammonia generation . . . 204
7.4.1 Amount of ammonia present within the domain . . . 205
7.4.2 Effect on the ammonia generation rate . . . 207
7.5 Analysis of the Uniformity Index . . . 209

7.6 Conclusions . . . . . 210
References . . . . . 212

**8 Maximum entropy principle applied to UWS sprays 213**
8.1 Introduction . . . . . 213
8.2 Theoretical background of the MEP . . . . . 214
8.3 Application of the MEP approach to UWS sprays . . . . . 218
8.4 Conclusions . . . . . 222
References . . . . . 223

**9 Conclusions and Future Work 227**
9.1 Introduction . . . . . 227
9.2 Conclusions . . . . . 227
9.2.1 Near-field study . . . . . 228
9.2.2 Far-field study . . . . . 230
9.3 Future work . . . . . 232

**Global Bibliography 235**