

## CONTENTS

---

<b>1</b>	<b>INTRODUCTION</b>	<b>1</b>
1.1	Context . . . . .	1
1.1.1	Energy mix . . . . .	1
1.1.2	The potential of wastes . . . . .	2
1.1.3	Wastes from automotive residues . . . . .	4
1.2	Fuels produced from Automotive Shredder Residues . . . . .	6
1.3	Combustion considerations . . . . .	10
1.4	Compression ignition and spark ignition . . . . .	11
1.5	Homogenous charge compression ignition . . . . .	12
1.6	Reactivity controlled compression ignition . . . . .	14
1.7	Objectives . . . . .	16
1.8	Thesis outline . . . . .	18
1.9	Publication . . . . .	21
<b>2</b>	<b>FROM CONVENTIONAL FUELS TO ASR FUELS</b>	<b>23</b>
2.1	Crude oil and petroleum products . . . . .	23
2.2	Hydrocarbon compounds . . . . .	24
2.2.1	Paraffins . . . . .	24
2.2.2	Olefins . . . . .	25
2.2.3	Naphthenes . . . . .	25
2.2.4	Aromatics . . . . .	26
2.3	Petroleum fractions . . . . .	27
2.4	Pyrolysis . . . . .	28
2.5	Experimental characterization techniques . . . . .	32
2.5.1	Characterization of the composition . . . . .	32
2.5.2	Characterization of the octane number . . . . .	34
2.5.3	Characterization of the cetane number . . . . .	38
2.5.4	Other properties . . . . .	38
2.6	Prediction methods applied to liquid fuels . . . . .	42
2.6.1	Prediction of the octane numbers . . . . .	42
2.6.2	Prediction of the cetane number . . . . .	47
2.6.3	Prediction of the composition . . . . .	50
2.6.4	Definition of surrogate fuels . . . . .	53
<b>3</b>	<b>METHODOLOGY</b>	<b>55</b>
3.1	Latin hypercube sampling . . . . .	55
3.2	Principal component analysis . . . . .	56
3.3	Artificial neural network . . . . .	59
3.4	Bayesian inference . . . . .	60
<b>4</b>	<b>FIRST INSIGHT OF ASR-DERIVED FUELS IN A COMPRESSION IGNITION ENGINE</b>	<b>63</b>
4.1	Introduction . . . . .	63
4.2	Post-processing of experimental data . . . . .	63
4.3	Comparison with conventional diesel . . . . .	64
4.4	Endurance test with silicon oxydes . . . . .	65
4.5	Endurance test without silicon oxydes . . . . .	68
4.5.1	Comparison of four fuels derived from ASR . . . . .	69
4.5.2	Endurance test . . . . .	71
4.6	conclusion . . . . .	74
<b>5</b>	<b>PREDICTION OF THE COMPOSITION OF ASR-DERIVED FUELS</b>	<b>77</b>
5.1	Introduction . . . . .	77

## CONTENTS

5.2	Description of the method . . . . .	78
5.2.1	Basis of the method . . . . .	78
5.3	Chemical Characterization and Chemical Database . . . . .	80
5.3.1	Chemical characterization . . . . .	80
5.3.2	Chemical database . . . . .	85
5.4	Selection and Characterization of the Properties . . . . .	87
5.4.1	Selection of the properties . . . . .	87
5.4.2	Characterization of the properties . . . . .	92
5.5	Mathematical Models and Resolution . . . . .	94
5.5.1	Pseudo-component definition . . . . .	94
5.6	Results and discussion . . . . .	97
5.6.1	Tuning of the molecule database . . . . .	97
5.6.2	Tuning of the weights . . . . .	100
5.7	Conclusion . . . . .	101
6	PREDICTION OF THE OCTANE NUMBERS WITH A BAYESIAN INFERENCE APPROACH	103
6.1	Introduction . . . . .	103
6.2	Method . . . . .	104
6.2.1	Example . . . . .	109
6.3	Results and discussion . . . . .	111
6.4	Conclusion . . . . .	115
7	PREDICTION OF THE OCTANE NUMBERS WITH AN ARTIFICIAL NEURAL NETWORK APPROACH	117
7.1	Introduction . . . . .	117
7.2	Composition of the studied fuels . . . . .	118
7.3	Properties of the studied fuels . . . . .	120
7.3.1	Thermodynamic properties . . . . .	121
7.3.2	Chemical properties . . . . .	122
7.3.3	Transport properties . . . . .	123
7.3.4	Octane numbers . . . . .	124
7.4	Variable selection and structure of the ANN . . . . .	125
7.5	Results . . . . .	126
7.6	Conclusion . . . . .	132
8	PREDICTION OF THE AUTO-IGNITION	135
8.1	Introduction . . . . .	135
8.2	Experimental section . . . . .	136
8.2.1	Fuel characterization . . . . .	136
8.2.2	Rapid compression machine . . . . .	138
8.3	Theoretical calculations . . . . .	141
8.4	Numerical simulation . . . . .	143
8.5	Results and discussion . . . . .	143
8.5.1	Ignition delays . . . . .	144
8.5.2	Atypical behaviour . . . . .	146
8.5.3	Formulation of a surrogate fuel . . . . .	148
8.6	Conclusion . . . . .	149
9	CONCLUSION	151
10	DISCUSSION AND PERSPECTIVES	155
	Bibliography	157
A	APPENDIX A: COMPOSITION OF THE ASR LIGHT FRACTION	173
B	APPENDIX B: NASA COEFFICIENTS	177
C	APPENDIX C: RESEARCH AND MOTOR OCTANE NUMBERS	179
D	APPENDIX D: TRAINING AND TESTING DATA	183