

Contents

Contents	V
List of figures	IX
List of tables	XIII
Notation	XV
Kurzfassung	XVII
Abstract	XIX
1 Introduction	1
1.1 Structure of this thesis	3
2 Current status of the environmental assessment of CO₂-based C1-chemicals	5
2.1 Introduction to CO ₂ conversion to C1-chemicals	6
2.1.1 Definition and utilization of C1-chemicals	6
2.1.2 Overview of CO ₂ conversion reactions to C1-chemicals	7
2.2 Introduction to life cycle assessment (LCA)	10
2.2.1 Attributional LCA (ALCA) vs consequential LCA (CLCA)	13
2.3 Review of LCA studies for CO ₂ conversion to C1-chemicals	15
3 Introducing a system-wide perspective for LCA	19
3.1 Interactions of CO ₂ -based processes with other life cycles	20
3.2 Competing processes for CO ₂ -based C1-chemicals	21
3.3 Multi-functionality	22
3.4 Use of renewable inputs	28
3.5 Maximum environmental impact reductions for CO ₂ -based processes	29
3.5.1 Environmental impact reductions	30
3.5.2 Maximum environmental impact reductions	31

4	CO₂-to-Chemical – Deriving the environmental impact reductions	33
4.1	Goal and scope definition	34
4.2	CO ₂ -based and fossil-based processes for C1-chemicals	36
4.2.1	CO ₂ -based processes	36
4.2.2	Fossil-based processes	38
4.2.3	Feedstock and utility supply processes	41
4.3	Environmental impacts of CO ₂ -based and fossil-based processes	43
4.4	Maximum environmental impact reductions for CO ₂ -based processes . .	47
4.4.1	Determination of maximum environmental impact reductions . .	47
4.4.2	Interpretation of maximum environmental impact reductions . .	49
4.4.3	Comparison of maximum environmental impact reductions . .	51
4.5	Conclusions	54
5	Power-to-Gas – Use of renewable electricity for CO₂-based processes	57
5.1	LCA method and data	58
5.1.1	Goal and scope definition	58
5.1.2	Process data for Power-to-Gas	61
5.2	Results and discussion	62
5.2.1	Steady-state operation of electrolysis	63
5.2.2	Part-load operation of electrolysis	68
5.3	Conclusions	70
6	Power-to-X – Assessment of utilization options for renewable electricity	73
6.1	LCA method for comparative assessment of Power-to-X systems	74
6.2	Comparison of environmental impact reductions for Power-to-X systems	77
6.2.1	Considered Power-to-X systems	77
6.2.2	Environmental impacts of Power-to-X systems	79
6.2.3	Identification of fossil-based processes replaced by Power-to-X systems	83
6.2.4	Global warming and fossil depletion impact reductions for Power-to-X systems	84
6.2.5	CO ₂ mitigation costs	88
6.3	Conclusions	90
7	CO₂ vs Biomass – Comparison of renewable carbon sources	91
7.1	Introduction	92

7.2	Optimization-based identification of environmentally beneficial process routes	92
7.2.1	Superstructure	92
7.2.2	Linear optimization model	94
7.3	Case study for methanol and methane production	94
7.3.1	Superstructure for case study	95
7.3.2	Global warming impacts for Wood-to-Methanol and Wood-to-Methane	97
7.3.3	Comparison of maximum global warming impact reductions for Wood-to-Methanol and Wood-to-Methane to alternative wood utilization	99
7.3.4	Comparison of CO ₂ and biomass as feedstock for C1-chemicals .	101
7.4	Conclusions	102
8	Summary and conclusions	105
A	Process data for C1-chemicals	111
A.1	Input and output data for CO ₂ -based processes	111
A.2	Input and output data for fossil-based processes	116
A.3	Input and output data for biomass-based processes	118
A.4	CO ₂ capture	121
B	LCA data	123
C	CO₂-to-Chemical	127
C.1	Breakdown of fossil depletion impacts for CO ₂ -based processes	127
C.2	Breakdown of global warming and fossil depletion impacts for fossil processes	129
C.3	Maximum environmental impact reductions with alternative natural gas supply	130
D	Power-to-Gas	135
D.1	Data for construction of electrolysis and hydrogen storage	135
D.2	Sensitivity analysis for maximum environmental impact reductions . .	136
D.2.1	Steady-state operation of electrolysis (use of grid electricity) . .	138
D.2.2	Part-load operation of electrolysis (use of 100 % renewable electricity)	140
D.3	Maximum reduction for further environmental impact categories . . .	141
D.3.1	Steady-state operation of electrolysis	141

D.3.2	Part-load operation of electrolysis	144
E	Power-to-X	145
E.1	Surplus electricity supply and demand	145
E.2	Data for considered Power-to-X systems and conventional processes . .	147
E.3	Results	151
F	Student theses completed within this work	161
	Bibliography	163