CONTENTS

Summary ..... **I**

Zusammenfassung ..... **III**

List of Figures ..... **VIII**

List of Tables ..... **XII**

Abbreviations and symbols ..... **XIV**

1 Introduction **1**

1.1 Background 3
1.2 Aim and scope 4
1.3 Methodology 6

2 Post-combustion CO_2 capture **9**

2.1 Process 10
2.2 Solvents 12
2.2.1 Amines 14
2.2.2 Solutions of alkali salts 20
2.2.3 Ammonia 21
2.2.4 Solutions of amino acid salts 24
2.2.5 Ionic liquids 24
2.3 Solvent selection 25

3 Semi-empirical column model **29**

3.1 Solvent properties 33
3.1.1 CO_2 solubility 34
3.1.2 Heat of absorption 38
3.1.3 Heat capacity 39
3.1.4 Density 40
3.2 Implementation 41
3.2.1 Mass balance, equilibrium, and summation equations 42
3.2.2 Enthalpy balance equations 45
3.3 Model validation 47
3.3.1 Absorber 50
3.3.2 Desorber 54

4 Model development 59

4.1 CO_2 capture unit 59
4.1.1 Absorber 63
4.1.2 Desorber 66
4.2 CO_2 compressor 67
4.3 Power plant 68
4.4 Implementation in EBSILON®*Professional* 72
4.5 Overall process 76
4.5.1 Supply of reboiler heat duty 76
4.5.2 Integration 79
4.5.3 Cooling system 83

5 Energetic evaluation of selected solvents 85

5.1 Basis of comparison 85
5.1.1 Net efficiency penalty and total power loss 86
5.1.2 Reboiler heat duty 86
5.2 Solvent characterisation 88
5.2.1 Temperature limits 88
5.2.2 CO_2 capacity 91
5.2.3 CO_2 capacity increase by overstripping 93
5.3 General impact of CCU on overall process 96
5.3.1 Reboiler temperature and steam quantity 96
5.3.2 Reboiler temperature and steam quality 98
5.3.3 Reboiler temperature, lean loading, and CO_2 compression . 100
5.3.4 Summary 103
5.4 Limitations of semi-empirical column model 104
5.5 Retrofit integration 106
5.5.1 Solution flow rate 106
5.5.2 Reboiler temperature 110
5.5.3 RLHX temperature difference 120
5.6 Retrofit integration with increased crossover design pressure 127
5.7 Greenfield integration 132

6 Conclusions 139

References **145**

A Annex **163**

A.1 Summary of key facts 163
A.2 CO_2 loading definition 164
A.3 Solvent properties 165
A.3.1 CO_2 solubility 165
A.3.2 Heat of absorption 170
A.3.3 Heat capacity 171
A.3.4 Density 174
A.4 Model validation data 176
A.5 Nomograms for graphical CO_2 capture process evaluation 178
A.6 Additional diagrams 182