

Contents

Contents	I
Notation	V
Kurzfassung	XII
Summary	XIII
Publications and Copyrights	XV
1 Introduction	1
2 Screening approaches for biorefinery processes	5
2.1 Biorefineries	5
2.2 Process development	6
2.3 Process screening approaches for biorefineries	8
2.4 Reaction Network Flux Analysis	11
2.4.1 Network construction and input data	12
2.4.2 Model formulation	13
2.4.3 Shortcomings	17
2.5 Consideration of separation steps	17
2.6 Value chain analysis	19
2.6.1 Biomass supply chain	20
2.6.2 Market models	21
2.7 Uncertainties at early design stage	23
2.8 Requirements for a novel screening method	24
3 Process Network Flux Analysis	27
3.1 PNFA development	27
3.1.1 Flux balance	31

3.1.2	Input data	32
3.2	Evaluation of processing pathways	33
3.2.1	Energy demand of pathways	34
3.2.2	Economic efficiency of pathways	43
3.2.3	Sustainability of pathways	48
3.2.4	Allocation	53
3.3	Supply chain design	55
3.4	Market and price modeling	58
3.5	Optimization problem formulation	60
3.5.1	RNFA problem	60
3.5.2	PNFA for processing pathways	61
3.5.3	PNFA for value chains	62
3.6	Summary and conclusions	64
4	PNFA benchmarking with literature, RNFA and conceptual design results	65
4.1	Cost and GWP comparison of PNFA and literature	66
4.1.1	Comparison of minimum selling prices	66
4.1.2	Comparison of investment costs	68
4.1.3	Comparison of global warming potential	70
4.2	Accuracy of the PNFA results for an ethanol production compared to RNFA and conceptual design	70
4.2.1	Conceptual process design for ethanol production	71
4.2.2	Conceptual design results	73
4.2.3	Comparison of RNFA, PNFA and conceptual design results	75
4.3	Summary and conclusions	76
5	Application of PNFA	79
5.1	Single-product biorefinery for fuel production	80
5.1.1	Reaction network	80
5.1.2	RNFA results	82
5.1.3	Analysis of separations	83
5.1.4	PNFA results	85
5.1.5	Sensitivity analysis	94
5.1.6	Heat integration	97
5.1.7	Biomass supply chain design	99
5.2	Analysis of fuel mixtures	107
5.3	Multi-product biorefinery for a co-production of fuel and chemicals	114
5.4	Summary and conclusions	116

6 Biorefinery improvement potential	119
6.1 Key improvement factors	119
6.2 Potential of biotechnology conversions	123
6.2.1 Process screening	125
6.2.2 Future improvement potential	129
6.2.3 Summary	130
7 Conclusions and outlook	131
A Separation models	137
B Green chemistry metrics	141
C Case study parameters	144
C.1 Overview parameters	144
C.2 Reaction network	147
C.3 Energy demand of separations	149
C.4 Properties	153
C.5 Active pathway fluxes	155
C.6 Supply chain data and design	158
C.7 Multi-product biorefinery	162
C.8 Mixtures	163
C.9 Fermentation data	163
C.10 Conceptual design data	170
Bibliography	173