

Table of Contents

1	Introduction.....	1
1.1	Energy Consumption in the Chemical Industry	1
1.2	State of the Art.....	4
1.3	Goal of the Thesis.....	7
1.4	Structure of the Thesis.....	9
2	Documentation based Models of Steam Consumption	10
2.1	Bottom-up Modeling.....	10
2.2	Standard Operating Procedures (SOPs).....	10
2.3	Model Development.....	12
2.3.1	Application Example	20
2.4	Model Uncertainty.....	28
2.4.1	Fuzzy Intervals	29
2.4.2	Application Example	30
3	Statistical Models	34
3.1	System Boundaries.....	34
3.2	Training and Validation Datasets	35
3.3	Stages of Process Design.....	37

3.4	Selection and Classification of Chemical Reactions..	38
3.5	Classification Models	39
3.5.1	Selection of Predictor Variables and Discretization of Target Attribute.....	41
3.5.2	Model Selection and Evaluation.....	46
3.5.3	Selection of Important Rules.....	48
3.6	Probability Density Function Models	50
4	Results Documentation based Approach	52
4.1	Case Study I.....	53
4.1.1	Dataset.....	53
4.1.2	Theoretical Energy Consumption.....	54
4.1.3	Energy Losses.....	55
4.1.4	Sensitivity and Uncertainty Analysis	56
4.1.5	Total Energy Consumption	60
4.2	Case Study II	62
4.2.1	Dataset.....	62
4.2.2	Total Energy Consumption	63
4.2.3	Top-down Energy Modeling	65

4.3	Case Study III	69
5	Results Classification Trees	71
5.1	Model Selection and Evaluation	71
5.2	Selection of Important Rules	78
6	Results Probability Density Function Models	85
6.1	Model Development	85
6.2	Model Evaluation per Reaction Type	89
6.3	Further Parameterization of the Models	91
7	Application of the Statistical Models.....	93
7.1	Case Study I	93
7.2	Case Study II	95
8	Conclusions and Outlook	107
8.1	Practical Relevance and Applications	107
8.2	Outlook	111
8.2.1	Extension of the Modeling Approaches to other Process Parameters	111
8.2.2	Optimization Problem for Selection of Classification Trees	112
	Nomenclature	113

Appendix 117

 A Supporting Information to Chapter 2 117

 B Supporting Information to Chapter 3 121

 C Supporting Information to Chapter 4 145

 D Supporting Information to Chapter 5 160

 E Supporting Information to Chapter 6 169

 F Supporting Information to Chapter 7 177

Bibliography 182

Curriculum Vitae 188