



This Is a Very Good Title That Illustrates What This Great Piece of Work Is All About and That Gives an Impression of What a Long Title Looks Like

vorgelegt von
First name second name
aus Berlin

von der Fakultät III – Prozesswissenschaften
der Technischen Universität Berlin
zur Erlangung des akademischen Grades

Doktor der Ingenieurwissenschaften
- Dr.-Ing. -

genehmigte Dissertation

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Tag der wissenschaftlichen Aussprache: 20. Dezember 2018

Berlin, 2018

*I dedicate this great thesis to my gold fish, which has
always been there for me*

Eidesstattliche Erklärung/Affidavit

Hiermit erkläre ich an Eides statt, dass ich die vorliegende Arbeit selbstständig und eigenhändig sowie ausschließlich unter Verwendung der aufgeführten Quellen und Hilfsmittel angefertigt habe.

FIRST NAME SECOND NAME

Berlin, 24. Dezember 2018

I hereby confirm that I prepared this thesis independently and by exclusive reliance on literature or tools indicated herein.

FIRST NAME SECOND NAME

Berlin, 24th December, 2018

Danksagung/Acknowledgements

Ein paar nette Worte / Some nice words...

Zusammenfassung/Abstract

Deutsch

Dies hier ist ein Blindtext zum Testen von Textausgaben. Wer diesen Text liest, ist selbst schuld. Der Text gibt lediglich den Grauwert der Schrift an. Ist das wirklich so? Ist es gleichgültig, ob ich schreibe: „Dies ist ein Blindtext“ oder „Huardest gefburn“? Kjift – mitnichten! Ein Blindtext bietet mir wichtige Informationen. An ihm messe ich die Lesbarkeit einer Schrift, ihre Anmutung, wie harmonisch die Figuren zueinander stehen und prüfe, wie breit oder schmal sie läuft. Ein Blindtext sollte möglichst viele verschiedene Buchstaben enthalten und in der Originalsprache gesetzt sein. Er muss keinen Sinn ergeben, sollte aber lesbar sein. Fremdsprachige Texte wie „Lorem ipsum“ dienen nicht dem eigentlichen Zweck, da sie eine falsche Anmutung vermitteln. Dies hier ist ein Blindtext zum Testen von Textausgaben. Wer diesen Text liest, ist selbst schuld. Der Text gibt lediglich den Grauwert der Schrift an. Ist das wirklich so? Ist es gleichgültig, ob ich schreibe: „Dies ist ein Blindtext“ oder „Huardest gefburn“? Kjift – mitnichten! Ein Blindtext bietet mir wichtige Informationen. An ihm messe ich die Lesbarkeit einer Schrift, ihre Anmutung, wie harmonisch die Figuren zueinander stehen und prüfe, wie breit oder schmal sie läuft. Ein Blindtext sollte möglichst viele verschiedene Buchstaben enthalten und in der Originalsprache gesetzt sein. Er muss keinen Sinn ergeben, sollte aber lesbar sein. Fremdsprachige Texte wie „Lorem ipsum“ dienen nicht dem eigentlichen Zweck, da sie eine falsche Anmutung vermitteln.

English

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Publications

This thesis is partially based on already published contributions. In the following, these are divided into Journal articles, papers within conference proceedings, oral presentations without papers, and a list of all supervised theses.

The following items do *not* appear in the references at the end of this dissertation when the \printpublication command is used! If you cite the reference in the text as well, it also appears at the end.

Theses are cited using a user-defined entry type in jabref called thesis in which you may enter the type as Bachelorarbeit, Masterarbeit, Bachelor's thesis, ... The entry type is part of the available .bib file in this template. If you want to create it on your own, it contains the entries author, title, school, year, type.

Journal Articles

- E. Esche, C. Hoffmann, M. Illner, D. Müller, S. Fillinger, G. Tolksdorf, H. Bonart, G. Wozny, and J.-U. Repke (2017). MOSAIC - Enabling Large-Scale Equation-Based Flow Sheet Optimization. *Chemie Ingenieur Technik* 89(5), 620–635. doi: 10.1002/cite.201600114

Conference Papers

- A. Penteado, H. R. Godini, E. Esche, G. Lovato, J. A. D. Rodrigues, and J.-U. Repke (2018). Optimal Design of a CO₂ Removal Section for

a Biogas-based Oxidative Coupling of Methane Process. In: *Blucher Chemical Engineering Proceedings*. Editora Blucher. doi: 10.5151 / cobeq2018-co.021

Oral Presentations Without Proceedings

- H. R. Godini, T. Karsten, C. Hoffmann, O. Görke, G. Wozny, and J.-U. Repke (2017). Integrated Membrane Reactors for Efficient Ethylene and Methanol Production. In: *Third European Workshop on Membrane Reactors, Verona, Italy*

Supervised Theses

- C. Hoffmann (2015). Real-time Optimization and Moving-horizon State Estimation for a Hydroformylation Plant. Masterarbeit. Technische Universität Berlin
- C. Hoffmann (2013). Simulation von Absorptionsprozessen mit ASPEN Plus für das Absorptionsmittel Methyldiethanolamin-Piperazin. Bachelorarbeit. Technische Universität Berlin

Contents

List of Figures	i
List of Tables	iii
List of Symbols	v
List of Abbreviations	vii
List of Algorithms	ix
1 Introduction	1
1.1 New Section	2
1.2 New Section	4
2 Theory	7
2.1 New Section	8
2.2 New Section	10
3 Methods	13
3.1 New Section	14
3.2 New Section	16
4 Results and Discussion	19
4.1 New Section	20
4.2 New Section	22
5 Conclusion and Outlook	25
5.1 New Section	26
5.2 New Section	28
References	I
A Appendix 1	A
B Appendix 2	C

List of Figures

1.1	Teeeeeeeeeeeeeeeest	2
2.1	Teeeeeeeeeeeeeeeest	8
3.1	Teeeeeeeeeeeeeeeest	14
4.1	Teeeeeeeeeeeeeeeest	20
5.1	Teeeeeeeeeeeeeeeest	26

List of Tables

1.1	Teeeeeeeeeeeeeeeest	4
2.1	Teeeeeeeeeeeeeeeest	10
3.1	Teeeeeeeeeeeeeeeest	16
4.1	Teeeeeeeeeeeeeeeest	22
5.1	Teeeeeeeeeeeeeeeest	28

List of Symbols

Greek Symbols

Symbol	Description	Unit
α	Non-randomness factor in NRTL-Modell	–
α	Parameter in Gleichung für Verdampfungsenthalpie	J mol^{-1}
α	Trennfaktor für binäre VLEs	–
Δ	Differenz	verschieden
Λ	Parameter in Wilson-Modell	–

Indices

Symbol	Description
i	Index für Komponenten
j	Index für Komponenten
k	Index der Strukturgruppe

Constants

Symbol	Description	Unit
R	Universelle Gaskonstante = 8.314 46	$\text{J mol}^{-1} \text{K}^{-1}$

Latin Symbols

Symbol	Description	Unit
A	Parameter in Antoine-Gleichung	–

List of Symbols

A	Porter-Parameter	-
B	Parameter in Antoine-Gleichung	K
B	Zweiter Virialkoeffizient (Leiden-Form)	$\text{m}^3 \text{mol}^{-1}$
B'	Zweiter Virialkoeffizient (Berlin-Form)	Pa^{-1}

Dimensionless Numbers

Symbol	Description	Definition
Re	Reynoldszahl	$\frac{wd\rho}{\eta}$

Operators

Symbol	Description	Definition
∇	Nabla-Operator	$\left[\frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_n} \right]^T$
rot	Rotationsoperator	$\text{rot } \vec{g} = \nabla \times \vec{g}$

Superscripts

Symbol	Description
E	Exzess
III	Phase/Zustand 3
II	Phase/Zustand 2
I	Phase/Zustand 1

Subscripts

Symbol	Description
0	Reinstoff
0	zu Beginn der Reaktion
c	Kritisch

List of Abbreviations

ab Active bounds

DAE Differential-algebraic equation (system)

SUNDIALS Suite of nonlinear and differential-algebraic equation solvers

List of Algorithms

1.1	Super-AlgoMan.	6
2.1	Super-AlgoMan.	12
3.1	Super-AlgoMan.	18
4.1	Super-AlgoMan.	24
5.1	Super-AlgoMan.	30

1 Introduction

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1 Introduction

need for special content, but the length of words should match the language.

Algorithm 1.1: Super-AlgoMan.

Data: ???**Result:** Hahahaha

initialization;

while möp **do**

bliblubla;

if höhöhö **then**

bipö;

bipö2;

else

ohhhhhhhhh;

end**end**

-
- (Coker, 2007), Coker (2007)
 - (Abrams and Prausnitz, 1975), Abrams and Prausnitz (1975)
 - (NIST Chemistry Webbook, 2017), NIST Chemistry Webbook (2017)
 - (Cuda, 2012), Cuda (2012)

2 Theory

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2 Theory

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3 Methods

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Unit 1	Unit 2	Unit 3
1	2	3
4	5	6

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3 Methods

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Algorithm 3.1: Super-AlgoMan.

Data: ???

Result: Hahahaha

initialization;

while möp **do**

 bliblubla;

if höhöhö **then**

 bipö;

 bipö2;

else

 ohhhhhhhhh;

end

end

- (Coker, 2007), Coker (2007)
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4 Results and Discussion

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4 Results and Discussion

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Data: ???

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 bliblubla;

if höhöhö **then**

 bipö;

 bipö2;

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5 Conclusion and Outlook

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5 Conclusion and Outlook

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Algorithm 5.1: Super-AlgoMan.

Data: ???**Result:** Hahahaha

initialization;

while möp **do**

bliblubla;

if höhöhö **then**

bipö;

bipö2;

else

ohhhhhhhhh;

end**end**

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A Appendix 1

Code A.1: Code example for AMPL.

```
1 reset;    # all blue words are keywords in this language
2             # they are defined in the file 05_Appendix/
3             a_CodeLanguageSpecifications.tex
4
5 model simulation.mod;
6 data simulation.dat;
7 include initial.dat;
8 option ipoptoptions "halt_on_ampl_error,yes";
9
10
11 solve;
```


B Appendix 2

Code B.1: Code example for Matlab.

```
1 clc
2 clear
3 close all
4
5 e0_param = 4;
6
7 j=0;
8 for i=1:e0_params % this loop is incredibly smart
9     if l==2
10         j=j+1;
11     else
12         j=j-1;
13     end
14 end
```