



# **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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2. Gutachterin: Prof. Dr.-Ing. Hans-Georg Wichtig

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.

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FIRST NAME SECOND NAME

Berlin, 24<sup>th</sup> 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 CO<sub>2</sub> 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

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# List of Symbols

## Greek Symbols

Symbol	Description	Unit
$\alpha$	Non-randomness factor in NRTL-Modell	–
$\alpha$	Parameter in Gleichung für Verdampfungsenthalpie	$\text{J mol}^{-1}$
$\alpha$	Trennfaktor für binäre VLEs	–
$\Delta$	Differenz	verschieden
$\Lambda$	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)	$\text{Pa}^{-1}$

## Dimensionless Numbers

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

## Operators

Symbol	Description	Definition
$\nabla$	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

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# 1 Introduction

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Unit 1	Unit 2	Unit 3
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4	5	6

## 1.2 New Section

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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)
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## 2 Theory

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## 2 Theory

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

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**while** möp **do**

bliblubla;

**if** höhöhö **then**

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## 3 Methods

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## d|b|t|a

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

## 3.2 New Section

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like "Huardest gefburn"? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language. Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like "Huardest gefburn"? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of

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### 3 Methods

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

---

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

## 4 Results and Discussion

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### 4.1 New Section

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like "Huardest gefburn"? Kjift – not

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#### 4 Results and Discussion

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

## 4.2 New Section

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#### 4 Results and Discussion

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

---

**Algorithm 4.1:** 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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## 5 Conclusion and Outlook

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

## 5.2 New Section

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## 5 Conclusion and Outlook

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

---

**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 let e0_param := 4;
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
```