



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, 25. 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, 25th 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

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 words should match the language.

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 und 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](https://doi.org/10.1002/cite.201600114)

Conference Papers

- A. Penteado, H. R. Godini, E. Esche, G. Lovato, J. A. D. Rodrigues und 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 und 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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Symbolverzeichnis

Griechische Symbole

Symbol	Beschreibung	Einheit
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	–

Indizes

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

Konstanten

Symbol	Beschreibung	Einheit
R	Universelle Gaskonstante = 8,314 46	$\text{J mol}^{-1} \text{K}^{-1}$

Lateinische Symbole

Symbol	Beschreibung	Einheit
A	Parameter in Antoine-Gleichung	–

Symbolverzeichnis

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}

Dimensionslose Kennzahlen

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

Operatoren

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

Superskripts

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

Subskripts

Symbol	Beschreibung
0	Reinstoff
0	zu Beginn der Reaktion
c	Kritisch

Abkürzungsverzeichnis

ab	Active bounds
DAE	Differential-algebraic equation (system)
SUNDIALS	Suite of nonlinear and differential-algebraic equation solvers

1 Guidelines

1.1 First Steps

- **carefully read this whole chapter**
- check whether you can compile this document without errors (this should always be the case as long as all necessary packages are installed)
- change the necessary entries in meta.tex (i.e. your name, matriculation number, etc.)
- add your own .bib file for your references or use the present one
- check whether biblatex and makeindex were set up correctly whether they are operational (see Sections 1.2.7 and 1.2.9)
- set the language of the document. Currently, you notice that this text is written in English while certain headings are in German. This is because the babel package is currently loaded with ngerman as default language (see Section 1.8).
- remove the guidelines chapter from this document by deleting it and removing it from the o_Text.tex file in the folder o3_Content
- start writing your thesis - good luck!

1.2 Template Structure

This section describes the use of this template. Questions remaining unanswered can be forwarded to Christian Hoffmann (c.hoffmann@tu-berlin.de).

1.2.1 Main Features

- valid for theses or dissertations
- can be used in German and English
- simple generation of list of symbols for latin, greek, etc. with the `nomentbl` package
- simple generation of list of abbreviations with the `acronym` package
- includes DOI/ISBN/URL automatically in references
- includes bibliography via `biblatex` and `biber`

1.2.2 Main Document

- is called `main.tex`
- this document must be executed in `LATEX`

1.2.3 01 _ Document _ administration

In this folder, the following files are located:

- a) `a_Packages.tex`
 - contains all packages, which are loaded
 - packags are sorted based on their application
- b) `b_Commands.tex`
 - contains further commands regarding formatting and look of the document
 - also sorted
- c) `c_Meta.tex`
 - contains meta information regarding author, etc.

- contains a boolean variable to select whether it is a dissertation or a bachelor/master thesis
- d) d_NomenclatureCommands.tex
- defines structure of the list of symbols
 - optional argument defines the class of a symbol (latin, greek, ...)
 - for the generation of the list of symbols, makeindex is used. A short instruction how to run makeindex correctly in texmaker is given below
- e) e_Header_Footer.tex
- defines headers and footer

1.2.4 02_Prematter

In this folder, the following files are located:

- a) a_Cover.tex
- creates the cover page
 - loads either a_Cover_BA_MA.tex (cover of a bachelor/master thesis) or a_Cover_Diss.tex (cover of a dissertation), depending on the value of `isDiss` set in c_Meta.tex
- b) b_Declaration.tex
- declaration that the thesis was written honestly
- c) c_Acknowledgements.tex
- thank important people
- d) d_Summary.tex
- summarize your thesis in German and English
- e) e_Nomenclature.tex
- enter all symbols and explain them

1 Guidelines

- examples are provided
- f) f_Abbreviations.tex
 - enter all abbreviations and explain them
 - examples are provided

1.2.5 02a_Dissertation_files

This folder contains files that are only needed for dissertations. They are only included if `isDiss` is set to `true`. Bachelor/Master theses do not have to consider them. However, if you want to dedicate your thesis to someone, you can of course include the dedication. In this folder, the following files are located:

- a) a_Dedication.tex
 - you can dedicate your thesis to someone
- b) b_Publications.tex
 - states all publications that were written in preparation of the dissertation

1.2.6 03_Content

In this folder, the following files are located:

- a) o_Text.tex
 - loads all single chapters
- b) X_iii.tex
 - contains the single chapters
 - can be split further if deemed necessary

1.2.7 04_Literature

In this folder, the following files are located:

- a) Bibliography.bib
 - contains the literature
 - uses bblatex for the generation of the bibliography
 - to make this work, bblatex (instead of bibtex) must be used
 - in texmaker, change the command in the preferences for bib(la)tex to (hot key standard is still F11)
"C:/path_to/biber.exe" %
 - for other L^AT_EXeditors, please see its respective documentation to find out how to use bblatex there
 - if you write your thesis on a Mac or a Linux distribution, the procedure is probably different. If you find out the right instructions, please forward us a brief summary (c.hoffmann@tu-berlin.de)

1.2.8 05_Appendix

In this folder, the following files are located:

- a) o_Appendix.tex
 - includes all single appendix chapters
- b) X_Appendix.tex
 - contains the Xth appendix
- c) a_CodeLanguageSpecifications
 - can be used to define a set of keywords and comment commands for a certain programming language

- if you want to apprehend your code in your thesis, you can either copy the code to a `lstlistings` environment (see example in Appendix/`1_Appendix.tex`) or even include your files
- more information can be found in the `lstlistings` documentation

1.2.9 Makeindex

- to compile the file correctly, `makeindex` and `biblatex` are used
- command line for `makeindex` (integrated in `texmaker`, hot key standard: F12):

```
"C:/path_to/makeindex.exe" %.nlo -s mynomentbl.list -o %.nls
```

- the necessary `mynomentbl.list` file is located in the template folder
- check your tex editor documentation to find out how to run `makeindex` in another software
- if you write your thesis on a Mac or a Linux distribution, the procedure is probably different. If you find out the right instructions, please forward us a brief summary (`c.hoffmann@tu-berlin.de`)

1.2.10 Compatibility with PDF/A

Dissertations are stored as PDF/A at the university library. To ensure compatibility of this template with PDF/A, the `pdfx` package is used with the option `a-1b`. The compiled PDF was successfully validated with Callas¹, as recommended by the university library². The output is shown in Fig. 1.1.

¹<https://conversion.ub.tu-berlin.de/>, December 2018

²https://www.ub.tu-berlin.de/fileadmin/pdf/Verlag/UV_pdfaDE.pdf, December 2018

Abb. 1.1: PDF/A validation on https://conversion.ub.tu-berlin.de/.

1.3 General Information

- a) the current „Prüfungsordnung“ overrides the following rules if they contradict the „Prüfungsordnung“.
- b) a Master’s thesis is a scientific-technical documentation that must satisfy requirements regarding structure and form. It should be precisely formulated and well-written, i.e. no orthographic or grammar mistakes, etc.
- c) the thesis should be logically structured.
- d) the thesis should present its scientific-technical content while remaining comprehensible. Hence, the author should repeatedly put him- or herself into the position of the reader and evaluate the thesis in this regard.
- e) the Figure, i.e. picture, diagram, photo, is preferred to long explanations.

- f) results must be tractable. Hence, the applied methods, assumptions, boundary conditions, experiments, and computer codes must be pointed out and explained in sufficient detail.
- g) calculations should be documented. This is of course difficult for large models. In this case, the code should be attached to the printed or digital appendix.
- h) the thesis should focus on the central themes and aspects. Other information should be referenced appropriately, but does not have to be repeated extensively.

1.4 Form

- a) the thesis must be written in German or English.
- b) sentences should be comprehensible. Germans tend to formulate complex phrases with many sub-clauses. This should be avoided.
- c) physical units must always be given and stated in SI units. Units must not be stated in brackets:
 - *WRONG:* Pressure P [Pa]
 - *RIGHT:* Pressure P in Pa

The only correct use of square brackets is shown here for the voltage: $[U] = V$, i.e. the unit of the voltage is volt.

- d) a list of symbols and a list of abbreviations must be included. This is done with the `nomentbl` and the `acronym` package in this template. Furthermore, symbols should be explained in the text after their first appearance. A list of algorithms or other lists can be added if necessary.
- e) Figures, Tables, and Equations must be numbered and must be referenced in the text. This is automatically done using the `caption` package (see section 1.9) and the `\ref` command. For example, a Figure is named Figure chapter.Num (Fig. 2.1). The numeration is done automatically in this template.

In addition, Figures and Tables must also be explained and discussed in the text.

- f) Figures should be chosen to support readability and comprehension. Especially, the most important details and relevant labels must be *readable*.
- g) extensive Tables or Figures that are repeatedly referenced in the text should be put in the appendix.
- h) information or data not generated by the author must always be referenced, see information on citations below.

1.5 Format

The format is fixed by this document. Of course, loading additional packages is possible, but aspects, such as font or font size, must remain unchanged.

Although we do not recommend it, writing the thesis in Microsoft Word or others is possible. In this case, the supplied Word template should be used.

1.6 Appearance

- a) the format of the page numbering is already specified and may not be changed.
- b) there is a maximum of four indenture levels in the text and a maximum of three levels in the table of contents.
- c) the sections of the appendix are numerated alphabetically in capital Latin letters. This is already specified in this template.
- d) important aspects can be emphasized with *italics*, **bold writing**, or using the *emphasize command* \emph. Underlining words should be avoided.

- e) paragraphs should not start in the last two lines of a page („Schusterjunge“ or orphen) or end in the first two lines of a page („Hurenkind“ or widow). This is done with the `nowidow` package.

1.7 References and Bibliography

Citations/references are used to

- document and justify one's own statements,
- differ between one's own statements and those made by others,
- help the reader to assess the origin of a statement

All information not generated by the author must be marked with a short reference, which is accompanied by the extensive reference in the bibliography. It is not important if this information appears directly or indirectly in the text.

We either use the authoryear or the numerical short citation. The most important rule is: The references must be complete and follow a consistent format. This is more important than following a specific citation style. If possible, the doi/ISBN of an article/book should be part of the citation. This is also included automatically in this template.

In the following, a few examples for the authoryear short reference are stated. For more information, the reader is referred to the documentation of the `biblatex` package. Biblatex is used because it is compatible with UTF8. Hence, Umlaute, such as ä, do not have to be rewritten as was the case in `bibtex`. Example: (Müller, 2018), see .bib file.

- (Coker, 2007), Coker (2007)
- (Abrams und Prausnitz, 1975), Abrams und Prausnitz (1975)
- (NIST Chemistry Webbook, 2017), NIST Chemistry Webbook (2017)

- (Cuda, 2012), Cuda (2012)

These commands are used as

- Abrams und Prausnitz (1975) stated that thermodynamics are great.
- Thermodynamics are great (Abrams und Prausnitz, 1975).

1.8 Language: English or German?

The language of this document is set with the `babel` package. The order of the loaded languages determines the default language. Usually, `ngerman` is default (and hence the *second*) language. The `babel` package automatically sets the right names for Tables and Figures, provides the correct hyphenation, and does more language-related things. In case the thesis is written in English, the order of the languages when loading the `babel` package must be changed.

If the language is English, it is recommended to change the output decimal marker for SI units (`siunitx` package) to a period. This can be changed in the `a_Packages.tex` file where the `siunitx` package is loaded.

1.9 Templates

1.9.1 Units

Units are very important. However, there are some rules when typesetting units. For example, they are never written in italics. They should also have the right space between them. For this purpose, the `siunitx` package is suggested.

Units can be written as $R = 8,314 \text{ J mol}^{-1} \text{ K}^{-1}$.

1.9.2 Figures

A template for a Figure is given in Fig. 1.2. Use the protected space ~ between Fig. and \ref. Figure 1.2 should not be abbreviated at the beginning of a sentence.



Abb. 1.2: This is the caption of the Figure in the text. It is placed below the Figure. It can be longer here and contain additional information, such as references or keys for the graphs. Note that one line captions are justified. A full stop is automatically added after the last sign.

1.9.3 Tables

A template for a Table is given in Tab. 1.1. Use the protected space ~ between Tab. and \ref. Table 1.1 should not be abbreviated at the beginning of a sentence.

Tab. 1.1: This is the caption of the Table in the text. It is placed above the table. It can be longer and contain additional information. Vertical lines should be avoided in tables. A full stop is automatically added after the last sign.

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

1.9.4 Equations

An exemplary Equation is given in Eq. 1.1. Use the protected space ~ between Eq. and \ref. Equation 1.1 should not be abbreviated at the beginning

of a sentence.

$$a = b. \quad (1.1)$$

1.9.5 Theorems, Lemmas, Proofs, Remarks, Definitions, and Algorithms

All of these items are introduced in the following. Note that frames and their colors are arbitrary. You might want to change the color or the linewidth. You can do this in the `b_Commands.tex` file.

Theorems: Theorems can be defined using the `amsthm` package in combination with the `mdframed` package for a possible frame. An exemplary Theorem is given in Theorem 1.1.

Theorem 1.1 : *Let f be a function whose derivative exists in every point, then f is a continuous function.*

Lemmas: Lemmas can be defined using the `amsthm` package in combination with the `mdframed` package for a possible frame. An exemplary Lemma is given in Lemma 1.1.

Lemma 1.1 : *Given two line segments whose lengths are a and b , respectively, there is a real number r such that $b = ra$.*

Proofs: Proofs can be defined using the `amsthm` package. They are typically not numbered as they follow a certain Theorem or Lemma.

Beweis. To prove it by contradiction, try and assume that the statement is false, proceed from there, and at some point, you will arrive at a contradiction. \square

Remarks: Remarks can be defined using the `amsthm` package in combination with the `mdframed` package for a possible frame. An exemplary Remark is given in Remark 1.1.

Remark 1.1 : *This statement is true, I guess.*

Definitions: Definitions can be defined using the `amsthm` package in combination with the `mdframed` package for a possible frame. An exemplary Definition is given in Def. 1.1. Equation 1.2 can also be referenced.

Definition 1.1 (What the definition defines): *This is a definition. It defines itself.*

$$c = \infty \quad (1.2)$$

Algorithms: Algorithms can be displayed using the `algorithm2e` package. An example is shown in Alg. 1.1.

Algorithmus 1.1: How to write algorithms

Data: this text

Result: how to write algorithm

initialization;

while *not at end of this document* **do**

 read current;

if *understand* **then**

 go to next section;

 current section becomes this one;

else

 go back to the beginning of current section;

end

end

1.9.6 Autorefs

The `hyperref` package also supplies an `\autoref` command that is linked to `babel`. In this case, Fig. or Tab. are localized and you do not have to worry what kind of float is referenced. As stated above, at the beginning of a sentence, the long version of an item should be used (the `\Autoref{label}` command was defined for this purpose):

- See Kap. 1. Kapitel 1 shows that ...
- See Abschn. 1.9. Abschnitt 1.9 shows that ...
- See Abschn. 1.2.9. Abschnitt 1.2.9 shows that ...
- See Abb. 1.2. Abbildung 1.2 shows that ...
- See Tab. 1.1. Tabelle 1.1 shows that ...
- See Gl. (1.1). Gleichung (1.1) shows that ...
- change language ...
- See Chap. 1. Chapter 1 shows that ...
- See Sec. 1.9. Section 1.9 shows that ...
- See Subsec. 1.2.9. Subsection 1.2.9 shows that ...
- See Fig. 1.2. Figure 1.2 shows that ...
- See Tab. 1.1. Table 1.1 shows that ...
- See Eq. (1.1). Equation (1.1) shows that ...

**1.10 The Sectioning
Command for Chapters
Supports not only
the Heading Text Itself
but also
a Short Version Whose
Use can be Controlled**

If your chapters or sections have long titles (which they should not have), you can use an optional argument for chapter or section commands to shorten it in the header. You can even manipulate the chapter or section title. Normally, the use of this option is not necessary.

2 Introduction

3 Theory

4 Methods

5 Results and Discussion

6 Conclusion and Outlook

Literatur

- Abrams, D. S. und J. M. Prausnitz (1975). Statistical thermodynamics of liquid mixtures: A new expression for the excess Gibbs energy of partly or completely miscible systems. *AIChE Journal* 21, 116–128. doi: 10.1002/aic.690210115 (zit. auf den S. 10, 11).
- Coker, A. K., Hrsg. (2007). *Ludwig's Applied Process Design for Chemical and Petrochemical Plants*. Gulf Professional Publishing. ISBN: 9780080469706 (zit. auf S. 10).
- Cuda, P. (2012). Exergoeconomic Analysis and Optimization of Organic Rankine Cycles. *Dissertation*. University of Ontario Institute of Technology. doi: 10.1016/j.energy.2012.01.064 (zit. auf S. 11).
- Müller, D. (2018). Übertriebene Parameterschätzung. *Chemie Ingenieur Technik* 10, 1–2 (zit. auf S. 10).
- NIST Chemistry Webbook (2017). *Benzene - Phase Change Data*. URL: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C71432&Units=SI&Mask=4%5C#Thermo-Phase> (letzter Zugriff 23.05.2016) (zit. auf S. 10).

A Anhang 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 Anhang 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
```