



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, 2019

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

Eidesstattliche Erklärung

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, 10. Januar 2019

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

FIRST NAME SECOND NAME

Berlin, 10th January, 2019

Danksagung

Ein paar nette Worte / Some nice words...

Zusammenfassung

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.

Schlüsselwörter: *Keyword1; Keyword2; Keyword3*

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.

Keywords: *Keyword1; Keyword2; Keyword3*

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 if the \printpublication command is used! If you cite the reference in the text as well, it also appears at the end.

Theses and dissertations are cited using a user-defined entry type in jabref called thesis in which you may enter the type as Bachelorarbeit, Masterarbeit, Dissertation, 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

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 Methylidiethanolamin-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

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	$\text{rot } \vec{g} = \nabla \times \vec{g}$

Superskripte

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

Subskripte

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**
- set the language of the document in the `a_Packages.tex` file with the `babel` package. 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 Abschn. 1.7).
- change the necessary entries in `c_Meta.tex` (e.g. your name, matriculation number, etc.), set the right value of the `isDiss` variable in this file
- check whether `biblatex` and `makeindex` were set up correctly (see Abschn. 1.8.1)
- check whether you can compile this document without errors (this should always be the case as long as all necessary packages are installed). This template was successfully compiled with a `texlive 2017` distribution. **Some problems appeared when users did not have the newest versions of the used packages of this template. If you run into trouble, please update all your packages.**¹
- remove the guidelines chapter from this document by deleting it and removing it from the `o_Text.tex` file in the folder `o3_Content`

¹<https://tex.stackexchange.com/questions/55437/how-do-i-update-my-tex-distribution>,
January 2019

1 Guidelines

- add your own .bib file for your references or use the present one (it is recommended to simply use the given one)
- start writing your thesis - good luck!
- note that not all of the shown items in the following sections *must* be part of your thesis. If a certain aspect does not apply to you, e.g. a List of Algorithms, just remove it from the thesis.

1.2 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.

1.3 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 are preferably 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 Abschn. 1.9) and the `\autoref` command (Abschn. 1.9.7). 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 comprehension. Especially, the most important details and relevant labels must be *readable*.

1 Guidelines

- 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. 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. The commands and some examples are shown in Abschn. 1.9.4.

1.4 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.

1.5 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 automatically achieved with the nowidow package in this template.

1.6 Template Structure

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

1.6.1 Main Features

- valid for theses or dissertations
- can be used with online editors, such as Overleaf, as well (see Abschn. 1.8.3)
- can be used in German and English
- simple generation of List of Symbols (Latin, Greek, etc.) with the nomencltbl package
- simple generation of List of Abbreviations with the acronym package
- includes bibliography via biblatex and biber
- includes DOI/ISBN/URL automatically in references

1.6.2 Main Document

- is called main.tex
- this document must be executed in L^AT_EX

1.6.3 01_Document_administration

The following files are located in this folder:

- a) a_Packages.tex
 - contains all packages, which are loaded
 - packages 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, ...)
 - makeindex is used for the generation of the List of Symbols. A short instruction how to run makeindex correctly in texmaker is given in Abschn. 1.8.1.
- e) e_Header_Footer.tex
 - defines headers and footer

1.6.4 02_Prematter

The following files are located in this folder:

- a) a_Cover_Diss.tex and a_Cover_BA_MA.tex
 - creates the cover page
 - main.tex 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
 - examples are provided
- f) f_Abbreviations.tex
 - enter all abbreviations and explain them
 - examples are provided

1.6.5 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. The following files are located in this folder:

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

1.6.6 03_Content

The following files are located in this folder:

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

1.6.7 04_Literature

The following files are located in this folder:

- a) Bibliography.bib
 - contains the literature

1.6.8 05_Appendix

The following files are located in this folder:

- 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

1.7 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.

1.8 Dependencies

1.8.1 Biblatex and Makeindex

- to compile the file correctly, `biblatex` and `makeindex` are used
- command line for setting up `biblatex` in `texmaker` (see Abb. 1.1):

1 Guidelines

a) Windows:

```
"C:/path_to/biber.exe" %
```

b) Linux:

```
"/usr/path_to/biber" %
```

c) MacOS:

```
"/usr/path_to/biber" %.bcf
```

– in texlive, biber is located in bin/win32.

– command line for setting up makeindex in texmaker (see Abb. 1.1):

a) Windows:

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

b) Linux:

```
"/usr/path_to/makeindex" %.nlo -s mynomentbl.list -o %.nls
```

c) MacOS:

```
"/usr/path_to/makeindex" %.nlo -s mynomentbl.list -o %.nls
```

– in texlive, makeindex is located in bin/win32

– Note that the paths for Mac or a Linux distribution have not been verified yet. If the path differs from what is stated here, please forward us the corrected instructions (c.hoffmann@tu-berlin.de)

– the necessary mynomentbl.list file is located in the template folder

– check your tex editor documentation to find out how to run bibtex (biber) and makeindex in another software

1.8.2 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 Callas², as

²<https://conversion.ub.tu-berlin.de/>, December 2018

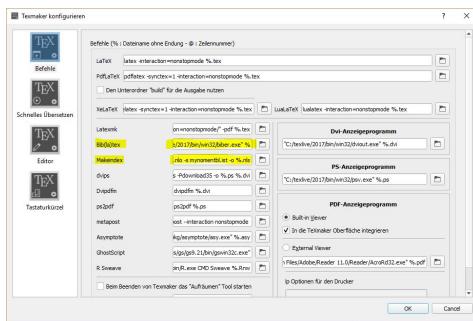


Abb. 1.1: Setting up biblatex and makeindex in texmaker. Zoom in if you need more details.

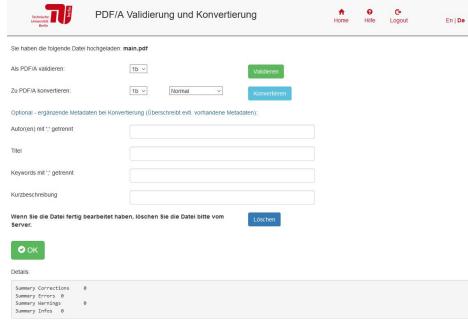


Abb. 1.2: PDF/A validation.

recommended by the university library³. Note that contrary to the descriptions given in the linked document in Fußnote 3, a specific color profile is *not* necessary if you use an up-to-date version of the `pdfx` package as it automatically includes a free color profile. Check the documentation of the `pdfx` package to find how to include other color profiles. Normally, the default should however suffice.

1.8.3 Support for Overleaf or other online editors

- this template was successfully tested with Overleaf, an online editor for \LaTeX documents⁴. If you would like to write in such an online environment, simply upload the template folder to a new empty project and compile it online. In this way, you do not have to install any \LaTeX distribution locally. **Note that this is not advised if you have sensitive data, e.g. from a company in the industry. In this case, your data should remain on your computer!**
- The only necessary change is the support for the `nomentbl` package. As this package needs `makeindex`, you have to tell the Overleaf compiler how to proceed. This information is contained in the `latextmkrc` file in this template folder. Simply upload the `latextmkrc` file to the Overleaf

³https://www.ub.tu-berlin.de/fileadmin/pdf/Verlag/UV_pdfaDE.pdf, December 2018

⁴<https://de.overleaf.com/>, January 2019

project and Overleaf should compile this file correctly. In some cases, you may first have to clear the cache to remove old temporary files⁵.

1.9 Templates

This section introduces templates for the typical elements of a thesis, such as figures, tables, equations, etc.

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.

- Numbers (`\num{number}`): 3,141 592 653 589 793
- Exponentials (`\num[number e 6]{number}`): $1,3 \cdot 10^6$
- Units (`\si{\unit}`): $\text{J mol}^{-1} \text{K}^{-1}$
- Numbers+units (`\SI{number}{\unit}`): $8,314 \text{ J mol}^{-1} \text{ K}^{-1}$
- Ranges (`\SIrange{number1}{number2}{\unit}`): 4 to 10 K.
- Uncertainty (`\num{Number(uncertainty)}`): $410,33 \pm 0,55$
- Uncertainty with units (`\SI{Number(uncertainty)}{\unit}`): $(410,33 \pm 0,55) \text{ J}$

⁵https://www.overleaf.com/learn/how-to/Clearing_the_cache, January 2019

1.9.2 Figures

A template for a Figure is given in Abb. 1.3. Abbildung 1.3 should not be abbreviated at the beginning of a sentence. Note that the often used `\ref` command is not used here. Instead, Abschn. 1.9.7 introduces the `\autoref` command. In addition, a short command for including figures was set up with the `xparse` package:

```
\myfigure [opt1] [opt2] {arg1} [opt3] {arg2} [opt4]
```

Therein,

- `opt1` is the preferred location of the float, e.g. `tbh`
- `opt2` is the fraction of the linewidth the figure should cover. It can be a value between `0` and `1`
- `arg1` is the file name of the figure
- `opt3` is the short caption for the List of Figures
- `arg2` is the caption of the figure in the text
- `opt4` is the label of the figure



Abb. 1.3: 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. Tabelle 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 Unit 1	Entry 2 Unit 2	Entry 3 Unit 3
1	2	3
4	5	6

1.9.4 References

In the following, a few examples of 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.

- Books: (Coker, 2007, S. 221), Coker (2007, S. 221)
- Articles: (Abrams und Prausnitz, 1975), Abrams und Prausnitz (1975)
- Online: (NIST Chemistry Webbook, 2017), NIST Chemistry Webbook (2017)
- Dissertations: (Cuda, 2012), Cuda (2012)
- Bachelor/Master thesis: (Hoffmann, 2015), Hoffmann (2015)

These commands are used as

- `\textcite{bibtexkey}`: „Abrams und Prausnitz (1975) stated that thermodynamics are great.“

- \parencite{bibtexkey}: „Thermodynamics are great (Abrams und Prausnitz, 1975).“

1.9.5 Equations

An exemplary Equation is given in Gl. (1.1). Gleichung (1.1) should not be abbreviated at the beginning of a sentence. The efficient used commands to generate the partial derivative were made with the `xparse` package.

$$\left(\frac{\partial^2 f}{\partial x^2} \right) = \left[\frac{\partial^4 g}{\partial x^4} \right]. \quad (1.1)$$

For important equations, you might want to use the `empheq` package:

$$E = mc^2 \quad (1.2)$$

1.9.6 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 Satz 1.1.

Satz 1.1 (What is theoremed): *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 Hilfssatz 1.1.

Hilfssatz 1.1 (What needs to be lemma'd): *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 numerated as they follow a certain Theorem or Lemma.

What needs to be proven. 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 Bem. 1.1.

Bemerkung 1.1 (What the remarker remarks): *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. Gleichung (1.3) can also be referenced.

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

$$c = \infty \quad (1.3)$$

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

1.9.7 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 remember whether you used Fig. or Figure or something else in the text. 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). Some short forms are equal to their long forms as there is not really a good abbreviation:

a) German ...

- ..., siehe Kap. 1. Kapitel 1 zeigt, dass ...
- ..., siehe Abschn. 1.9. Abschnitt 1.9 zeigt, dass ...
- ..., siehe Abschn. 1.8.1. Abschnitt 1.8.1 zeigt, dass ...
- ..., siehe Abb. 1.3. Abbildung 1.3 zeigt, dass ...

1 Guidelines

- ..., siehe Tab. 1.1. Tabelle 1.1 zeigt, dass ...
- ..., siehe Gl. (1.1). Gleichung (1.1) zeigt, dass ...
- ..., siehe Satz 1.1. Satz 1.1 zeigt, dass ...
- ..., siehe Hilfssatz 1.1. Hilfssatz 1.1 zeigt, dass ...
- ..., siehe Bem. 1.1. Bemerkung 1.1 zeigt, dass ...
- ..., siehe Def. 1.1. Definition 1.1 zeigt, dass ...
- ..., siehe Alg. 1.1. Algorithmus 1.1 zeigt, dass ...

b) English ...

- ..., see Chap. 1. Chapter 1 shows that ...
- ..., see Sec. 1.9. Section 1.9 shows that ...
- ..., see Subsec. 1.8.1. Subsection 1.8.1 shows that ...
- ..., see Fig. 1.3. Figure 1.3 shows that ...
- ..., see Tab. 1.1. Table 1.1 shows that ...
- ..., see Eq. (1.1). Equation (1.1) shows that ...
- ..., see Theorem 1.1. Theorem 1.1 shows that ...
- ..., see Lemma 1.1. Lemma 1.1 shows that ...
- ..., see Remark 1.1. Remark 1.1 shows that ...
- ..., see Def. 1.1. Definition 1.1 shows that ...
- ..., see Alg. 1.1. Algorithm 1.1 shows that ...

1.9.8 Acronyms and Abbreviations

New acronyms must typically be explained at their first appearance in the text. The \ac command uses the defined acronyms (see List of Abbreviations) for doing that. For example, the **Suite of nonlinear and differential-algebraic equation solvers** (SUNDIALS) is explained here, but not afterwards because SUNDIALS was already defined. The same is true for a **Differential-algebraic equation (system)** (DAE). Later on, we just write DAE systems. It seems to be more to write, but thus you make sure that an abbreviations is explained

only at its first appearance ... even if you change your text completely. In addition, you link them to the List of Abbreviations.

1.9.9 Chemistry and Chemical Reactions

Sometimes it is necessary to state chemical reactions or molecules. For this purpose, the `chemfig` and the `mhchem` package are used as shown in Abb. 1.4.

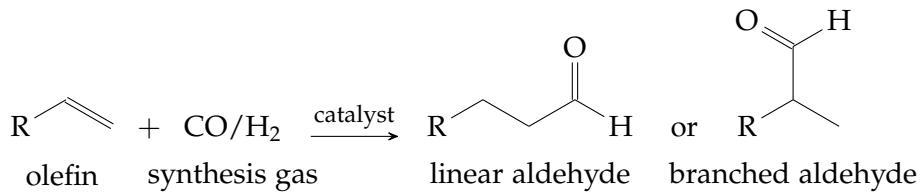


Abb. 1.4: Hydroformylation reaction scheme to demonstrate the two chemistry packages (based on some reference).

**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

Some introducing words ...

2.1 Motivation and Objective

Why this subject is important and what will be shown ...

2.2 Literature Review

What are relevant researchers/publications in this field and why is their work important for this thesis?

2.3 Outline of Work

What will happen in the next chapters?

3 Theoretical Background

Some introducing words ...

In this chapter, all fundamentals that are necessary to understand this work are introduced.

4 Methods

5 Results and Discussion

6 Conclusion and Outlook

Some introducing words ...

6.1 Conclusion

6.2 Outlook and Future Directions

Literaturverzeichnis

- 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. 14, 15).
- Coker, A. K., Hrsg. (2007). *Ludwig's Applied Process Design for Chemical and Petrochemical Plants*. Gulf Professional Publishing. ISBN: 9780080469706 (zit. auf S. 14).
- 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. 14).
- Hoffmann, C. (2015). Real-time Optimization and Moving-horizon State Estimation for a Hydroformylation Plant. *Masterarbeit*. Technische Universität Berlin (zit. auf S. 14).
- Müller, D. (2018). Übertriebene Parameterschätzung. *Chemie Ingenieur Technik* 10, 1–2 (zit. auf S. 14).
- 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. 14).

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
```


C Appendix 3

Especially in the appendix, it is common that long tables appear, which contain experimental or simulated data. For this purpose, the `longtable` environment can be used. The `\autoref` command to reference tables works for them as well (Tab. C.1).

Tab. C.1: This is a longtable, because it is a long table.

Ragged right	Ragged left	Justified	Parbox
Result A	Result B	Result C	Result D
Text.	Text.	Text.	Longer text to create li- ne breaks.
Text.	Text.	Text.	Longer text to create li- ne breaks.
Text.	Text.	Text.	Longer text to create li- ne breaks.
Text.	Text.	Text.	Longer text to create li- ne breaks.
Text.	Text.	Text.	Longer text to create li- ne breaks.
Text.	Text.	Text.	Longer text to create li- ne breaks.

C Appendix 3

Text.	Text.	Text.	Longer text to create li- ne breaks.
Text.	Text.	Text.	Longer text to create li- ne breaks.
Text.	Text.	Text.	Longer text to create li- ne breaks.

Tab. C.2: The caption of a long table on the first page.

Ragged right	Ragged left	Justified	Parbox
Result A	Result B	Result C	Result D
Text.	Text.	Text.	Longer text to create li- ne breaks.
Text.	Text.	Text.	Longer text to create li- ne breaks.
Text.	Text.	Text.	Longer text to create li- ne breaks.
Text.	Text.	Text.	Longer text to create li- ne breaks.
Text.	Text.	Text.	Longer text to create li- ne breaks.
Text.	Text.	Text.	Longer text to create li- ne breaks.
Text.	Text.	Text.	Longer text to create li- ne breaks.

Continued on next page

Tab. C.2 (continued).

Ragged right	Ragged left	Justified	Parbox
Result A	Result B	Result C	Result D
Text.	Text.	Text.	Longer text to create li- ne breaks.
Text.	Text.	Text.	Longer text to create li- ne breaks.