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Title

Tesi di Laurea Magistrale in
Engineering Physics - Ingegneria Fisica

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Abstract

Here goes the Abstract in English of your thesis followed by a list of keywords. The Abstract is a concise summary of the content of the thesis (single page of text) and a guide to the most important contributions included in your thesis. The Abstract is the very last thing you write. It should be a self-contained text and should be clear to someone who hasn't (yet) read the whole manuscript. The Abstract should contain the answers to the main scientific questions that have been addressed in your thesis. It needs to summarize the adopted motivations and the adopted methodological approach as well as the findings of your work and their relevance and impact. The Abstract is the part appearing in the record of your thesis inside POLITesi, the Digital Archive of PhD and Master Theses (Laurea Magistrale) of Politecnico di Milano. The Abstract will be followed by a list of four to six keywords. Keywords are a tool to help indexers and search engines to find relevant documents. To be relevant and effective, keywords must be chosen carefully. They should represent the content of your work and be specific to your field or sub-field. Keywords may be a single word or two to four words.

Keywords: here, the keywords, of your thesis

Abstract in lingua italiana

Qui va l'Abstract in lingua italiana della tesi seguito dalla lista di parole chiave.

Parole chiave: qui, vanno, le parole chiave, della tesi

Contents

Introduction

Writing the introduction to your physics master's thesis on lithium-ion batteries is an important step, and you've made a good start by highlighting the connection between lithium-ion batteries and addressing climate change and CO2 emissions. Here's a more detailed outline of what you might include in your introduction:

1. **Introduction to the Climate Change Problem**: - Begin by providing an overview of the global climate change issue and the environmental consequences of increased carbon dioxide (CO2) emissions. - Mention the growing urgency to reduce greenhouse gas emissions to mitigate the effects of climate change, including extreme weather events, rising sea levels, and other ecological disruptions.

2. **Transportation Sector's Role in Emissions**: - Discuss the role of the transportation sector in contributing to CO2 emissions. Emphasize the significance of this sector in the context of the climate change problem.

3. **Need for Sustainable Solutions**: - Highlight the need for sustainable energy solutions to address the environmental challenges posed by the transportation sector. Mention the increasing demand for electric vehicles (EVs) as an alternative to internal combustion engine vehicles.

4. **Role of Lithium-Ion Batteries**: - Introduce the importance of lithium-ion batteries in the context of the EV industry. Explain their significance as the primary energy storage technology for electric vehicles.

5. **Key Advantages of Lithium-Ion Batteries***: - Enumerate the key advantages of lithium-ion batteries, such as high energy density, rechargeability, and relatively low environmental impact compared to traditional fossil fuels.

6. **Thesis Statement and Objectives**: - Present your thesis statement, which could be something like, "This master's thesis aims to explore the role of lithium-ion batteries in mitigating CO2 emissions from the transportation sector, focusing on their technological aspects, environmental impact, and potential for widespread adoption."

7. **Outline of the Thesis**: - Provide a brief overview of how your thesis is structured,

including the main sections and the order in which you'll address various aspects of lithium-ion batteries, their applications, and their environmental impact.

8. **Significance of the Research**: - Conclude the introduction by emphasizing the importance of your research in contributing to the understanding of lithium-ion batteries' role in addressing climate change and CO2 emissions in the transportation sector.

Remember to make your introduction engaging and clear, setting the stage for the rest of your thesis. It should give the reader a sense of the significance of the topic and motivate them to continue reading to learn more about your research and its implications.

Certainly, in addition to climate change, there are several related and important topics that you might mention in your introduction to provide a more comprehensive context for your thesis. Here are a few additional topics you can consider including:

1. **Energy Transition and Decarbonization**: - Discuss the broader context of the global energy transition and the decarbonization of various sectors, including transportation. - Highlight the goals of reducing greenhouse gas emissions and transitioning to cleaner and more sustainable energy sources.

2. **Challenges in Electrification**: - Address the challenges and barriers associated with the electrification of transportation, such as infrastructure development, range anxiety, and cost considerations. - Discuss how lithium-ion batteries play a role in addressing these challenges.

3. **Global Adoption of Electric Vehicles**: - Highlight the adoption of electric vehicles in different regions of the world and their contribution to reducing CO2 emissions in the transportation sector.

These additional topics can help provide a more comprehensive and holistic context for your thesis. You can choose to incorporate them into your introduction as needed to make the narrative more complete and engaging.

1 | Lithium-ion batteries

The Earth stands at a critical juncture in its history, where the consequences of human activity on the environment have reached a crossroads of global significance. Climate change, driven primarily by the relentless emission of greenhouse gases, has manifested itself in increasingly severe weather patterns, rising sea levels, and ecological disruptions. The urgency of the situation cannot be overstated, as nations grapple with the complex challenge of reducing carbon dioxide (CO_2) emissions to mitigate the impending climate crisis [8, 10, 13].

The dire need for sustainable energy solutions has never been more evident. Various sectors of the economy are challenged to reduce their carbon footprint in order to restrict their impact on climate change. The transport sector was responsible for 23% of global emissions from fuel combustion in 2021 and emerges as a critical contributor to the climate change predicament [4].

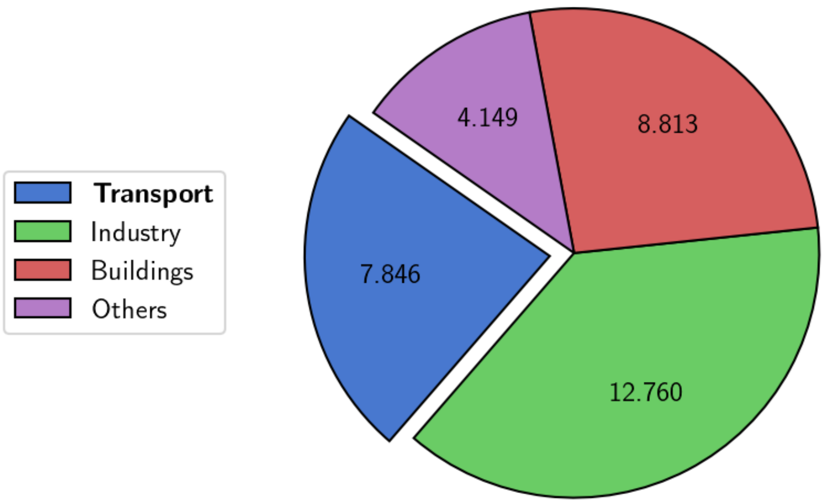

Figure 1.1: 2021 Global CO_2 emissions from fuel combustion by sector [$GtCO_2$]. Source: IEA (2023) [4].

As societies evolve and the global population continues to grow, the demand for transportation, particularly in the form of automobiles and other fossil-fuel-reliant means, has risen dramatically. Innovative solutions are crucial to decouple the connection between personal mobility and CO_2 emissions. Electric vehicles (EVs) have emerged as a promising alternative to traditional internal combustion engine vehicles. They offer the potential to revolutionize the way we commute, significantly diminishing the transportation sector's contribution to carbon emissions.

At the heart of the electric vehicle industry's transformation lie lithium-ion batteries (LIBs). These energy storage devices have rapidly gained prominence as the primary means of powering EVs [12, 15]. The suitability of LIBs for this role is driven by their impressive energy density, rechargeability, and relatively low environmental impact compared to conventional fossil fuels [5]. As we explore the potential of lithium-ion batteries, it becomes evident that their development and adoption may hold the key to mitigating the environmental impact of the transportation sector.

The shortcomings of LIBs are their narrow operational temperature range and charge-discharge rates. The capacity of the battery degrades faster if working at a high temperature, and the lifetime is shortened, too [6, 7]. When LIBs adre subjected to conditions outside of their design window, they may fail through a rapid self-heating or thermal runaway, which may ignite the sorrounding materials [9]. Hence, LIBs require meticolous safety testing in order to guarantee safe use in all usage frameworks. Safety tests must produce reliable parameters to enable satisfactory evaluation and classification of safe battery specifications. The consumer and industrial market demands safe, low-cost, high-power batteries produced with low environmental impact, using sustainable components that enable easy recycling [2].

In the following sections the functioning of lithium-ion batteries is described, followed by a discussion of the safety and degradation issues that arise in LIBs.

1.1. Overview

A lithium-ion battery consists of two electrodes, an electrolyte, a separator, two current collectors and a metal casing. The positive and negative electrode materials are powders that are applied as coatings on current collector foils, resulting in composite electrodes. The ion-conducting electrolyte (containing a dissociated lithium conducting salt) is situated between two electrodes. The separator, an electrolyte-permeable membrane to electrically isolate the two electrodes, is also in that position.

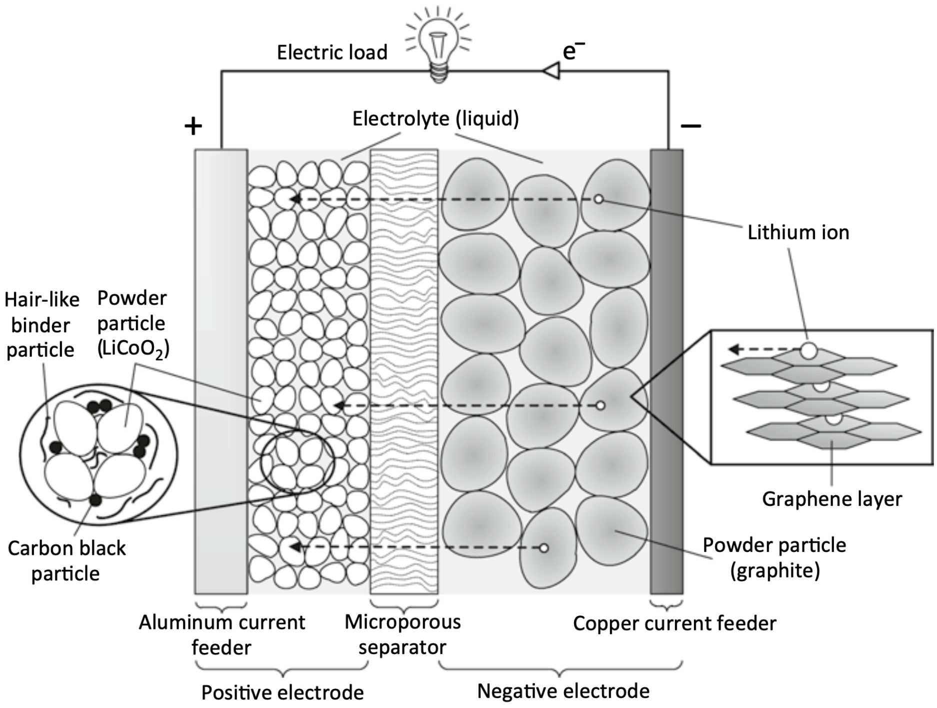

Figure 1.2: Components of a traditional lithium-ion battery during discharging. Source: Korthauer (2018) [5].

The electrolyte conducts the ionic component of the chemical reaction between the anode and the cathode, but it forces the electronic component to traverse an external circuit where it does work. Metallic current collectors deliver electronic current from/to the redox centers of the electrodes to/from the external circuit. These elements are used to produce cylindrical, prismatic and pouch cells. Depending on the application, a single battery cell is used or several cells are connected in series in a module. Also, a parallel connection is possible, dependent on the required capacity. Several connected modules form a battery system for auto-motive applications [3, 5].

1.1.1. Positive Electrode

Lithium transition metal compounds are employed as positive electrode materials. These composites can develop mixed crystals over an ample composition range and can deintercalate lithium ions from the structure during the charging process. The traditional positive electrode material is lithiated cobalt oxide, $LiCoO_2$. It has a layered structure with alternating cobalt, oxygen, and lithium ion layers. During charging, lithium leaves the crystal (deintercalation); during discharging, it returns (intercalation). However, only 50% of the lithium may be utilized. If more than half of the lithium leaves the crystal, the structure may collapse and liberate oxygen. This can cause thermal runaway, as oxygen is able to burn the electrolyte. For complete discharging, the reaction at the positive electrode is:

$$2Li_{0.5}CoO_2 + Li^+ + e^- \rightarrow 2LiCoO_2 \quad (1.1)$$

Thus for one mole (7 g) of active lithium, two moles (189 g) of $Li_{0.5}CoO_2$ are needed as host for lithium during discharge.

The use of cobalt oxide as positive electrode material is not safe. If it is kept "fully" charged as $Li_{0.5}CoO_2$, it reacts slowly with the electrolyte, thus losing performance. If it is slightly overcharged, there is a clear loss in capacity and service life. In case of severe overcharging, the cobalt oxide crystal collapses which can cause thermal runaway and fire. Overcharging easily happens, as there is no obvious voltage difference between normal charging and overcharging. Cobalt oxide is expensive, as cobalt ore is scarce. This problem is getting worse as the demand grows. Economics of scale do not apply here. Last but not least, cobalt is toxic.

The main commercial alternatives for cobalt oxide are listed in Table 1.1. Each of the alternative materials solves some of the problems but they all are compromises. LMO is safer and very cheap but has a limited service life. NCM is safer and cheaper, but has a sloping discharge voltage. NCA is cheaper and lighter (more specific capacity, mAh/g) but it is hardly safer. LFP is very safe and slightly cheaper, but it gives 0.5 V lower voltage than cobalt oxide. At the moment, NCM and LFP seem to be the most promising candidates for large-scale batteries.

Compound	Abbreviation	Chemical structure
Manganese oxide	LMO	$LiMn_2O_4$
Nickel manganese cobalt oxide	NCM	$LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$
Nickel cobalt aluminum oxide	NCA	$LiNi_{0.8}Co_{0.15}Al_{0.15}O_2$
Iron phosphate	LFP	$LiFePO_4$

Table 1.1: Commercial alternatives for cobalt oxide. Source: Korthauer (2018) [5].

1.1.2. Negative Electrode

By far the most common negative electrode material is graphitic carbon. It has carbon atoms in parallel graphene layers. During charging, the lithium ions are intercalated into the graphite, between its layers. During discharging, lithium leaves the graphite. Unlike cobalt oxide, graphite is stable even without lithium, so it can be almost completely discharged. For complete discharging, the reaction at the negative electrode is:

$$\mathrm{LiC_6} \rightarrow \mathrm{Li}^+ + e^- + 6\mathrm{C} \tag{1.2}$$

Thus for one mole (7 g) of active lithium, there are six moles (72 g) of carbon that act as host for the lithium during charging.

Graphite as negative electrode is not safe either. For graphite, the lithium intercalation potential is only about 80 mV more positive than the lithium metal plating potential. Even a small design failure or charging error causes deposition of metallic lithium on the electrode surface. Small amounts of metallic lithium increase the reactivity of the graphite surface, thus consuming electrolyte in secondary reactions. Large amounts of deposited lithium metal can grow as metallic peaks, "dendrites", that short-circuit the negative and positive electrodes. This might cause excess heating and ignite the electrolyte resulting in a fire.

The potential of lithiated graphite is far beyond the stability window of the common electrolytes. During the first charging of the battery, graphite reacts with the electrolyte, building a protective layer on the graphite surface. This solid electrolyte interface (SEI) layer should prevent further secondary reactions. However, some secondary reactions take place throughout the lifetime of the battery, reducing its cyclic and calendar life. Some commercial alternatives for graphite exist. Soft and hard carbons are used due to their slightly more positive intercalation potentials. This means less risk of lithium metal deposition and a possibility of faster charging. However, the energy density is considerably lower when these materials are used. Lithium titanate is a very safe negative electrode material with an amazingly long service life, but the 1.4 V lower cell voltage limits the use of lithium titanate to very few applications. The newest commercial alternative, silicon, gives a formidable energy density, but low stability limits its service life.

Graphite is cheap and lightweight, especially when compared to cobalt oxide. Therefore, it can be expected that graphite retains its position as standard negative electrode material in the near future.

1.1.3. Electrolyte

Electrolytes are an essential component of a lithium-ion battery. The interplay of solvent, conducting salt, and the respective additives forms a complex system. This system must be diligently chosen, and its characteristics must be combined in the most efficient way. At the same time, the electrolyte is not an independent component of the cell. It needs to be chosen in dependence on the materials for the anode and the cathode side. That, in turn, calls for close collaboration between the electrolyte manufacturer and the cell and battery developers. New challenges stem from the new materials of the next-generation batteries, e.g., high-voltage cathodes that demand suitably stable electrolytes not exhibiting a degradation tendency even at such potential levels. In addition to that, these electrolytes should ensure a passivation of the current collectors, which is a challenge on the cathode side at higher potentials. Alongside all these technological requirements, to realize future applications in electric mobility and stationary energy storage, it must be assured that the necessary numbers can actually be produced. [1, 5, 11, 14]

1.1.4. Separator

1.1.5. Current Collectors

1.1.6. Cell Geometries and Designs

1.2. Safety and Degradation

2 | Synchrotron X-Ray Imaging

3 | Useful Things

This document is intended to be both an example of the Polimi LaTeX template for Master Theses, as well as a short introduction to its use. It is not intended to be a general introduction to LaTeX itself, and the reader is assumed to be familiar with the basics of creating and compiling LaTeX documents.
The cover page of the thesis must contain all the relevant information: title of the thesis, name of the Study Programme and School, name of the author, student ID number, name of the supervisor, name(s) of the co-supervisor(s) (if any), academic year. The above information are provided by filling all the entries in the command `\puttitle{}` in the title page section of this template.
Be sure to select a title that is meaningful. It should contain important keywords to be identified by indexer. Keep the title as concise as possible and comprehensible even to people who are not experts in your field. The title has to be chosen at the end of your work so that it accurately captures the main subject of the manuscript.
Since a thesis might be a substantial document, it is convenient to break it into chapters. You can create a new chapter as done in this template by simply using the following command

```
\chapter{Title of the chapter}
```

followed by the body text.
Especially for long manuscripts, it is recommended to give each chapter its own file. In this case, you write your chapter in a separated `chapter_n.tex` file and then include it in the main file with the following command

```
\input{chapter_n.tex}
```

It is recommended to give a label to each chapter by using the command

```
\label{ch:chapter_name}%
```

where the argument is just a text string that you'll use to reference that part as follows: *Chapter 3 contains* AN INTRODUCTION TO . . . .
If necessary, an unnumbered chapter can be created by

```
\chapter*{Title of the unnumbered chapter}
```

In this chapter additional useful information is reported.

3.1. Sections and subsections

Chapters are typically subdivided into sections and subsections, and, optionally, subsubsections, paragraphs and subparagraphs. All can have a title, but only sections and subsections are numbered. A new section is created by the command

```
\section{Title of the section}
```

The numbering can be turned off by using `\section*{}`.
A new subsection is created by the command

```
\subsection{Title of the subsection}
```

and, similarly, the numbering can be turned off by adding an asterisk as follows

```
\subsection*{}
```

3.2. Equations

This section gives some examples of writing mathematical equations in your thesis.

Maxwell's equations read:

$$\begin{cases} \nabla \cdot \boldsymbol{D} = \rho, & (3.1a) \\ \nabla \times \boldsymbol{E} + \dfrac{\partial \boldsymbol{B}}{\partial t} = \mathbf{0}, & (3.1b) \\ \nabla \cdot \boldsymbol{B} = 0, & (3.1c) \\ \nabla \times \boldsymbol{H} - \dfrac{\partial \boldsymbol{D}}{\partial t} = \boldsymbol{J}. & (3.1d) \end{cases}$$

Equation (3.1) is automatically labeled by `cleveref`, as well as Equation (3.1a) and Equation (3.1c). Thanks to the `cleveref` package, there is no need to use `\eqref`. Remember that Equations have to be numbered only if they are referenced in the text.

Equations (3.2), (3.3), (3.4), and (3.5) show again Maxwell's equations without brace:

$$\nabla \cdot \boldsymbol{D} = \rho, \tag{3.2}$$

$$\nabla \times \boldsymbol{E} + \frac{\partial \boldsymbol{B}}{\partial t} = \mathbf{0}, \tag{3.3}$$

$$\nabla \cdot \boldsymbol{B} = 0, \tag{3.4}$$

$$\nabla \times \boldsymbol{H} - \frac{\partial \boldsymbol{D}}{\partial t} = \boldsymbol{J}. \tag{3.5}$$

Equation (3.6) is the same as before, but with just one label:

$$\begin{cases} \nabla \cdot \boldsymbol{D} = \rho, \\ \nabla \times \boldsymbol{E} + \dfrac{\partial \boldsymbol{B}}{\partial t} = \mathbf{0}, \\ \nabla \cdot \boldsymbol{B} = 0, \\ \nabla \times \boldsymbol{H} - \dfrac{\partial \boldsymbol{D}}{\partial t} = \boldsymbol{J}. \end{cases} \tag{3.6}$$

3.3. Figures, Tables and Algorithms

Figures, Tables and Algorithms have to contain a Caption that describe their content, and have to be properly reffered in the text.

3.3.1. Figures

For including pictures in your text you can use `TikZ` for high-quality hand-made figures, or just include them as usual with the command

```
\includegraphics[options]{filename.xxx}
```

Here xxx is the correct format, e.g. `.png`, `.jpg`, `.eps`, ...

Figure 3.1: Caption of the Figure to appear in the List of Figures.

Thanks to the `\subfloat` command, a single figure, such as Figure 3.1, can contain multiple sub-figures with their own caption and label, e.g. Figure 3.2a and Figure 3.2b.

(a) One PoliMi logo.

(b) Another one PoliMi logo.

Figure 3.2: This is a very long caption you don't want to appear in the List of Figures.

3.3.2. Tables

Within the environments `table` and `tabular` you can create very fancy tables as the one shown in Table 3.1.

Title of Table (optional)

	column 1	**column 2**	**column 3**
row 1	1	2	3
row 2	α	β	γ
row 3	alpha	beta	gamma

Table 3.1: Caption of the Table to appear in the List of Tables.

You can also consider to highlight selected columns or rows in order to make tables more readable. Moreover, with the use of `table*` and the option `bp` it is possible to align them at the bottom of the page. One example is presented in Table 3.2.

	column1	**column2**	**column3**	**column4**	**column5**	**column6**
row1	1	2	3	4	5	6
row2	a	b	c	d	e	f
row3	α	β	γ	δ	ϕ	ω
row4	alpha	beta	gamma	delta	phi	omega

Table 3.2: Highlighting the columns

	column1	**column2**	**column3**	**column4**	**column5**	**column6**
row1	1	2	3	4	5	6
row2	a	b	c	d	e	f
row3	α	β	γ	δ	ϕ	ω
row4	alpha	beta	gamma	delta	phi	omega

Table 3.3: Highlighting the rows

3.3.3. Algorithms

Pseudo-algorithms can be written in LaTeX with the `algorithm` and `algorithmic` packages. An example is shown in Algorithm 3.1.

Algorithm 3.1 Name of the Algorithm

Initial instructions
for $for - condition$ **do**
    Some instructions
    if $if - condition$ **then**
        Some other instructions
    end if
end for
while $while - condition$ **do**
    Some further instructions
end while
Final instructions

3.4. Theorems, propositions and lists

3.4.1. Theorems

Theorems have to be formatted as:

Theorem 3.1. *Write here your theorem.*

Proof. If useful you can report here the proof.

3.4.2. Propositions

Propositions have to be formatted as:

Proposition 3.1. *Write here your proposition.*

3.4.3. Lists

How to insert itemized lists:

- first item;
- second item.

How to insert numbered lists:

1. first item;
2. second item.

3.5. Use of copyrighted material

Each student is responsible for obtaining copyright permissions, if necessary, to include published material in the thesis. This applies typically to third-party material published by someone else.

3.6. Plagiarism

You have to be sure to respect the rules on Copyright and avoid an involuntary plagiarism. It is allowed to take other persons' ideas only if the author and his original work are clearly mentioned. As stated in the Code of Ethics and Conduct, Politecnico di Milano *promotes the integrity of research, condemns manipulation and the infringement of* *intellectual property*, and gives opportunity to all those who carry out research activities to have an adequate training on ethical conduct and integrity while doing research. To be sure to respect the copyright rules, read the guides on Copyright legislation and citation styles available at:

`https://www.biblio.polimi.it/en/tools/courses-and-tutorials`

You can also attend the courses which are periodically organized on "Bibliographic citations and bibliography management".

3.7. Bibliography and citations

Your thesis must contain a suitable Bibliography which lists all the sources consulted on developing the work. The list of references is placed at the end of the manuscript after the chapter containing the conclusions. We suggest to use the BibTeX package and save the bibliographic references in the file `Thesis_bibliography.bib`. This is indeed a database containing all the information about the references. To cite in your manuscript, use the `\cite{}` command as follows:

4 | Conclusions and future developments

A final chapter containing the main conclusions of your research/study and possible future developments of your work have to be inserted in this chapter.

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A | Appendix A

If you need to include an appendix to support the research in your thesis, you can place it at the end of the manuscript. An appendix contains supplementary material (figures, tables, data, codes, mathematical proofs, surveys, . . .) which supplement the main results contained in the previous chapters.

B | Appendix B

It may be necessary to include another appendix to better organize the presentation of supplementary material.

List of Figures

List of Tables

List of Symbols

Variable	Description	SI unit
$\boldsymbol{u}$	solid displacement	m
$\boldsymbol{u}_f$	fluid displacement	m

Acknowledgements

Here you might want to acknowledge someone.