Mathematical Modeling of Lithium-ion Batteries and Improving Mathematics Learning Experience for Engineering Students

By
Mohammadmoein Moradi
B.Sc., Imam Khomeini International University (IKIU), 2014

Submitted to the graduate degree program in Mechanical Engineering and the Graduate Faculty
of the University of Kansas in partial fulfillment of the requirements
for the degree of Master of Science.

Thesis Advisor and Committee Chair: Dr. Lin Liu

Committee Member: Dr. Carl Luchies

Committee Member: Dr. Christopher Depcik

Date Defended: 12 December 2017

The thesis committee for Mohammadmoein Moradi certifies that
this is the approved version of the following thesis:

Mathematical Modeling of Lithium-ion Batteries and Improving Mathematics Learning Experience for Engineering Students

Committee Chair: Lin Liu

Date Approved: 30 January 2018

Abstract

Increase in the world's energy consumption along with the environmental impacts of conventional sources of energy (gas, petroleum, and coal) makes the shift to clean energy sources unavoidable. To address the energy needs of the world, using clean energy sources would not provide the sufficient answer to the world's energy issues if it is not accompanied by developing energy storage systems that are capable of storing energy efficiently. Lithium-ion batteries are the main energy storage devices that are developed to satisfy the ever-growing energy needs of the modern world. However, there are still important features of Li-ion battery systems (such as the battery microstructural effects) that need to be studied to a broader extent. In this regard, some of the battery microstructural phenomena, such as the formation of solid electrolyte interface, is believed to be the main reason behind battery degradation and drop in performance. Previous studies have focused on the experimental and computational investigation of micro- and macro- structural features of the Li-ion battery; however, further study is needed to focus on incorporating the effects of microscale features of the Li-ion batteries into the total response of the battery system. In the present work, the details of developing a multiscale mathematical model for a Li-ion battery system is explained, and a multiscale model for the battery system is developed by employing variational multiscale modeling method. The developed model is capable of considering the effects of the battery microstructural features (e.g., the random shape of the active material particles) on the total battery performance. In the developed multiscale framework, the microstructural effects are accounted for in the governing equations of the battery macroscale with the help of Green's function and variational formulation. This part of the present work provides a clear framework for understanding the details and process of developing a multiscale mathematical model for a Li-ion battery system.

Learning mathematics is essential in engineering education and practice. With increasing number of students and emergence of online/distance learning programs, it is critical to look for new approaches in teaching mathematics that different in content development and design. Special consideration should be in place in designing an online program for teaching mathematics to ensure students' success and satisfaction in the engineering curriculum. Previous investigations studied the effects of enrolling in online programs on students' achievement. However, more implementations of such educational frameworks are needed to recognize their shortcomings and enhance the quality of online learning programs. In addition, the idea of the blended classroom should be put into practice to a further extent to ensure the high-quality development of online instructional content. In this work, an online learning program was provided for engineering students enrolled in an introductory engineering mechanics course. Online interactive instructional modules were developed and implemented in the targeted engineering course to cover prerequisite mathematical concepts of the course. Students with access to the developed online learning modules demonstrated improvement in their learning and recommended employing such modules to teach fundamental concepts in other courses. This part of the work improves the understanding

of the development process of the online learning modules and their implementation in lecture-based classrooms.

Acknowledgments

I would like to take the opportunity to express my gratitude to all who have provided help and assistance during my graduate studies and writing of my thesis.

I would like to first thank my advisor and committee chair, Dr. Lin Liu for his support during the last two and a half years, and my committee members, Dr. Carl Luchies and Dr. Christopher Depcik for their invaluable help, time, and insights.

I would also like to express my sincerest and deepest gratitude and appreciation to my family, especially my parents, for their endless and priceless support.

I would also like to thank all my friends, especially Morteza Alipanahrostami, Nourouddin Sharifi, Masoud Farahmand, Ali Rahmati, Shayan Akbari, Hossein Seyfollahzadeh, Javad Namazian, Hamid Ghasemi, and Mohammad Kazemi who supported and helped me during my master's studies from the beginning to the end.

TABLE OF CONTENTS

Abstract....iii

Acknowledgments....v

List of Figures....x

List of Tables....xii

PART I. Mathematical Modeling of Lithium-ion Batteries....1

Chapter 1. Introduction....1

1.1 Motivation....1

1.2 Energy Conversion Systems....3

1.2.1 Fuel Cells....4

1.3 Energy Storage Systems (ESSs)....6

1.3.1 Lithium-ion Battery (LIB)....7

1.4 Research Objectives....8

1.5 Thesis Part I Organization....8

1.6 References....8

Chapter 2. Literature Review....12

2.1 Introduction....12

2.2 LIB Configurations....12

2.3 LIB Mathematical Modeling....14

2.4 Electrochemical Modeling and Analysis....16

2.5 Multiscale Nature of LIBs....18

2.6 Multiscale Modeling Methods....19

2.7 Conclusion....23

2.8 References....23

Chapter 3. Variational Multiscale Modeling of LIB....38

3.1 Introduction....38

3.2 Methods....40

3.2.1 LIB Electrochemical Modeling....40

3.2.2 Stabilized Methods and Multiscale Modeling....41

3.2.3 Variational Multiscale Modeling....44

3.3 Conclusion....49

3.4 Appendix....50

3.5 References....50

Chapter 4. Conclusion and Scientific Contribution....55

4.1 Conclusion....55

4.1.1 Summary....55

4.1.2 Variational Multiscale Modeling of LIB....55

4.2 Scientific Contributions....55

4.3 Future Work Recommendation....56

PART II. Online Learning in Engineering Education: Theory and Practice....57

Chapter 1. Introduction....57

1.1 Motivation....57

1.2 Engineering Education....60

1.3 Research Objectives....60

1.4 Thesis Part II Organization....60

1.5 References....60

Chapter 2. Literature Review....62

2.1 Online and Distance Learning....62

2.2 Technology Integrated Classrooms....63

2.3 Online Learning: Background Theories....63

2.4 Online Interactive Instructional Modules 68
2.5 Conclusion 69
2.6 References..........70
Chapter 3. Identifying Important Aspects in Developing Interactive Instructional Videos ..77
3.1 Introduction..........77
3.2 Methodology..........78
3.3 Results and Discussion 80
3.3.1 Videos 80
3.3.2 Limitations..........82
3.3.3 Future Work..........83
3.4 Conclusion 83
3.5 References..........83
Chapter 4. Enhancing the Teaching-Learning Effectiveness: Creating Online Interactive Instructional Modules 86
4.1 Introduction..........86
4.1.1 Prior Knowledge 86
4.1.2 Benefits of Online Supplementary Instruction 87
4.1.2.1 Individualized, Self-Paced Instruction..........87
4.1.2.2 Presence in Online Instruction..........87
4.1.2.3 Cognitive Apprenticeship 88
4.1.3 Integrating Self-Testing into Study Sessions..........89
4.2 Methods..........89
4.2.1 Procedure 89
4.2.2 Participants..........90
4.2.3 Modules..........91

4.2.4 Measures 91

4.2.4.1 Questionnaire: Demographic, Academic, and Social Background Data 91

4.2.4.2 Pre- and Post- Quiz 91

4.2.4.3 Pre- and Post- Test 92

4.2.4.4 Survey 92

4.2.5 Data Analysis 92

4.3 Results and Discussion 93

4.4 Conclusion 98

4.5 References 98

Chapter 5. Conclusion and Scientific Contribution 103

5.1 Conclusion 103

5.1.1 Summary 103

5.1.2 Identifying Important Aspects in Developing Interactive Instructional Videos 103

5.1.3 Enhancing the Teaching-Learning Effectiveness: Creating Online Interactive Instructional Modules 103

5.2 Scientific Contributions 104

5.3 Future Work Recommendations 104

List of Figures

PART I. Mathematical Modeling of Lithium-ion Batteries

Figure 1.1. World Energy Consumption (quadrillion Btu) for OECD* and non-OECD countries, 1991-2040 [15]..1

Figure 1.2. OECD and non-OECD net electricity generation (trillion kilowatt-hours), 1990-2040 [15]...2

Figure 1.3. World net electricity generation by fuel (trillion kilowatt-hours), 2012-40 [15]......2

Figure 1.4. U.S. net electricity generation from select fuels (billion kilowatt-hours) [16] 3

Figure 1.5. Solar cells in a solar farm, South Burlington VT [29] 4

Figure 1.6. Environmental benefits of the SOFC [44]...5

Figure 1.7. An electrical power profile, illustrating the demand variation over a 24-hour period [47]...6

Figure 1.8. Schematic of a battery structure [47]..7

Figure 2.1. Comparison of different battery systems (volumetric and gravimetric energy density) [2]..12

Figure 2.2. A common LIB schematic [6]...13

Figure 2.3. Schematic of a simple electrical circuit model of a LIB [75]...................................15

Figure 2.4. LIB schematic during discharge [79]...16

Figure 2.5. Multiscale character of an electrode of a LIB [123]...19

Figure 3.1. SEM image of a LIB cathode [26] 39

Figure 3.2. Schematic diagram of decomposing battery domain for application of VMM in LIB simulation..45

PART II. Online Learning in Engineering Education: Theory and Practice

Figure 1.1. Overall higher education enrollment: fall 2014 [3]...58

Figure 1.2. Student enrollment in distance education courses exclusively: fall 2014 [3] 59

Figure 2.1. Models for incorporation of online learning in educational curriculum [11]...........62

Figure 2.2. Student engagement against the length of the videos [120].....................................69

Figure 3.1. Camtasia start screen 79

Figure 3.2. Screenshots of quizzing, markers, and callouts features of Camtasia 80

Figure 3.3. Menu and quiz in the video 81

Figure 3.4. Feedback and callout 82

Figure 4.1. Flowchart of the study 90

Figure 4.2. Participants' age distribution 94

Figure 4.3. Participants' performance overall the two tests....94

Figure 4.4. Distribution of survey questions feedback in percentages 96

List of Tables

PART I. Mathematical Modeling of Lithium-ion Batteries

Table 3.1. List of symbols..50

PART II. Online Learning in Engineering Education: Theory and Practice

Table 1.1. Enrollment in degree-granting postsecondary institutions (in thousands), from fall 2000 through fall 2016 [1]..57

Table 1.2. Total fall enrollment in degree-granting postsecondary institutions (in thousands), from 2000 through 2016 [1]..58

Table 4.1. Age of participants in two groups (α=0.05)..93

Table 4.2. Mean, median and standard deviation of test scores 95

Table 4.3. t-test results for the collected data (α=0.05) 95

Table 4.4. Survey results..95

PART I. Mathematical Modeling of Lithium-ion Batteries

Chapter 1. Introduction

1.1 Motivation

Energy consumption and consequential environmental issues are primary concerns in modern days that need to be addressed. There have been efforts in finding energy sources other than conventional fossil fuels [1, 2] that are clean and sustainable. Policies have been proposed by some countries, China in particular [3], to reduce the amount of emission and pollution caused by energy consumption in a specific period. Additionally, there have been investigations regarding job market changes in case of shifting from traditional sources of energy, such as fossil fuels, to cleaner and more sustainable, renewable energy sources [4-9] with some reports claiming benefits and positive results on economic and job growth [10-14]. One major factor in the search for new and clean energy sources is the increasing demand for energy in the world. According to a 2016 International Energy Outlook (IEO) report [15], the world consumption of energy is projected to rise from “549 quadrillion British thermal units (Btu) in 2012 to 629 quadrillion Btu in 2020” (see Figure 1.1).

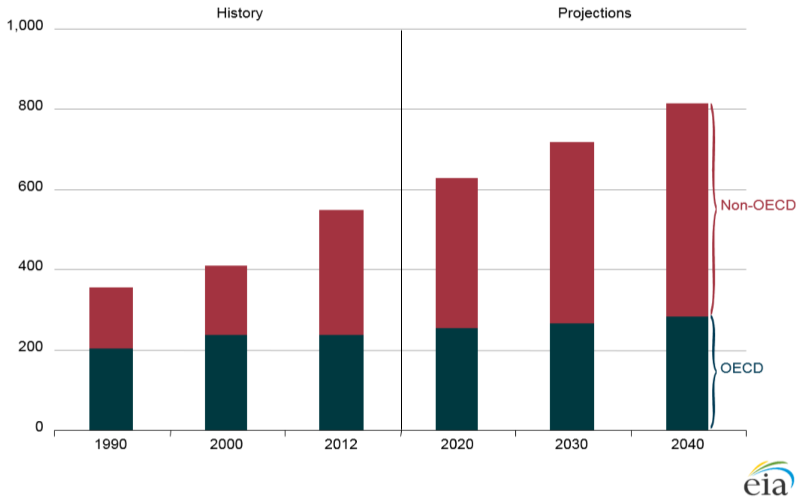


Figure 1.1. World Energy Consumption (quadrillion Btu) for OECD* and non-OECD countries, 1991-2040 [15]

* Countries that are members of the Organisation for Economic Co-operation and Development

According to the IEO report [15], there is an increase in the production of electricity in the world (Figure 1.2). Furthermore, the increase in electricity generation is accompanied by increasing usage of renewable energy sources for electricity production. This increase has led to the recognition of renewable sources as the fastest-growing source of energy for generating electricity with a 2.9% projected annual increase from 2012 to 2040; see Figure 1.3.

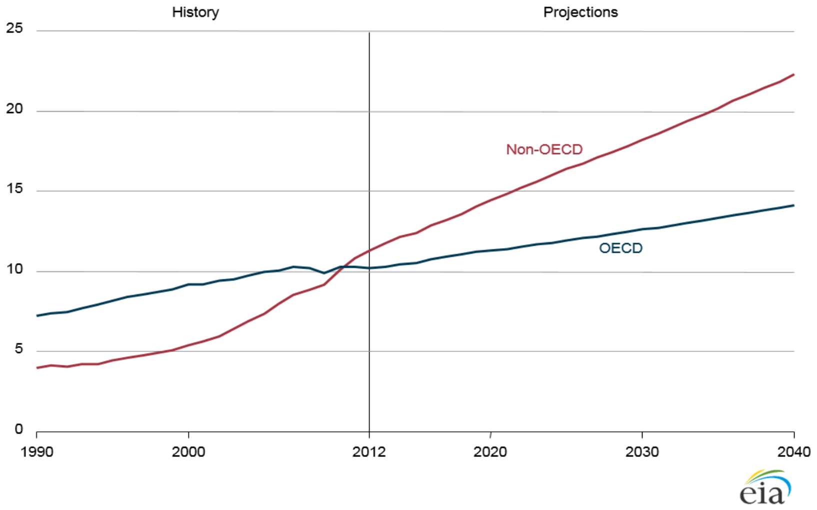


Figure 1.2. OECD and non-OECD net electricity generation (trillion kilowatt-hours), 1990-2040 [15]

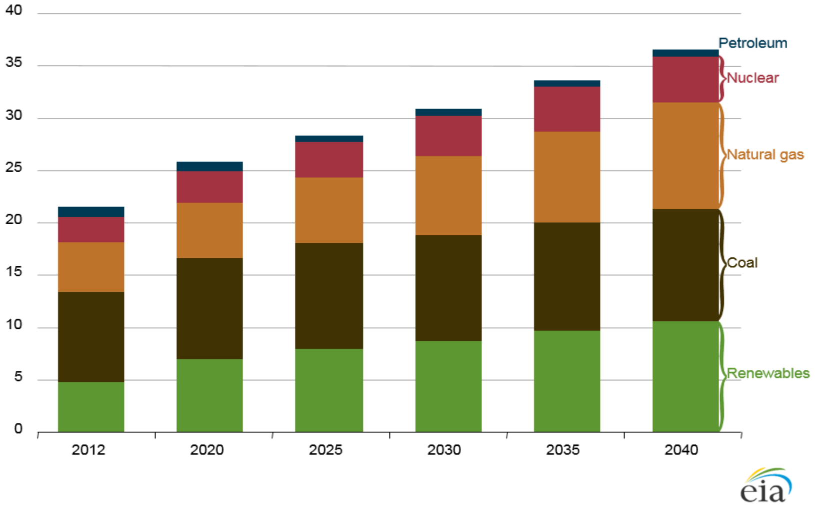


Figure 1.3. World net electricity generation by fuel (trillion kilowatt-hours), 2012-40 [15]

The same trend in the contribution of renewables in electricity generation can be noticed in a recently released report from the U.S. Energy Information Administration [16]. As can be noted from Figure 1.4, the increasing trend in the utilization of renewable sources indicates that a shift from petroleum to renewable sources is inevitable.

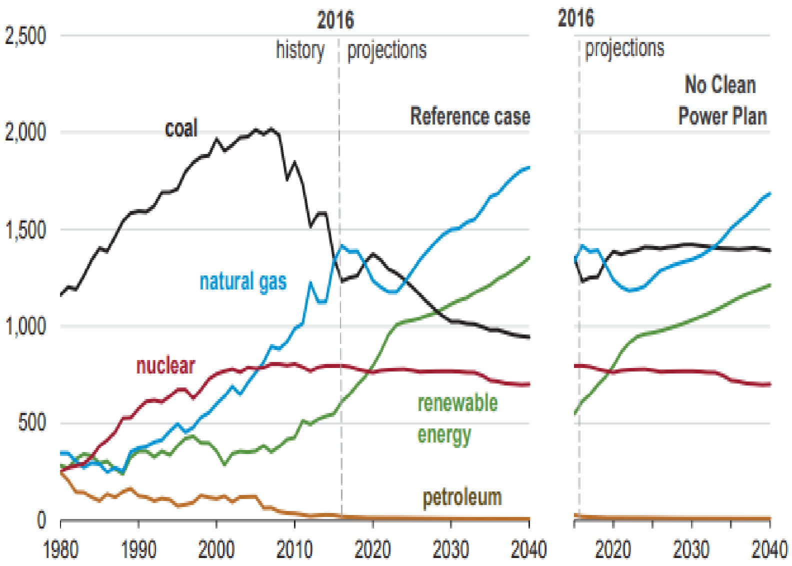


Figure 1.4. U.S. net electricity generation from select fuels (billion kilowatt-hours) [16]

Besides energy supply, energy generation is another important subject in the energy demand and supply chain. Energy storage devices have been developed to provide answers to the important issue of energy storage, and batteries emerged as one of the prominent devices used to store electrical energy. Understanding the behavior and characteristics of such devices is decisive for design and manufacturing processes. While experimental studies are important in studying any battery system, there also needs to be a computational framework to study cases which are expensive, either regarding monetary or time resources, to be experimentally investigated. The importance of simulation and computational analysis is undeniable in the design and optimization of a battery system. It should also be noted that there should be a careful examination of developed models and frameworks so that the computational model represents the actual system with reasonable accuracy. There have been efforts to make battery models more accurate and close to real systems and a variety of models have been proposed in the literature [17-28]. Therefore, developing models of battery systems that are more realistic and close to real systems is of substantial importance in both battery modeling and simulation.

1.2 Energy Conversion Systems

Development and utilization of energy conversion systems will tremendously help in meeting the increasing demands of energy consumption in the modern world. Therefore, along with the research on energy storage, the concept of energy conversion has also been the topic of investigation for decades. Transforming energy from one form to a desired energy form for a certain application is the basis of energy conversion systems. Windmills are some of the early examples of energy conversion systems which date back to centuries ago. More advanced conversion systems have been developed since, with the main focus being on transforming different forms of energy into electricity and providing electrical power. To mention Some of the examples of the more advanced energy conversion systems, one can point out solar cells (Figure 1.5) and fuel cells.

Figure 1.5. Solar cells in a solar farm, South Burlington VT [29]

Unlike traditional energy conversion systems, such as internal combustion engines, advanced energy conversion systems (e.g., fuel cells) follow a direct conversion method. Such modern systems transform the initial form of energy directly to electricity without transforming the primary energy to an intermediate state (e.g., thermal energy) in the conversion process. Since the system characteristics of fuel cells match the features of battery systems closely, a brief review of such systems is presented in the next part of this chapter.

1.2.1 Fuel Cells

Since the invention in 1839 by William Grove, fuel cell design and application have been improved and expanded significantly. As noted by Grove [30], fuel cells are capable of working with various reactants, including ethylene, carbon monoxide, and hydrogen. But Grove's fuel cells were not practical for power production from hydrogen and oxygen [31]. Mond and Langer tried to improve Grove's work by improving the performance of the cell [32]. Mond and Langer improved the structure of the Grove's cell electrodes by giving them a porous structure, and thus, their fuel cell has this one feature in common with modern low-temperature fuel cells [31]. Further development of fuel cells was made following the work of Baur [31] that improved the operating temperature of fuel cells compared to the work of Mond and Langer. The application of fuel cells expanded in the 20th century, as the cell developed by Bacon [33], was modified by Pratt and Whitney and eventually used in Apollo lunar missions [31].

There are different types of fuel cells. A brief description of some the common types of fuel cell systems are presented as follow:

- Phosphoric Acid Fuel Cell: These types are the common available fuel cells. They generate electricity at around 40% efficiency. Along with fossil fuels such as gasoline, hydrogen can also be used as the fuel in this type of fuel cells.

- Proton Exchange Membrane Fuel Cell: Proton exchange membrane or PEM fuel cells are most suitable for applications that quick changes in power demand is required. They are also mostly operative at low temperatures.

- Molten Carbonate Fuel Cell: Operating at higher temperatures compared to PEMs, these fuel cells use a broad range of fuels: from hydrogen to natural gas and marine diesel. The main applications of these systems have been identified to be in providing electrical power for electrical utility systems.

- Solid Oxide Fuel Cell: As one of the most efficient types of fuel cell systems, solid oxide fuel cell (SOFC) has been the subject of investigation in previous studies [34-43]. The important characteristic of the SOFC is its capability to generate electricity at 60% efficiency [44]. SOFC also is environmentally friendly as can be noted from Figure 1.6 that demonstrates the pollutions emitted from an SOFC system. The SOFC can operate at very high temperatures. But since operating at high temperatures would decrease the performance of these cells, there have been efforts to lower the cell operating temperature [45]. Additionally, research has been done in studying the effects of microstructural evolution on the SOFC performance [46].

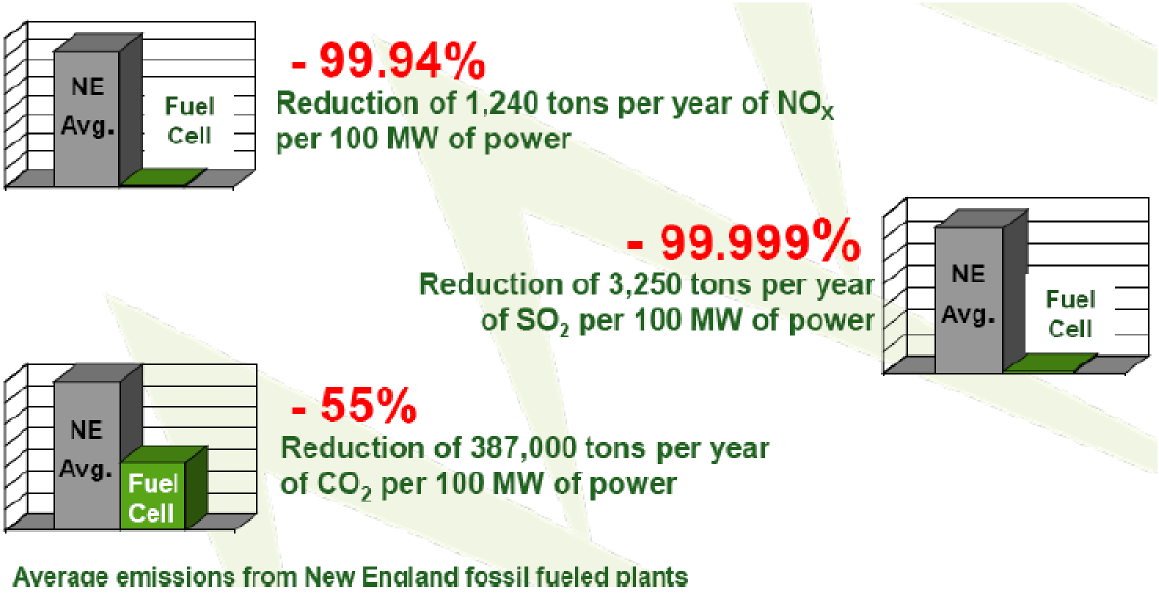


Figure 1.6. Environmental benefits of the SOFC [44]

1.3 Energy Storage Systems (ESSs)

The history of energy storage dates back to pre-history when energy was saved in stars like the Sun, and humans used that energy through radiation and solar heating. With the rise in energy demand and environmental concerns about using fossil fuels and nuclear energy, a shift from conventional energy sources to renewable sources seems unavoidable. Utilizing renewable energy sources for everyday usage is a significantly important issue. Therefore, energy storage is of critical importance in making the shift from conventional sources as smooth as possible. The important role of ESSs in reducing and managing electrical demands at peak time is undeniable. As demonstrated by a typical electrical power profile as illustrated in Figure 1.7 [47], the ESS can be charged during the low demand hours and released when the electrical demand reaches its peak level.

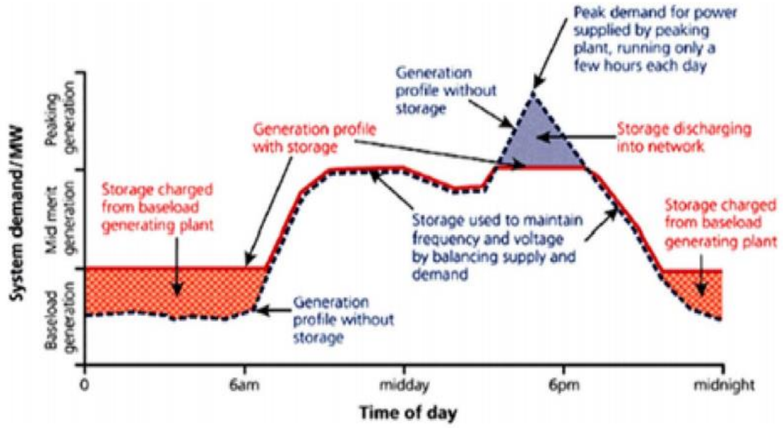


Figure 1.7. An electrical power profile, illustrating the demand variation over a 24-hour period [47]

There are many different types of ESSs such as pumped-storage hydroelectricity, superconducting magnetic energy storage, gas holder, grid energy storage, and gravitational potential energy storage with solid masses. However, the main types of ESSs capable of storing electrochemical energy are batteries, fuel cells, and capacitors.

The history of developing these types of ESSs dates back to 2200 years ago [48]. A discovered clay pot Baghdad, Iraq, is the first known battery. Alessandro Volta's work in creating a photovoltaic cell in the 19th century, the Daniell cell, and the Leclanché cell can be mentioned as the noticeable developments in the history of battery systems production. The lead acid batteries were the first type of batteries. Further advances in battery development led to the evolution of lead-acid battery into Lithium-ion battery [47], which is the focus of this thesis.

1.3.1 Lithium-ion Battery (LIB)

Energy plays an important, if not the most important, role in our everyday life. From small living organs to big infrastructure and machines, everything needs the energy to continue functioning normally. Therefore, securing reliable energy sources is the ultimate goal for every country in the world. There would be no growth and development in any sector without a dependable energy supply that can support such progress. However, supplying energy is not the only goal anymore. There are genuine concerns over the condition of our living environment. Consuming energy from unclean energy sources such as fossil fuels affect our environment with a damaging impact. Global warming, water, air, and soil pollutions are the prominent headlines of the reports on environmental issues. With the rapid pace of technology advancements, an increase in energy demands seems inevitable, and as such, there have been efforts to take renewable energy sources into account in engineering designs [49, 50]. LIBs are one of the leading examples of scientific efforts to address concerns over energy supply and storage. Batteries are comprised of two solid electrodes, namely anode, and cathode illustrated in a simple schematic in Figure 1.8.

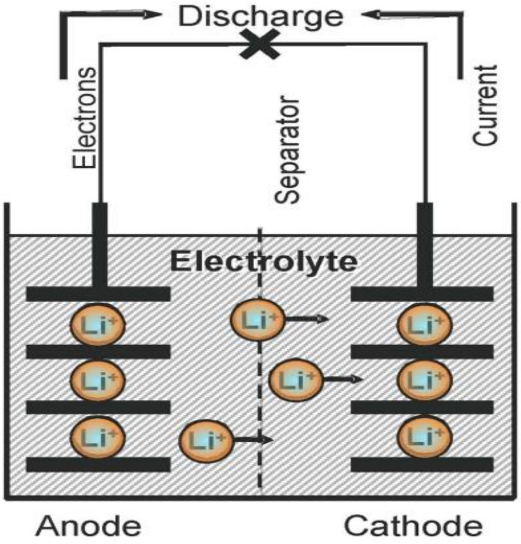


Figure 1.8. Schematic of a battery structure [47]

The basis for the development of LIBs was founded in the Ford Motor Company in the 1970s when scientists found that solid compounds can be used to store and release lithium ions [51, 52]. On discharge, electrons flow from the anode through an external circuit to the cathode. Another flow in the same direction is happening at the same time in the electrolyte, in which cations flow from anode to cathode. The high energy capacity and long cycle life of these batteries make them a reliable choice in today’s demanding markets. The application of these battery systems becomes broader every day as they can be used as an energy provider source in almost every device around us; from smartphones and electric toothbrushes to electric cars and airplanes. Considering the important role of LIBs in modern day life, there need to be extensive numerical and experimental studies on these batteries to ensure a safer and more durable design. As a physical system that has important mass transfer phenomena at the microscale level, a numerical model of this system must include the effect of the microscale phenomena in the macroscale response of the system. Therefore, multiscale analysis of a LIB is essential to have a more accurate mathematical model for the design and analysis of such battery systems.

1.4 Research Objectives

This part of the thesis is focused on developing a mathematical framework for the modeling and simulation of a LIB system. The basis of modeling the battery system has been accomplished by using a novel modeling technique called variational multiscale modeling (VMM). This method of modeling employs conventional techniques and concepts of finite element analysis (FEA) – such as variational formulation, basis functions, etc. – in solving partial differential equations (PDEs) describing a special class of physical systems. These systems have important multiscale phenomena in different spatial and/or temporal domain. Therefore, a special method of analysis capable of considering the multiscale effect of such phenomena in the total response of the system should be included in the analysis of multiscale systems. The previous research employed this method of analysis in the modeling of multiple systems. However, this study is exclusively focused on the development of such modeling framework from a mathematical standpoint. Therefore, the mathematical foundation for performing VMM is developed, and necessary details and steps in constructing the mathematical model are provided.

1.5 Thesis Part I Organization

The remaining portion of this part is divided into three chapters. Chapter 2 is a comprehensive literature review on Lithium-ion batteries and mathematical modeling of such physical systems. In Chapter 3, a framework for constructing a multiscale model of LIBs is developed and presented. Chapter 4 includes a summary of part I, scientific contribution, and suggestions for future research.

1.6 References

1. Kothari, R., et al., *Fermentative hydrogen production–An alternative clean energy source.* Renewable and Sustainable Energy Reviews, 2012. **16**(4): p. 2337-2346.
2. Stambouli, A.B. and E. Traversa, *Solid oxide fuel cells (SOFCs): a review of an environmentally clean and efficient source of energy.* Renewable and sustainable energy reviews, 2002. **6**(5): p. 433-455.
3. Yuan, J., et al., *China's 2020 clean energy target: Consistency, pathways and policy implications.* Energy Policy, 2014. **65**: p. 692-700.
4. Llera, E., et al., *Forecasting job creation from renewable energy deployment through a value-chain approach.* Renewable and Sustainable Energy Reviews, 2013. **21**: p. 262-271.
5. Blyth, W., et al., *Low carbon jobs: The evidence for net job creation from policy support for energy efficiency and renewable energy.* London: UK Energy Research Centre, 2014.

6. Simas, M. and S. Pacca, *Assessing employment in renewable energy technologies: A case study for wind power in Brazil.* Renewable and Sustainable Energy Reviews, 2014. **31**: p. 83-90.
7. Carley, S., et al., *Energy-based economic development.* Renewable and Sustainable Energy Reviews, 2011. **15**(1): p. 282-295.
8. Connolly, D., H. Lund, and B.V. Mathiesen, *Smart Energy Europe: The technical and economic impact of one potential 100% renewable energy scenario for the European Union.* Renewable and Sustainable Energy Reviews, 2016. **60**: p. 1634-1653.
9. Blazejczak, J., et al., *Economic effects of renewable energy expansion: A model-based analysis for Germany.* Renewable and Sustainable Energy Reviews, 2014. **40**: p. 1070-1080.
10. Kammen, D.M., K. Kapadia, and M. Fripp, *Putting renewables to work: How many jobs can the clean energy industry generate.* 2004.
11. Bhattacharya, M., et al., *The effect of renewable energy consumption on economic growth: Evidence from top 38 countries.* Applied Energy, 2016. **162**: p. 733-741.
12. Shahbaz, M., et al., *Does renewable energy consumption add in economic growth? An application of auto-regressive distributed lag model in Pakistan.* Renewable and Sustainable Energy Reviews, 2015. **44**: p. 576-585.
13. Inglesi-Lotz, R., *The impact of renewable energy consumption to economic growth: A panel data application.* Energy Economics, 2016. **53**: p. 58-63.
14. Apergis, N. and J.E. Payne, *Renewable energy consumption and economic growth: Evidence from a panel of OECD countries.* Energy Policy, 2010. **38**(1): p. 656-660.
15. Administration, E.I. and G.P. Office, *International Energy Outlook: 2016 with Projections to 2040*. 2016: U.S. Government Printing Office.
16. Administration, U.S.E.U.S.E.I. and P.H. Press, *Annual Energy Outlook 2017 with Projections to 2050*. 2017: CreateSpace Independent Publishing Platform.
17. Zou, Y., et al., *Combined State of Charge and State of Health estimation over lithium-ion battery cell cycle lifespan for electric vehicles.* Journal of Power Sources, 2015. **273**: p. 793-803.
18. Yuan, S., H. Wu, and C. Yin, *State of Charge Estimation Using the Extended Kalman Filter for Battery Management Systems Based on the ARX Battery Model.* Energies, 2013. **6**(1): p. 444.
19. Ouyang, M., et al., *Enhancing the estimation accuracy in low state-of-charge area: A novel onboard battery model through surface state of charge determination.* Journal of Power Sources, 2014. **270**: p. 221-237.
20. Li, S.E., et al., *An electrochemistry-based impedance model for lithium-ion batteries.* Journal of Power Sources, 2014. **258**: p. 9-18.
21. Sabatier, J., et al., *Lithium-ion batteries modeling: A simple fractional differentiation based model and its associated parameters estimation method.* Signal Processing, 2015. **107**: p. 290-301.
22. Mastali Majdabadi, M., et al., *Simplified electrochemical multi-particle model for LiFePO4 cathodes in lithium-ion batteries.* Journal of Power Sources, 2015. **275**: p. 633-643.
23. Sung, W. and C.B. Shin, *Electrochemical model of a lithium-ion battery implemented into an automotive battery management system.* Computers & Chemical Engineering, 2015. **76**: p. 87-97.

24. Bartlett, A., et al., *Electrochemical model-based state of charge and capacity estimation for a composite electrode lithium-ion battery.* IEEE Transactions on Control Systems Technology, 2016. **24**(2): p. 384-399.
25. Bizeray, A.M., et al., *Lithium-ion battery thermal-electrochemical model-based state estimation using orthogonal collocation and a modified extended Kalman filter.* Journal of Power Sources, 2015. **296**: p. 400-412.
26. Han, X., et al., *Simplification of physics-based electrochemical model for lithium ion battery on electric vehicle. Part II: Pseudo-two-dimensional model simplification and state of charge estimation.* Journal of Power Sources, 2015. **278**: p. 814-825.
27. Northrop, P.W., et al., *Efficient simulation and model reformulation of two-dimensional electrochemical thermal behavior of lithium-ion batteries.* Journal of The Electrochemical Society, 2015. **162**(6): p. A940-A951.
28. Li, J. and M.S. Mazzola, *Accurate battery pack modeling for automotive applications.* Journal of Power Sources, 2013. **237**: p. 215-228.
29. MacKay, D.J., *Solar energy in the context of energy use, energy transportation and energy storage.* Philos Trans A Math Phys Eng Sci, 2013. **371**(1996): p. 20110431.
30. Grove, W.R., *The correlation of physical forces*. 1874: Longmans, Green.
31. Appleby, A.J., *From Sir William Grove to today: fuel cells and the future.* Journal of Power Sources, 1990. **29**(1): p. 3-11.
32. Mond, L. and C. Langer, *A new form of gas battery.* Proceedings of the Royal Society of London, 1889. **46**: p. 296-304.
33. A.M. Adams, F.T. Bacon, and R.G.H. Watson, *Fuel Cells.* W. Mitchell Jr. (Ed.), Academic Press, New York, 1963: p. p. 129.
34. Abdullah, T. and L. Liu, *Peak Power Optimization of Solid Oxide Fuel Cells with Particle Size and Porosity Grading.* ECS Transactions, 2014. **61**(13): p. 33-46.
35. Liu, L. *Modeling of Solid Oxide Fuel Cells with Linear and Nonlinear Functionally Graded Electrodes*. in *Meeting Abstracts*. 2014. The Electrochemical Society.
36. Liu, L., G.-Y. Kim, and A. Chandra, *Modeling of Ni–CGO anode in a solid oxide fuel cell deposited by spray pyrolysis.* Journal of Power Sources, 2012. **210**: p. 129-137.
37. Liu, L., et al., *Modeling of solid oxide fuel cells with particle size and porosity grading in anode electrode.* Fuel Cells, 2012. **12**(1): p. 97-108.
38. Liu, L., et al., *Microstructural and electrochemical impedance study of nickel–Ce0.9Gd0.1O1.95 anodes for solid oxide fuel cells fabricated by ultrasonic spray pyrolysis.* Journal of Power Sources, 2011. **196**(6): p. 3026-3032.
39. Liu, L., G.-Y. Kim, and A. Chandra, *Fabrication of solid oxide fuel cell anode electrode by spray pyrolysis.* Journal of Power Sources, 2010. **195**(20): p. 7046-7053.
40. Liu, L., G.-Y. Kim, and A. Chandra, *Modeling of thermal stresses and lifetime prediction of planar solid oxide fuel cell under thermal cycling conditions.* Journal of Power Sources, 2010. **195**(8): p. 2310-2318.
41. Liu, L., G.-Y. Kim, and A. Chandra, *Deposition of Porous Anode Electrode of a Solid Oxide Fuel Cell by Ultrasonic Spray Pyrolysis.* 2010(44045): p. 311-317.
42. Liu, L., G.-Y. Kim, and A. Chandra, *Life Prediction of a Solid Oxide Fuel Cell Under Thermal Cycling Conditions.* 2009(48814): p. 247-255.
43. Abdullah, T. and L. Liu, *Phase field simulation coupling microstructural evolution and crack propagation during performance degradation of solid oxide fuel cells.* ECS Transactions, 2015. **66**(2): p. 207-217.

44. Liu, L., *Solid oxide fuel cell reliability and performance modeling and fabrication by spray pyrolysis*. 2011: Iowa State University.
45. Abdullah, T. and L. Liu, *Simulation-based microstructural optimization of solid oxide fuel cell for low temperature operation.* International Journal of Hydrogen Energy, 2016. **41**(31): p. 13632-13643.
46. Abdullah, T. and L. Liu, *Meso-Scale Phase-Field Modeling of Microstructural Evolution in Solid Oxide Fuel Cells.* Journal of The Electrochemical Society, 2016. **163**(7): p. F618-F625.
47. Whittingham, M.S., *History, Evolution, and Future Status of Energy Storage.* Proceedings of the IEEE, 2012. **100**(Special Centennial Issue): p. 1518-1534.
48. Dănilă, E. and D.D. Lucache, *HISTORY OF THE FIRST ENERGY STORAGE SYSTEMS.*
49. Momeni, A.F., et al., *Effect of Prestressing Wire Indentation Type on the Development Length and Flexural Capacity of Pretensioned Concrete Crossties.* 2015(56451): p. V001T01A026.
50. Momeni, A.F., et al., *Effect of Concrete Release Strength on the Development Length and Flexural Capacity of Members Made With Different Prestressing Strands.* 2016(49675): p. V001T01A017.
51. Yao, Y.-F.Y. and J. Kummer, *Ion exchange properties of and rates of ionic diffusion in beta-alumina.* Journal of Inorganic and Nuclear Chemistry, 1967. **29**(9): p. 2453IN12467-24662475.
52. Whittingham, M. and R. Huggins, *the thermodynamic and transport properties of a number of materials. However, these studies have been restricted essentially to systems utilizing electrolytes containing mobile silver or copper ions at low temperatures, and oxygen ions at high temperatures. Transport measurements have been made on single crystals of beta alumina, which has the nominal formula MAZ 1.1017 where M is usually a monovalent cation, to test its suitability as.* Solid State Chemistry: Proceedings, 1972. **364**: p. 139.

Chapter 2. Literature Review

2.1 Introduction

LIBs are the top choice in the battery market, as they account for 63% of the total worldwide sales in portable batteries [1]. The popularity of LIBs originates to their outstanding features such as high energy storage, a longer lifetime compared to other battery systems, lighter weight, and easier transportation as a result, and flexibility in design [2] (for a comparison see Figure 2.1). Therefore, there need to be substantial efforts in investigating the performance and electrochemical characteristics of LIBs as well as their safety while in use.

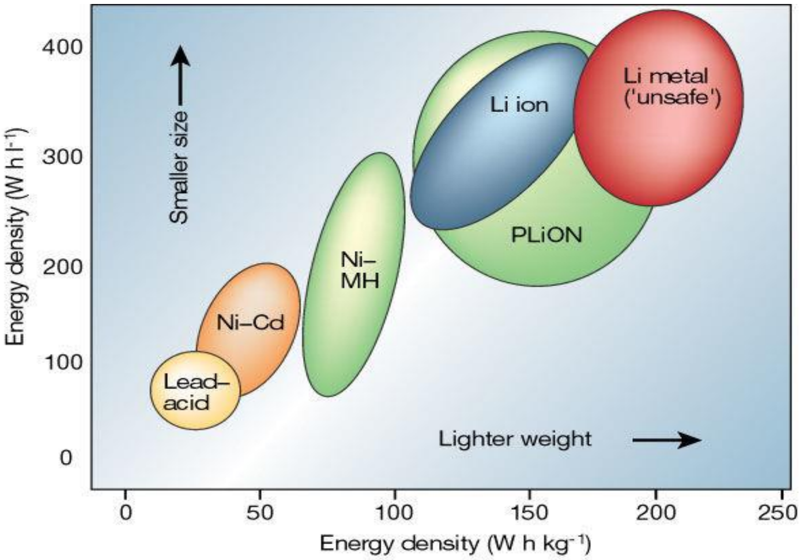


Figure 2.1. Comparison of different battery systems (volumetric and gravimetric energy density) [2]

2.2 LIB Configurations

There are multiple different materials used as components for either the electrode or electrolyte in the configuration of LIBs. For instance, TiS_2 was used as a positive electrode and lithium metal as a negative electrode, while the electrolyte was chosen to be the electrolyte [3, 4]. The most common structure of LIBs contain a graphite anode (MCMB or mesocarbon microbeads), a lithium metal oxide cathode (such as $LiCoO_2$) and an electrolyte which consists of a lithium salt (e.g., $LiPF_6$) and an organic solvent (EC-DMC or ethylene carbonate-dimethyl carbonate) that are embedded in a separator felt [5]. In most cases the operating process of LIBs is as follows:

$$yC + LiMO_2 \leftrightarrows Li_xC_y + Li_{(1-x)}MO_2,\ x \sim 0.5,\ y = 6,\ \text{voltage} \sim 3.7\ \text{VDC} \qquad (2.1)$$

in which the insertion and extraction of lithium ions are reversible between the solid electrolytes [6].

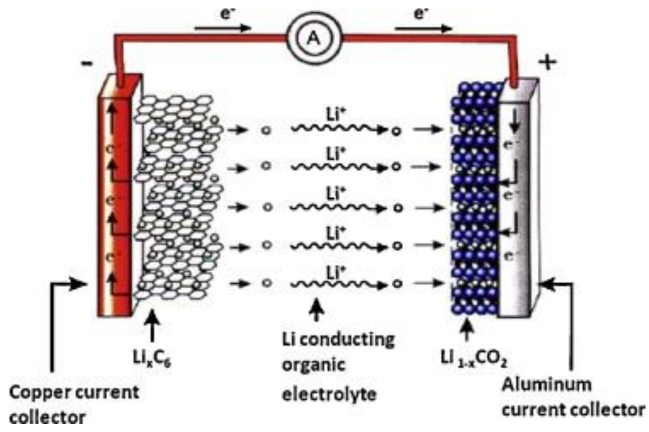


Figure 2.2. A common LIB schematic [6]

There is still ongoing research in finding new materials for either positive or negative electrode. For positive electrode material choice, it is important first to determine the type of the battery system and whether it is a lithium-metal or lithium-ion type battery [7]. As for the negative electrode, there were efforts in finding an alternative material to carbon-based electrodes that have larger capacities and provides more positive voltages (discovery of lithium transition-metal nitrides are one of the results of these efforts) [8]. Recent advances in designing LIB structures aim to improve the battery performance. In regards to some examples of such efforts, one can point to a design employing a self-heating mechanism capable of improving the battery performance at low temperatures [9], a watermelon inspired design which offers improvement in the properties of silicon/carbon (Si/C) anodes [10], a honeycomb-cobweb inspired core-shell structure which enhances the rate capability of Si/C anodes [11], the addition of zirconium to improve the cycling stability [12], and using silicon-iron (Si-Fe) based nanomaterials to minimize the volume expansion of anode during lithium ion insertion/extraction cycles [13].

Although the ongoing process in LIBs seems like a simple ion exchange between the two electrodes, there are much more complexities in battery system reactions description and analysis. Anode and cathode decomposition is one of the main processes in LIBs happening during charge and discharge cycles. The decomposition of the electrodes and consumption of electrolyte mass along with gas production and solid electrolyte interface (SEI) layer growth leads to battery capacity fade and safety hazards which are not the desired circumstances in a battery system. Therefore, these processes must be carefully controlled to ensure a reliable battery performance [14]. As such, there have been multiple efforts to model and study the LIB systems that account for battery degradation mechanisms, models and experimental studies such as a dynamic capacity degradation model, on-line electrochemical mass spectrometry, ex-situ nuclear magnetic resonance (NMR), scanning electron microscope (SEM) imaging, and differential voltage analysis [15-20].

2.3 LIB Mathematical Modeling

Numerical techniques are employed for developing a mathematical model of complex systems where analytical methods cannot provide a solution. In such cases, it is inevitable to take a theoretical/computational approach to investigate the considered system. The efficiency of the numerical techniques mainly depends on the technique, complexity of the system and the boundary conditions [21]. In computational studies, a complete model can often be developed based on experimental data collected from experimental studies. LIB systems are no exception in this matter, as the complexities in their structure and cost of the experimental procedure often make their experimental studies too expensive to be carried out. Therefore, many researchers and scholars tried to study such systems by taking a theoretical approach [22-24].

Deriving a mathematical model for a battery system usually consists of the following steps: 1) defining a variable(s) that is going to be investigated, 2) deriving/determining the governing equations for variable(s), 3) defining boundary and initial conditions for the equations and 4) choosing the appropriate solution method for solving the mathematical model. For example, De Vidts and White [25] demonstrated porous electrodes governing equations derived by employing volume-averaging techniques. Additionally, a model that coupled micro- and macro- scales of the battery system based on volume-averaging techniques was developed by Wang, Gu, & Liaw [26]. Assumptions taken into account during the development of a mathematical model should be carefully examined so that the results of the model can make physical sense. As noted by Jain and Weidner [27], an implicitly made assumption can result in a substantial error in material balance calculations. Looking for analytical methods is the first step in solving the governing equations of the model [28, 29]. Separation of variables, conformal mapping and perturbation methods are some of the analytical methods used for solving battery models. The perturbation method was employed by Morbidelli [30] to obtain a solution for non-linear governing equations of a chemical system.

The control volume, finite element method, and finite difference method are the most common methods employed in the numerical solution of the battery systems. As reported in several previous publications [31-44], the finite difference has been used as one of the most common methods in numerical analysis. However, the finite difference method shows some discrepancy in mass balance solutions in some cases [45, 46]. Therefore, the finite volume method was employed to avoid this issue [45-50]. For example, Botte, Ritter, & White [51] have demonstrated that the finite volume method produces more accurate results for boundary value problems with boundary conditions defined as fluxes. However, the authors [51] indicated that the finite difference method was still better for cases with a small number of mesh nodes. As for systems consisted of irregularities in geometry or heterogeneous material structure, the finite element method provides a better solution [52]. Finite element modeling has been employed in several research efforts, e.g., modeling a cylindrical LIB cell [53], developing battery thermal models [54], and three-dimensional stress analysis for a Li-ion half-cell [55]. Orthogonal projections and Chebyshev orthogonal collocations [56] can be mentioned as some of the recent efforts in the estimation of LIB model parameters [57].

The modeling efforts focused on different areas in the analysis of LIB systems. A number of studies focused on modeling LIBs' safety by modeling battery operation (with inclusion of ageing) [58-61], other reports developed thermal runaway models [62-64], some studies focused on investigating the electrical behavior of LIBs by developing electrical circuit models [65-68] (see Figure 2.3); and the thermal behavior of LIBs has been the subject of investigation in multiple publications [69-71]. Equivalent circuit modeling has been employed in several previous research for modeling batteries. The small number of parameters and the clarity and simplicity in applying the method can be recognized as the advantages of this modeling method, while the limitation in displaying current and voltage can be pointed out as the main drawback of this method [72]. The incorporation of the battery electrochemical properties in the equivalent circuit models to enhance the accuracy of these models was offered by Sparacino, Reed, Kerestes, Grainger, & Smith [73]. Furthermore, Hu, Li, & Peng [74] compared equivalent circuit models for LIBs. They reported the suitability of RC models for LINMC cells while suggested RC models with one-state hysteresis are more appropriate for $LiFePO_4$ cells.

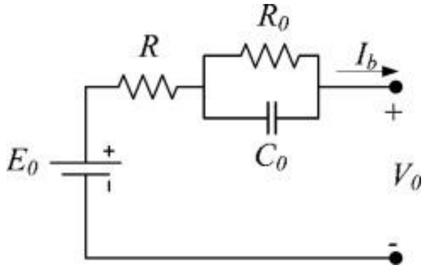


Figure 2.3. Schematic of a simple electrical circuit model of a LIB [75]

As stated by various previous research [75-78], electrochemical models are the most accurate models for optimization studies of LIBs and understanding the behavior of electrochemical systems. An electrochemical model was developed by the work of Newman's research group (see Figure 2.4) which used microscopic and macroscopic data (such as concentration distribution and battery current respectively) to predict the discharge behavior of a LIB [79].

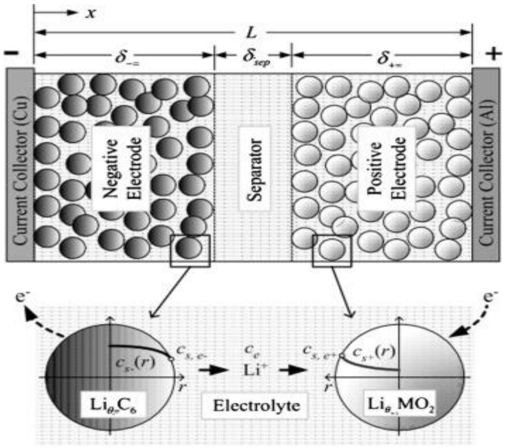


Figure 2.4. LIB schematic during discharge [79]

2.4 Electrochemical Modeling and Analysis

Mathematical modeling of battery systems has been accomplished by employing a variety of modeling methods [80, 81], such as least-squares approximation formulation and electrothermal modeling. The least-square approximation was employed by Casacca and Salameh [82] to model a lead-acid battery. A comparative study between electrothermal and electrochemical modeling methods by Fink and Kaltenegger [83] recognized the higher calculation time as a downside of electrochemical modeling, and the need for large number of fitting parameters as a disadvantage of electrothermal modeling. Additionally, Fink and Kaltenegger [83] realized the capability of the electrochemical modeling that allows for investigation of different material properties as one of the main advantages of electrochemical modeling. The electrochemical modeling method has been vastly employed in multiple previous research efforts, such as battery power management and optimization studies [84-91].

Electrodes in Li-ion batteries contain a porous structure which increases the surface area, allowing chemical reactions to occur within a small space. Furthermore, the porous structure of the electrodes decreases the negative effects of slow electrochemical reactions by increasing the area between the battery's solid and liquid phases [92]. The complex geometry of the porous media has led to practical difficulties in developing a robust model of the battery system [93]. Newman and Tiedemann developed the porous electrode theory from a macroscopic scale standpoint [92]. The governing equations were obtained by using continuous and average quantities to simplify the geometric complexities. The LIB pseudo 2-dimensional model was developed and presented by Doyle, Fuller, & Newman [79] through combining the porous electrode and concentrated solution theories. The developed pseudo 2-dimensional model has remained the most popular LIB model since its development day [93] and has been extensively examined and validated [94]. The one-directional intercalation process of ions was modeled as ions moving through the surface of spherical particles which are surrounded by the electrolyte. Therefore, a 1-dimensional modeling approach was employed [79, 95, 96]. The validity of this model is vastly confirmed such that the model results are often used as a standard in cases where dependable experimental data is not available [97-99].

The Doyle-Fuller-Newman model that was developed in 1993 [79] was one of the first attempts at developing an electrochemical model of a LIB system. It was developed further in successive years to model and simulate different types of intercalation batteries such as lithium-metal, lithium-ion, and nickel metal-hybrid systems. The battery system that is considered in this model is composed of three sections: 1) Anode, 2) Separator and 3) Cathode. Lithium ions can move freely (by diffusing through a separator) between the cathode and the anode by passing the separator. However, the separator does not allow a path for electron movement between the electrodes of the battery. The electrodes are also composed of multiple parts such as solid particles, electrolyte, gas, pores, and a binder. The governing equations of this battery system are as follows [95]:

Mass transfer in the solid phase:

$$\frac{\partial c_s}{\partial t} = \mathrm{D}_s^{eff} . \frac{\partial^2 c_s}{\partial r^2} \tag{2.2}$$

where c_s is the concentration of lithium ions in the solid phase. The mass balance equation in the electrolyte:

$$\frac{\partial c_e}{\partial t} = \mathrm{D}_e^{eff} \Delta c_e + \frac{i_e(1 - t_+)}{F} \tag{2.3}$$

c_e is the Li-ion concentration in the electrolyte and D_e^{eff}:

$$\mathrm{D}_e^{eff} = D \frac{c_T}{c_o} \left(1 + \frac{dln\gamma_\pm}{dlnm}\right) \tag{2.4}$$

The current in the solution phase, i_e, is given by Ohm's law:

$$i_e = -\sigma_e^{eff} \nabla \emptyset_e + \frac{2RT}{F}(1 - t_+)\sigma_e^{eff} \nabla ln c_e \tag{2.5}$$

The rate of the chemical reactions in the interface between electrode and electrolyte is dependent on lithium ion concentration and the solid and solution potential. In order to relate the current and surface overpotential, we have the Butler-Volmer equation as:

$$\begin{aligned} i_n = j_n F = i_0 \Bigg[& exp\left(\frac{\alpha_a F(\emptyset_s - \emptyset_e - U - R_{SEI} F j_n)}{RT}\right) \\ & - exp\left(\frac{\alpha_c F(\emptyset_s - \emptyset_e - U - R_{SEI} F j_n)}{RT}\right)\Bigg] \end{aligned} \tag{2.6}$$

where R_{SEI} is the resistance induced by the formation of a solid layer at the interface of electrode-electrolyte. This layer is called solid electrolyte interface (SEI) and is one of the important degradation mechanisms in LIB systems such that a considerable number of published work have been focused on modeling the formation and study the effect of SEI layer on battery performance [100-110]. For the charge balance equation, we have:

$$-\nabla.\left(\sigma_s^{eff}\nabla\emptyset_s\right)=0 \quad (2.7)$$

where σ_s^{eff} is the effective electrode conductivity and $\emptyset_s$ is the solid state potential.

The idea of simplifying the pseudo-2D model was proposed by introducing a single particle model [111]. In the single particle model, the two electrodes are modeled as two spherical particles and the potential, and concentration changes in the liquid phase are not considered [111]. Providing a simple model which leads to low computational cost [93] in addition to the capability of life modeling [112] and real-time estimation of the LIB [113] are the main advantages of the single particle method. For cases of thick electrodes or simulation of high discharge rates, the single particle model must be carefully adjusted to the electrolyte properties, one of the features of this method that has been identified as the model limitation [76]. There have been efforts in the further development of this method of modeling to overcome the drawbacks of the single particle method [114-116].

The main challenges in developing simplified/reduced pseudo-2D models are summarized in the following [93]: Model reduction is mostly based on fitting techniques, such that the model parameters are fitted to a polynomial profile. However, there are concerns over these fitting techniques, as there are not certain criteria for determining which parameters should be fitted and which should be calculated. Also, most of the model parameters of a LIB demonstrate a nonlinear behavior, especially if the effect of multiscale phenomena is included. However, the fitting techniques in model reduction efforts typically do not account for this nonlinear response as the parameters are only fitted to simple continuous functions. The change in battery characteristics due to aging should also be considered in simplified models, especially in cases of real-time simulation and monitoring of the battery system. In addition, the Doyle-Fuller-Newman model and the models based on his work, consider the microscale mass transfer of lithium ions in the form of limiting the formation of the electrode particles into certain shapes such as spherical, cylindrical, and planar [79, 117-121]. Although these types of simplifications provided acceptable numerical answers, the model was not a realistic one, as the shape of the particles were random, and the solid particles do not form a regular geometrical shape. Also, based on the porous electrode theory developed by Newman and Tiedemann [92], the interface area of the electrode and electrolyte, and the properties in the electrode are averaged values, and no consideration had been given to the variables that can be defined exclusively in the microscale domain of the problem. Further study based on these assumptions tried addressing these simplifications by developing a model with different particle sizes [122], but the model still lacked the consideration for including the microscale response in the total behavior of the system.

2.5 Multiscale Nature of LIBs

It is clear that LIBs are multiscale and multiphysics systems. As it is illustrated in Figure 2.5, the electrode of a LIB made of $LiFePO_4$ represents a multiscale system at different length scales [123].

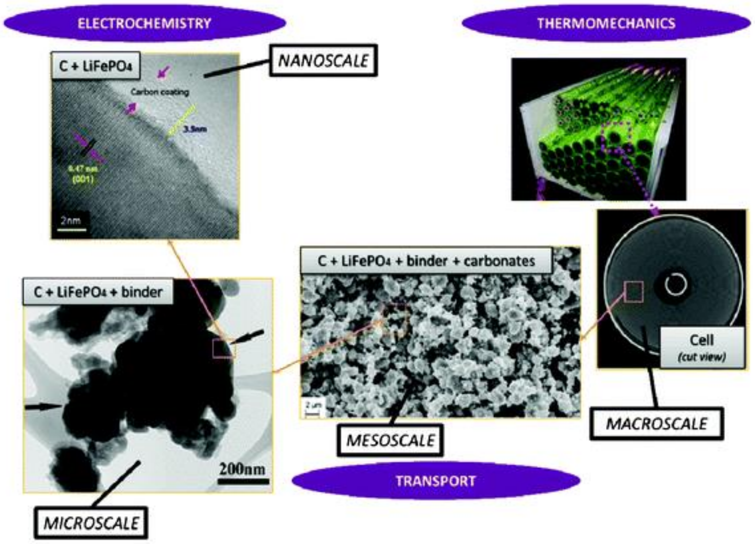


Figure 2.5. Multiscale character of an electrode of a LIB [123]

LIBs are strongly considered as multiscale physical systems since there are strong effects imposed on the behavior of the systems that are caused by changes in the microstructure of the LIB. The structure of LIB electrodes and its details have a critical effect on the LIB performance and lifespan [124-127]; e.g., electrodes that provide a small area reduce the safety risks associated with LIB systems [128]. Additionally, the microstructural formation of LIB electrodes has a significant impact on battery performance by providing diffusion pathways for lithium ions, active material and interfacial surface area [126, 129-132]. The failures of pseudo-2D models to simulate some battery phenomena are induced by the heterogeneity of battery structure, such as ineffectiveness of Bruggeman’s relation in capturing electrode tortuosity [133-136], which raises the need to develop mathematical models of LIBs that can capture the effects of battery microstructure.

2.6 Multiscale Modeling Methods

Accurate description of physical phenomena at different length and time scales is required for the discovery and development of new materials. All engineering materials and systems are heterogeneous at some scales. These heterogeneities are the cause of nonlinear behavior of the material or the system under study, such as phase changes, microstructural evolution, crack propagation, etc. [137-140]. Therefore, development of predictive multiscale models that can provide a better understanding of new materials’ properties and the processing conditions that create them is needed [141]. To achieve a predictive model, it is critical to fully resolve the heterogeneities existing at the microscale domain of the problem. Various phases of heterogeneity are presented at the microstructure, such as voids, inclusions, crystals, etc. which could have various sizes and shapes [141].

PART I: Mathematical Modeling of Lithium-ion Batteries

Conventional methods of modeling are focused merely on one scale. If the macroscale response of a problem is of interest, then a continuum model of the problem will be developed, and constitutive models are used if the microscale analysis of a problem is being performed. These methods lead to acceptable results when there is a simple system under investigation. For complex systems, either some assumptions should be made for the sake of system simplification -and thus, a less realistic model- or there should be a more robust method of modeling, which can couple different length scales of the problem or at least integrate the microscale effects into the full system response. Multiscale modeling methods are developed to accomplish more accurate mathematical models. It is very important to consider developing multiscale models for complex systems. The importance of multiscale modeling can be recognized from awarding the Noble Prize in Chemistry to researchers because of their efforts in developing a multiscale model for a chemical system [142-144].

Before the birth of the multiscale modeling methods, Eshelby [145, 146] introduced a modeling approach called micromechanics analysis. This approach was based on assigning a value to any subscale discrepancy in the continuum and considering the continuum scale composed of representative volume elements (RVE). Micromechanics method of analysis then became the foundation of many numerical methods, such as the homogenization theory, Mura-Tananka method [147], and mean-field theory [148]. To couple the atomistic and electronic scale simulations, researchers employed both concurrent and hierarchical multiscale modeling methods [149]. Additionally, density functional matters were coupled with embedded-atom model potentials to track the dislocation changes at atomic scales [150, 151].

There are different multiscale analysis methods developed to analyze a complex system. For example, in stochastic multiscale modeling, the main idea is to treat fast and slow evolving variables separately [152-156]. Therefore, to treat the separated variables, the governing equation should be studied for different timescales. Separating variables results in the coupling of the fast and slow variable and hence, dealing with the interfaces of the models at different scales [157]. As for treating model interfaces, two classes of methods are suggested [158-160]. The first is a sequential method, where one first solves the problem for the whole model and provides explicit information on slow and fast variables. Then, by using the results of the model solution, a reduced model for the slow variables is defined. The concurrent (mixed-resolution) method is the second type of methods in treating interface of models at different scales, which is explained later in this section. Furthermore, flexible partitioning has been used in multiscale modeling [161-163] in dealing with model interfaces. Most models use a fixed partition as they treat different scales completely separately. It has been demonstrated that this method of meshing is not always the efficient method of modeling since switching between the fine and coarse models facilitate information exchange, which has been proven to be helpful in some analysis [164].

Based on the problem formulation, the multiscale methods are categorized into the following classes:

- Concurrent methods, in which different parts of the system are modeled at different scales [165, 166], i.e., different governing equations at different scales [167-175]. One main issue of this method is ensuring that the scales are properly coupled through defining boundary conditions carefully [157].
- Hierarchical methods, which are a class of methods where hierarchical scales of the problem are coupled together at the same part of the problem domain, e.g., through building structure-property relations [176]. The coupling between different scales is achieved through averaging or on a parameter identification basis. Computational homogenization is an example of a hierarchical multiscale method which is based on integration over the domain in small scales [141].
- Hybrid methods, which determine properties of different scales. These methods include, but are not limited to multigrid methods [177], quasi-continuum methods [178], and generalized finite element methods [179].

Some of the multiscale modeling techniques include, but are not limited to adaptive mesh refinement, the multigrid method, domain decomposition methods, the heterogeneous multiscale method, and the variational multiscale method [180]. Sustaining the heterogeneities of a physical system or materials structure can be accomplished either by statistical analysis or image-based modeling. An image-based method was applied in combination with finite element analysis to perform a multiscale modeling study of the microstructure of engineering alloys [181]. Detailed complexities of the system are achieved through innovative imaging techniques in image-based multiscale modeling. The imaging technique is typically selected based on the material composition [141]. For example, the computed tomography method is used for dense materials [182, 183] while imaging of polycrystalline metals, metal alloys, and fuel cells is achieved by serial sectioning techniques [184-186]. Statistical models also play a major role in multiscale modeling studies by helping in ascertaining of important subscale features [149]. Macroscopic properties have been assumed as statistical averages of their microscopic counterparts, which is the basis of statistical physics [187]. Moreover, there are two assumptions to be satisfied in order to identify macroscopic features as the averages of microscopic properties: 1) in investigating a property, the volume under examination should be macroscopically small and microscopically large, and 2) the measurement of the macroscopic property should be macroscopically short but microscopically long [187, 188].

A number of the multiscale modeling methods are purely originated from a mathematical standpoint, such as the Percolation theory, dimensional analysis, and fractal analysis [149]. For example, the dimensional analysis was used by Barenblatt [189] for describing the method of scaling relationships. Asymptotic expansions was employed to capture the multiscale behavior of an elastic spherical shell through the application of nonlocal functionals [190]. Regarding the percolation theory, Otsubo [191] established particle sizes in a polymeric system suspension by the application of that theory. In another effort, distribution of porosities in a ceramic was reported by using a percolation-based model [192].

Multiscale modeling of batteries has been done in both temporal and spatial scales. Time-scale separation for multiscale analysis of a LIB [193-198], multiscale modeling based on spatial variable separation [197, 199-204], and multiscale modeling based on imaging techniques (nano-scale X-Ray tomography, 3D CT imaging, etc.) [205-207] are some of the reported types of LIB multiscale analysis. Recent case studies in multiscale modeling of LIBs include, but are not limited to: variational multiscale enrichment modeling for the study of the microstructure of LIBs [208], multiscale modeling of SEI layer growth [197], modeling of LIB aging [209], modeling the damage evolution in LIBs [210], cycle degradation modeling [211], correlative multiscale tomography/X-ray microscopy modeling [212, 213], LIB thermal runaway modeling [214], investigation of electrical conduction in LIB [215], study on the impact of particle sizes on LIB charging [216], and research on discharge behavior of LIBs [217].

The approaches to multiscale problems are founded on two assumptions: 1) the assumption of self-similarity across different scales of the system/material, and 2) the assumption of capturing the effects of microscale on macroscale by averaging on the microscale [218]. Clearly these approaches do not work for 1) problems where we are faced with different properties at different scales, and therefore the self-similarity approach is not valid, and 2) problems where the behavior of the phenomena is strongly dependent on the details of the microstructure, and consequently, the averaged microscale property does not represent the corresponding macroscale quantity [219]. Moreover, the solid failure occurs under non-equilibrium conditions and therefore, statistical mechanics approaches do not hold anymore as they are only valid in equilibrium conditions [218].

Global-local multiscale methods are the most appropriate methods in the multiscale analysis for capturing the behavior of the system when there are serious changes in material/system property over small areas of the material/system domain [220]. Some of these global-local techniques origin back to the work of Mote [221]. The following can be named as a few proposed global-local numerical approaches: the global-local finite element method [222-225], the generalized finite element method [226], the S-version finite element method [227], and multiscale coupling based on Lagrange multiplier method [228]. Based on the work presented in [229, 230], VMM was introduced. The basic idea of VMM is decomposing the problem response field into coarse and fine components, the former of which is solved in part of the domain which is consisted of coarse meshes while either semi-analytical approaches obtain the solution of the latter (variational projection, Green's function) [231, 232] or direct numerical solutions (DNS) [220]. In semi-analytical approaches, the global-local characteristic of the system is not strictly resolved as the fine-scale field remains unresolved. However, for DNS-based methods, the fine-scale is resolved by directly obtaining the residual response on a network of fine meshes [220]. DNS methods are the basis for the later developed multiscale modeling methods, including the numerical subgrid upscaling method [233, 234] and the variational multiscale enrichment (VME) method [235, 236].

The numerical subgrid upscaling method was used by Arbogast [233] in the formulation of a problem of flow through porous media. The numerical Green's function was employed in the process of obtaining the solution for fine-scale response field. Another work in employing the numerical subgrid upscaling scheme is the work accomplished by Juanes and Dub [237] to provide solutions for problems pertaining porous media flow. An extension for the VMM was proposed by Garikipati and Hughes [231] to investigate strain localization for cases of plastic deformations presence. The authors [231] used variational projection for evaluating the fine-scale behavior. Embedding fine-scale strain gradient theories within the variational multiscale formulation were demonstrated by Garikipati [238]. Further developments of VMM include but not limited to the work of Masud and Xia [239] which constructed a stabilized mixed FEM for VMM, incorporation of meshfree methods into the VMM for solving an elastoplastic deformation by Yeon and Youn [240], and one of the recent works presented by Oskay [235] which proposed the VME method. The innovation of the proposed method by Oskay [235] is its capability to allow the existence of subgrid heterogeneity. The main drawback in the VME approach is the development of efficient algorithms for resolving microstructure (such as [241, 242]), that avoids obtaining a full response in the enrichment (fine-scale) regions of the problem domain. The exclusion of fine-scale full resolution response field in VME approaches has also been noted by [220] as the critical factor in the practical application of the VME method.

Based on the nature of the problem and the capability of the method in considering microscale effects on the total response of the problem, the VMM was employed for the analysis of a LIB system, and a mathematical framework on how to apply this method in modeling LIB systems was developed. The details of this method are covered thoroughly in Chapter 3 of this part of the thesis.

2.7 Conclusion

Therefore, a mathematical model capable of deriving a multiscale analysis of LIBs will be presented. Variational multiscale modeling is employed in deriving the multiscale form of the governing equations. Physical spatial variables are decomposed into two separate variables, micro/fine- and macro/coarse- scale variables. These variables are linked to each other such that the determined microscale variable is being considered as an approximation error measurement in the macroscale equation.

2.8 References

1. *Hooked on Lithium.* The Economist, 2002.
2. Tarascon, J.M. and M. Armand, *Issues and challenges facing rechargeable lithium batteries.* Nature, 2001. **414**(6861): p. 359-367.
3. Whittingham, M.S., *Electrical energy storage and intercalation chemistry*. Science, 1976. **192**(4244): p. 1126-1127.
4. Whittingham, M.S., *Chalcogenide battery*. 1977, US Patent 4,009,052.
5. van Schalkwijk, W. and B. Scrosati, *Advances in lithium-ion batteries*. 2007: Springer Science & Business Media.
6. Scrosati, B. and J. Garche, *Lithium batteries: Status, prospects and future.* Journal of Power Sources, 2010. **195**(9): p. 2419-2430.

7. Guyomard, D., T. Osaka, and M. Datta, *New trends in electrochemical technology: energy storage systems for electronics.* Gordon & Breach Science Publishers, 2000. **9**: p. 253-350.
8. Shodai, T., et al., *Study of Li3− xMxN (M: Co, Ni or Cu) system for use as anode material in lithium rechargeable cells.* Solid State Ionics, 1996. **86**: p. 785-789.
9. Wang, C.-Y., et al., *Lithium-ion battery structure that self-heats at low temperatures.* Nature, 2016. **529**(7587): p. 515.
10. Xu, Q., et al., *Watermelon-Inspired Si/C Microspheres with Hierarchical Buffer Structures for Densely Compacted Lithium-Ion Battery Anodes.* Advanced Energy Materials, 2017. **7**(3).
11. Wu, J., et al., *A honeycomb-cobweb inspired hierarchical core–shell structure design for electrospun silicon/carbon fibers as lithium-ion battery anodes.* Carbon, 2016. **98**: p. 582-591.
12. Wang, D., et al., *Role of zirconium dopant on the structure and high voltage electrochemical performances of LiNi0.5Co0.2Mn0.3O2 cathode materials for lithium ion batteries.* Electrochimica Acta, 2016. **188**: p. 48-56.
13. Fukata, N., et al., *Lithium ion battery anodes using Si-Fe based nanocomposite structures.* Nano Energy, 2016. **26**: p. 37-42.
14. DOE, *Report of the Basic Energy Sciences Workshop on Electrical Energy Storage.* July 2007.
15. Ouyang, M., et al., *A dynamic capacity degradation model and its applications considering varying load for a large format Li-ion battery.* Applied Energy, 2016. **165**: p. 48-59.
16. Gasteiger, H.A. *Fundamental Aspects of Lithium Ion Battery Materials Degradation Mechanisms*. in *Meeting Abstracts*. 2016. The Electrochemical Society.
17. Ren, D., et al., *Degradation Identification of Individual Components in the LiyNi1/3Co1/3Mn1/3O2-LiyMn2O4 Blended Cathode for Large Format Lithium Ion Battery.* Energy Procedia, 2017. **105**: p. 2698-2704.
18. Hu, C., et al. *On-Board Analysis of Degradation Mechanisms of Lithium-Ion Battery Using Differential Voltage Analysis*. in *ASME 2016 International Design Engineering Technical Conferences and Computers and Information in Engineering Conference*. 2016. American Society of Mechanical Engineers.
19. Smith, K., et al. *Life prediction model for grid-connected Li-ion battery energy storage system*. in *American Control Conference (ACC), 2017*. 2017. IEEE.
20. Yan, D., et al., *Durability comparison of four different types of high-power batteries in HEV and their degradation mechanism analysis.* Applied Energy, 2016. **179**: p. 1123-1130.
21. Botte, G.G., V.R. Subramanian, and R.E. White, *Mathematical modeling of secondary lithium batteries.* Electrochimica Acta, 2000. **45**(15): p. 2595-2609.
22. Xu, J., et al., *Computational model of 18650 lithium-ion battery with coupled strain rate and SOC dependencies.* Applied Energy, 2016. **172**: p. 180-189.
23. Trembacki, B., et al., *Mesoscale Modeling of Lithium-Ion Battery Electrodes: Computational Requirements and the Role of Polymeric Binders*. 2016, Sandia National Laboratories (SNL-NM), Albuquerque, NM (United States); Sandia National Laboratories, Livermore, CA.
24. Saw, L.H., et al., *Computational fluid dynamic and thermal analysis of Lithium-ion battery pack with air cooling.* Applied Energy, 2016. **177**: p. 783-792.

25. De Vidts, P. and R.E. White, *Governing equations for transport in porous electrodes.* Journal of the Electrochemical Society, 1997. **144**(4): p. 1343-1353.
26. Wang, C., W. Gu, and B. Liaw, *Micro-Macroscopic Coupled Modeling of Batteries and Fuel Cells I. Model Development.* Journal of the Electrochemical Society, 1998. **145**(10): p. 3407-3417.
27. Jain, M. and J.W. Weidner, *Material Balance Modification in One-Dimensional Modeling of Porous Electrodes.* Journal of The Electrochemical Society, 1999. **146**(4): p. 1370-1374.
28. Carslow, H. and J. Jaeger, *Conduction of Heat In Sol Ids, Oxford University Press*. 1959, Oxford.
29. Crank, J., *The mathematics of diffusion*. 1979: Oxford university press.
30. Morbidelli, M., *Mathematical methods in chemical engineering*. 1997: Oxford University Press on Demand.
31. Ciarlet, P.G. and J.-L. Lions, *Handbook of numerical analysis*. Vol. 8. 1990: Gulf Professional Publishing.
32. Davis, M.E., *Numerical methods and modeling for chemical engineers*. 2013: Courier Corporation.
33. Pozrikidis, C., *Numerical computation in science and engineering*. Vol. 6. 1998: Oxford university press New York.
34. Pozrikidis, C. and J.H. Ferziger, *Introduction to theoretical and computational fluid dynamics.* Physics Today, 1997. **50**: p. 72.
35. De Vidts, P. and R.E. White, *A semi-analytical solution method for linear partial differential equations.* Computers & chemical engineering, 1992. **16**(10-11): p. 1007-1009.
36. Haran, B.S. and R.E. White, *A semianalytical technique for solving nonlinear partial differential equations.* Computer Applications in Engineering Education, 1996. **4**(3): p. 229-240.
37. Subramanian, V.R. and R.E. White. *A semi-analytical method for predicting current and potential distributions*. 1999.
38. White, R.E., *On Newman's numerical technique for solving boundary value problems.* Industrial & Engineering Chemistry Fundamentals, 1978. **17**(4): p. 367-369.
39. Van Zee, J., M.A. Edmund, and R.E. White, *Application of Newman's Technique to Coupled, Nonlinear Partial Differential Equations.* Industrial & Engineering Chemistry Fundamentals, 1980. **19**(4): p. 438-440.
40. Nguyen, T. and R.E. White, *A finite difference procedure for solving coupled, nonlinear elliptic partial differential equations.* Computers & chemical engineering, 1987. **11**(5): p. 543-546.
41. Curtis, D., T. Evans, and R.E. White, *A Comparison of Newman's Numerical Technique and deBoor's Algorithm.* Journal of the Electrochemical Society, 1989: p. 3392.
42. Preisig, H. and R.E. White, *On the design of a simple solver for nonlinear two-point boundary value problems.* Computers & chemical engineering, 1990. **14**(2): p. 179-196.
43. Matlosz, M. and J. Newman, *Solving 1-D boundary-value problems with BandAid: A functional programming style and a complementary software tool.* Computers & chemical engineering, 1987. **11**(1): p. 45-61.
44. Fan, D. and R.E. White, *Modification of Newman's BAND (J) Subroutine to Multi-Region Systems Containing Interior Boundaries: MBAND.* Journal of the Electrochemical Society, 1991. **138**(6): p. 1688-1691.

45. Patankar, S., *Numerical heat transfer and fluid flow, Hemisphere Publ.* Corp., New York, 1980.
46. West, A. and T. Fuller, *Influence of rib spacing in proton-exchange membrane electrode assemblies.* Journal of applied electrochemistry, 1996. **26**(6): p. 557-565.
47. Varga, R.S., *Matrix iterative analysis*. Vol. 27. 2009: Springer Science & Business Media.
48. Stark, R.H., *Rates of convergence in numerical solution of the diffusion equation.* Journal of the ACM (JACM), 1956. **3**(1): p. 29-40.
49. Marchuk, G.I., *Numerical methods for nuclear reactor calculations*. Soviet journal of atomic energy. Supplement ;1958, no. 3-4. 1959, New York: Consultants Bureau. 295 p.
50. Versteeg, H.K. and W. Malalasekera, *An introduction to computational fluid dynamics: the finite volume method*. 2007: Pearson Education.
51. Botte, G.G., J.A. Ritter, and R.E. White, *Comparison of finite difference and control volume methods for solving differential equations.* Computers & Chemical Engineering, 2000. **24**(12): p. 2633-2654.
52. Gresho, P.M. and R.L. Sani, *Incompressible flow and the finite element method. Volume 1: Advection-diffusion and isothermal laminar flow*. 1998: John Wiley and Sons, Inc., New York, NY (United States). Medium: X; Size: 300 p.
53. Raffler, M., et al., *Finite element model approach of a cylindrical lithium ion battery cell with a focus on minimization of the computational effort and short circuit prediction.* Journal of Power Sources, 2017. **360**: p. 605-617.
54. Wang, Z., J. Ma, and L. Zhang, *Finite element thermal model and simulation for a cylindrical Li-ion battery.* IEEE Access, 2017. **5**: p. 15372-15379.
55. Wu, L., Y. Wen, and J. Zhang, *Three-Dimensional Finite Element Study on Li Diffusion Induced Stress in FIB-SEM Reconstructed LiCoO 2 Half Cell.* Electrochimica Acta, 2016. **222**: p. 814-820.
56. Bizeray, A.M., et al., *Lithium-ion battery thermal-electrochemical model-based state estimation using orthogonal collocation and a modified extended Kalman filter.* Journal of Power Sources, 2015. **296**(Supplement C): p. 400-412.
57. Moura, S.J., N.A. Chaturvedi, and M. Krstic. *PDE estimation techniques for advanced battery management systems—Part I: SOC estimation*. in *American Control Conference (ACC), 2012*. 2012. IEEE.
58. Northrop, P.W., et al., *Efficient simulation and reformulation of lithium-ion battery models for enabling electric transportation.* Journal of The Electrochemical Society, 2014. **161**(8): p. E3149-E3157.
59. Vetter, J., et al., *Ageing mechanisms in lithium-ion batteries.* Journal of Power Sources, 2005. **147**(1): p. 269-281.
60. Verma, P., P. Maire, and P. Novák, *A review of the features and analyses of the solid electrolyte interphase in Li-ion batteries.* Electrochimica Acta, 2010. **55**(22): p. 6332-6341.
61. Broussely, M., et al., *Main aging mechanisms in Li ion batteries.* Journal of Power Sources, 2005. **146**(1): p. 90-96.
62. Maleki, H. and J.N. Howard, *Internal short circuit in Li-ion cells.* Journal of Power Sources, 2009. **191**(2): p. 568-574.
63. Fang, W., P. Ramadass, and Z. Zhang, *Study of internal short in a Li-ion cell-II. Numerical investigation using a 3D electrochemical-thermal model.* Journal of Power Sources, 2014. **248**: p. 1090-1098.

64. Zhao, W., G. Luo, and C.-Y. Wang, *Modeling nail penetration process in large-format Li-ion cells.* Journal of The Electrochemical Society, 2015. **162**(1): p. A207-A217.
65. Gao, L., S. Liu, and R.A. Dougal, *Dynamic lithium-ion battery model for system simulation.* IEEE transactions on components and packaging technologies, 2002. **25**(3): p. 495-505.
66. González-Longatt, F.M. *Circuit based battery models: A review*. in *Proceedings of 2nd Congreso IberoAmericano De Estudiantes de Ingenieria Electrica, Puerto la Cruz, Venezuela*. 2006.
67. Saw, L., Y. Ye, and A. Tay, *Electro-thermal characterization of Lithium Iron Phosphate cell with equivalent circuit modeling.* Energy Conversion and Management, 2014. **87**: p. 367-377.
68. Daowd, M., et al. *Battery models parameter estimation based on MATLAB/Simulink®*. in *Proceedings of the 25th Electric Vehicle Symposium (EVS-25), Shenzhen, China*. 2010.
69. Pals, C.R. and J. Newman, *Thermal modeling of the lithium/polymer battery I. Discharge behavior of a single cell.* Journal of the Electrochemical Society, 1995. **142**(10): p. 3274-3281.
70. Al Hallaj, S., et al., *Thermal modeling and design considerations of lithium-ion batteries.* Journal of Power Sources, 1999. **83**(1): p. 1-8.
71. Kumaresan, K., G. Sikha, and R.E. White, *Thermal model for a Li-ion cell.* Journal of the Electrochemical Society, 2008. **155**(2): p. A164-A171.
72. Macdonald, J.R. and E. Barsoukov, *Impedance spectroscopy: theory, experiment, and applications.* History, 2005. **1**(8).
73. Sparacino, A.R., et al. *Survey of battery energy storage systems and modeling techniques*. in *Power and Energy Society General Meeting, 2012 IEEE*. 2012. IEEE.
74. Hu, X., S. Li, and H. Peng, *A comparative study of equivalent circuit models for Li-ion batteries.* Journal of Power Sources, 2012. **198**(Supplement C): p. 359-367.
75. Jaguemont, J., L. Boulon, and Y. Dubé, *A comprehensive review of lithium-ion batteries used in hybrid and electric vehicles at cold temperatures.* Applied Energy, 2016. **164**: p. 99-114.
76. Ramadesigan, V., et al., *Modeling and simulation of lithium-ion batteries from a systems engineering perspective.* Journal of The Electrochemical Society, 2012. **159**(3): p. R31-R45.
77. Hu, X., S. Li, and H. Peng, *A comparative study of equivalent circuit models for Li-ion batteries.* Journal of Power Sources, 2012. **198**: p. 359-367.
78. Fotouhi, A., et al., *A review on electric vehicle battery modelling: From Lithium-ion toward Lithium–Sulphur.* Renewable and Sustainable Energy Reviews, 2016. **56**: p. 1008-1021.
79. Doyle, M., T.F. Fuller, and J. Newman, *Modeling of galvanostatic charge and discharge of the lithium/polymer/insertion cell.* Journal of the Electrochemical Society, 1993. **140**(6): p. 1526-1533.
80. Moradi, M. and L. Liu. *Towards a More Realistic Model: Variational Multiscale Modeling of Lithium-Ion Battery*. in *Meeting Abstracts*. 2017. The Electrochemical Society.
81. Moradi, M. and L. Liu. *Variational Multiscale Modeling of Charge Transport in Li Metal Battery*. in *Meeting Abstracts*. 2015. The Electrochemical Society.

82. Casacca, M.A. and Z.M. Salameh, *Determination of lead-acid battery capacity via mathematical modeling techniques.* IEEE Transactions on Energy Conversion, 1992. **7**(3): p. 442-446.

83. Fink, C. and B. Kaltenegger. *Comparison of Electrochemical and Electrothermal Models for Lithium-Ion Batteries Used in 3D Simulation*. in *Meeting Abstracts*. 2014. The Electrochemical Society.

84. Lin, X., et al., *A comprehensive capacity fade model and analysis for Li-ion batteries.* Journal of The Electrochemical Society, 2013. **160**(10): p. A1701-A1710.

85. Liu, L., et al., *A thermal-electrochemical model that gives spatial-dependent growth of solid electrolyte interphase in a Li-ion battery.* Journal of Power Sources, 2014. **268**(Supplement C): p. 482-490.

86. Liu, C. and L. Liu, *PMP-Based Fuel Cell Hybrid Vehicle Power Management Considering Battery Current Constraint and Battery Health Analysis*. 2015, SAE Technical Paper.

87. Liu, C. and L. Liu. *Improve Battery Safety for Hybrid Electric Vehicles through Multi-Objective Optimization of Battery Design and Hybridization Level*. in *Meeting Abstracts*. 2015. The Electrochemical Society.

88. Liu, C. and L. Liu, *Improving Battery Safety for Electric Vehicles through the Optimization of Battery Design Parameters.* ECS Transactions, 2015. **69**(20): p. 5-15.

89. Liu, C. and L. Liu. *Optimizing Battery Design for Fast Charging through a Genetic Algorithm Based Multi-Objective Optimization Framework.* in *Meeting Abstracts*. 2017. The Electrochemical Society.

90. Liu, C. and L. Liu, *Optimal Design of Li-Ion Batteries through Multi-Physics Modeling and Multi-Objective Optimization.* Journal of The Electrochemical Society, 2017. **164**(11): p. E3254-E3264.

91. Liu, C. and L. Liu, *Optimizing Battery Design for Fast Charge through a Genetic Algorithm Based Multi-Objective Optimization Framework.* ECS Transactions, 2017. **77**(11): p. 257-271.

92. Newman, J. and W. Tiedemann, *Porous‐electrode theory with battery applications.* AIChE Journal, 1975. **21**(1): p. 25-41.

93. Jokar, A., et al., *Review of simplified Pseudo-two-Dimensional models of lithium-ion batteries.* Journal of Power Sources, 2016. **327**: p. 44-55.

94. Newman, J. and K.E. Thomas-Alyea, *Electrochemical systems*. 2012: John Wiley & Sons.

95. Thomas, K.E., J. Newman, and R.M. Darling, *Mathematical modeling of lithium batteries*, in *Advances in lithium-ion batteries*. 2002, Springer. p. 345-392.

96. Doyle, C.M., *Design and simulation of lithium rechargeable batteries.* Lawrence Berkeley National Laboratory, 2010.

97. Smith, K.A., C.D. Rahn, and C.-Y. Wang, *Control oriented 1D electrochemical model of lithium ion battery*. Energy Conversion and Management, 2007. **48**(9): p. 2565-2578.

98. Dao, T.-S., C.P. Vyasarayani, and J. McPhee, *Simplification and order reduction of lithium-ion battery model based on porous-electrode theory.* Journal of Power Sources, 2012. **198**(Supplement C): p. 329-337.

99. Klein, R., et al., *Electrochemical model based observer design for a lithium-ion battery.* IEEE Transactions on Control Systems Technology, 2013. **21**(2): p. 289-301.

100. Lin, X., L. Liu, and P. Guan. *Phase Field Modeling of SEI layer morphology in Li-Ion Batteries*. in *Meeting Abstracts*. 2014. The Electrochemical Society.

101. Guan, P., X. Lin, and L. Liu, *Phase-Field Simulations of Solid Electrolyte Interface Morphology Evolution.* ECS Transactions, 2014. **61**(27): p. 29-41.
102. Liu, L. and M. Zhu, *Modeling of SEI layer growth and electrochemical impedance spectroscopy response using a thermal-electrochemical model of Li-ion batteries.* ECS Transactions, 2014. **61**(27): p. 43-61.
103. Guan, P. and L. Liu, *Lithium-ion Diffusion in Solid Electrolyte Interface (SEI) Predicted by Phase Field Model.* MRS Online Proceedings Library Archive, 2015. **1753**.
104. Guan, P., L. Liu, and X. Lin, *Simulation and experiment on solid electrolyte interphase (SEI) morphology evolution and lithium-ion diffusion.* Journal of The Electrochemical Society, 2015. **162**(9): p. A1798-A1808.
105. Guan, P. and L. Liu. *Phase Field Modeling of Lithium-Ion Diffusion and Crack Formation in the Solid Electrolyte Interphase of Silicon-Based Lithium-Ion Battery*. in *Meeting Abstracts*. 2015. The Electrochemical Society.
106. Guan, P. and L. Liu, *Phase-field Simulation of Lithium Ion Diffusion in Solid Electrolyte Interphase.* ECS Transactions, 2015. **66**(9): p. 81-91.
107. Guan, P. and L. Liu. *The Role of Porosity-Graded Electrode in Mitigating Performance Degradation of High Voltage Lithium-Ion Battery*. in *Meeting Abstracts*. 2017. The Electrochemical Society.
108. Liu, L. and P. Guan, *The Role of Porosity-Graded Electrode in Mitigating Performance Degradation of High Voltage Lithium-Ion Battery.* ECS Transactions, 2017. **77**(11): p. 321-329.
109. Liu, L., P. Guan, and C. Liu, *Experimental and Simulation Investigations of Porosity Graded Cathodes in Mitigating Battery Degradation of High Voltage Lithium-Ion Batteries.* Journal of The Electrochemical Society, 2017. **164**(13): p. A3163-A3173.
110. Liu, L. and M. Moradi, *Towards a More Realistic Battery Model: Variational Multiscale Modeling of Li-Ion Batteries.* ECS Transactions, 2017. **77**(11): p. 273-291.
111. Zhang, D., B.N. Popov, and R.E. White, *Modeling lithium intercalation of a single spinel particle under potentiodynamic control.* Journal of The Electrochemical Society, 2000. **147**(3): p. 831-838.
112. Ning, G. and B.N. Popov, *Cycle life modeling of lithium-ion batteries.* Journal of The Electrochemical Society, 2004. **151**(10): p. A1584-A1591.
113. Santhanagopalan, S., et al., *Review of models for predicting the cycling performance of lithium ion batteries.* Journal of Power Sources, 2006. **156**(2): p. 620-628.
114. Tanim, T.R., C.D. Rahn, and C.-Y. Wang, *A temperature dependent, single particle, lithium ion cell model including electrolyte diffusion.* Journal of Dynamic Systems, Measurement, and Control, 2015. **137**(1): p. 011005.
115. Rahimian, S.K., S. Rayman, and R.E. White, *Extension of physics-based single particle model for higher charge–discharge rates.* Journal of Power Sources, 2013. **224**: p. 180-194.
116. Rajabloo, B., M. Désilets, and Y. Choquette. *Parameter Estimation of Single Particle Model Using COMSOL Multiphysics® and MATLAB® Optimization Toolbox*. in *Proceedings of the 2015 COMSOL Conference in Boston*.
117. Fuller, T.F., M. Doyle, and J. Newman, *Simulation and optimization of the dual lithium ion insertion cell.* Journal of the Electrochemical Society, 1994. **141**(1): p. 1-10.

118. DOYLE , M. and J. NEWMAN *Analysis of capacity–rate data for lithium batteries using simplified models of the discharge process.* Journal of Applied Electrochemistry, 1997. **27**(7): p. 846-856.
119. Wang, Q., et al., *Thermal runaway caused fire and explosion of lithium ion battery.* Journal of Power Sources, 2012. **208**: p. 210-224.
120. Gomadam, P.M., et al., *Mathematical modeling of lithium-ion and nickel battery systems.* Journal of Power Sources, 2002. **110**(2): p. 267-284.
121. Song, J. and M.Z. Bazant, *Effects of nanoparticle geometry and size distribution on diffusion impedance of battery electrodes.* Journal of The Electrochemical Society, 2013. **160**(1): p. A15-A24.
122. Darling, R. and J. Newman, *Modeling a porous intercalation electrode with two characteristic particle sizes.* Journal of The Electrochemical Society, 1997. **144**(12): p. 4201-4208.
123. Franco, A.A., *Multiscale modelling and numerical simulation of rechargeable lithium ion batteries: concepts, methods and challenges.* Rsc Advances, 2013. **3**(32): p. 13027-13058.
124. Jensen, K.M., et al., *X-ray diffraction computed tomography for structural analysis of electrode materials in batteries.* Journal of The Electrochemical Society, 2015. **162**(7): p. A1310-A1314.
125. Tariq, F., et al., *Three-dimensional high resolution X-ray imaging and quantification of lithium ion battery mesocarbon microbead anodes.* Journal of Power Sources, 2014. **248**: p. 1014-1020.
126. Kashkooli, A.G., et al., *Multiscale modeling of lithium-ion battery electrodes based on nano-scale X-ray computed tomography.* Journal of Power Sources, 2016. **307**: p. 496-509.
127. Poizot, P., et al., *Nano-sized transition-metal oxides as negative-electrode materials for lithium-ion batteries.* Nature, 2000. **407**(6803): p. 496-499.
128. Derrien, G., et al., *Nanostructured Sn–C composite as an advanced anode material in high-performance Lithium-ion batteries.* Advanced Materials, 2007. **19**(17): p. 2336-2340.
129. Dillon, S.J. and K. Sun, *Microstructural design considerations for Li-ion battery systems.* Current Opinion in Solid State and Materials Science, 2012. **16**(4): p. 153-162.
130. Ebner, M., et al., *X-ray tomography of porous, transition metal oxide based lithium ion battery electrodes.* Advanced Energy Materials, 2013. **3**(7): p. 845-850.
131. Zhou, J., et al., *Magnetite/graphene nanosheet composites: interfacial interaction and its impact on the durable high-rate performance in lithium-ion batteries.* Rsc Advances, 2011. **1**(5): p. 782-791.
132. Nguyen, C.C. and S.-W. Song, *Interfacial structural stabilization on amorphous silicon anode for improved cycling performance in lithium-ion batteries.* Electrochimica Acta, 2010. **55**(8): p. 3026-3033.
133. Wang, C.-W. and A.M. Sastry, *Mesoscale modeling of a Li-ion polymer cell.* Journal of The Electrochemical Society, 2007. **154**(11): p. A1035-A1047.
134. Gupta, A., et al., *Effective transport properties of LiMn2O4 electrode via particle-scale modeling.* Journal of The Electrochemical Society, 2011. **158**(5): p. A487-A497.
135. Kehrwald, D., et al., *Local tortuosity inhomogeneities in a lithium battery composite electrode.* Journal of The Electrochemical Society, 2011. **158**(12): p. A1393-A1399.
136. Chung, D.-W., et al., *Validity of the Bruggeman relation for porous electrodes.* Modelling and Simulation in Materials Science and Engineering, 2013. **21**(7): p. 074009.

137. Zaoui, A., *Continuum micromechanics: survey*. Journal of Engineering Mechanics, 2002. **128**(8): p. 808-816.
138. Nemat-Nasser, S. *Retrospect and Prospect: Micromechanics*. in *Engineering Mechanics*. ASCE.
139. Ortiz, M., *Computational micromechanics.* Computational Mechanics, 1996. **18**(5): p. 321-338.
140. Tvergaard, V., *Studies of the micromechanics of materials.* Eur. J. Mechanics A/solids, 1997. **16**(special): p. 5-24.
141. Matouš, K., et al., *A review of predictive nonlinear theories for multiscale modeling of heterogeneous materials.* Journal of Computational Physics, 2017. **330**: p. 192-220.
142. Karplus, M., *Development of multiscale models for complex chemical systems: from H+ H2 to biomolecules (Nobel lecture).* Angewandte Chemie International Edition, 2014. **53**(38): p. 9992-10005.
143. Levitt, M., *Birth and future of multiscale modeling for macromolecular systems (Nobel Lecture).* Angewandte Chemie International Edition, 2014. **53**(38): p. 10006-10018.
144. Warshel, A., *Multiscale modeling of biological functions: from enzymes to molecular machines (nobel lecture).* Angewandte Chemie International Edition, 2014. **53**(38): p. 10020-10031.
145. Eshelby, J.D. *The determination of the elastic field of an ellipsoidal inclusion, and related problems*. in *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*. 1957. The Royal Society.
146. Eshelby, J. *The elastic field outside an ellipsoidal inclusion*. in *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*. 1959. The Royal Society.
147. Mori, T. and K. Tanaka, *Average stress in matrix and average elastic energy of materials with misfitting inclusions.* Acta metallurgica, 1973. **21**(5): p. 571-574.
148. Hill, R., *Continuum micro-mechanics of elastoplastic polycrystals.* Journal of the Mechanics and Physics of Solids, 1965. **13**(2): p. 89-101.
149. Horstemeyer, M.F., *Multiscale Modeling: A Review*, in *Practical Aspects of Computational Chemistry: Methods, Concepts and Applications*, J. Leszczynski and M.K. Shukla, Editors. 2010, Springer Netherlands: Dordrecht. p. 87-135.
150. Ghosez, P. and J. Junquera, *Handbook of theoretical and computational nanotechnology.* American Scientific, Stevenson Ranch, CA, 2006: p. 623-728.
151. Lu, G., E.B. Tadmor, and E. Kaxiras, *From electrons to finite elements: A concurrent multiscale approach for metals.* Physical Review B, 2006. **73**(2): p. 024108.
152. Liu, Y., et al., *Computational microstructure characterization and reconstruction for stochastic multiscale material design.* Computer-Aided Design, 2013. **45**(1): p. 65-76.
153. Chakraborty, A. and S. Rahman, *Stochastic multiscale models for fracture analysis of functionally graded materials.* Engineering Fracture Mechanics, 2008. **75**(8): p. 2062-2086.
154. Ganapathysubramanian, B. and N. Zabaras, *A stochastic multiscale framework for modeling flow through random heterogeneous porous media.* Journal of Computational Physics, 2009. **228**(2): p. 591-618.
155. Geißendörfer, M., et al., *Stochastic multiscale modeling of metal foams.* Probabilistic Engineering Mechanics, 2014. **37**: p. 132-137.

156. Babuška, I. and M. Motamed, *A fuzzy-stochastic multiscale model for fiber composites: A one-dimensional study*. Computer Methods in Applied Mechanics and Engineering, 2016. **302**: p. 109-130.
157. Zhou, H.-X., *Theoretical frameworks for multiscale modeling and simulation.* Current opinion in structural biology, 2014. **25**: p. 67-76.
158. Ayton, G.S., W.G. Noid, and G.A. Voth, *Multiscale modeling of biomolecular systems: in serial and in parallel.* Current Opinion in Structural Biology, 2007. **17**(2): p. 192-198.
159. Sherwood, P., B.R. Brooks, and M.S. Sansom, *Multiscale methods for macromolecular simulations.* Current opinion in structural biology, 2008. **18**(5): p. 630-640.
160. Saunders, M.G. and G.A. Voth, *Coarse-graining of multiprotein assemblies.* Current opinion in structural biology, 2012. **22**(2): p. 144-150.
161. Heyden, A., H. Lin, and D.G. Truhlar, *Adaptive partitioning in combined quantum mechanical and molecular mechanical calculations of potential energy functions for multiscale simulations.* The Journal of Physical Chemistry B, 2007. **111**(9): p. 2231-2241.
162. Heyden, A. and D.G. Truhlar, *Conservative Algorithm for an Adaptive Change of Resolution in Mixed Atomistic/Coarse-Grained Multiscale Simulations.* Journal of Chemical Theory and Computation, 2008. **4**(2): p. 217-221.
163. Nielsen, S.O., et al., *Recent progress in adaptive multiscale molecular dynamics simulations of soft matter.* Physical Chemistry Chemical Physics, 2010. **12**(39): p. 12401-12414.
164. Saunders, M.G. and G.A. Voth, *Coarse-graining methods for computational biology.* Annual review of biophysics, 2013. **42**: p. 73-93.
165. Warshel, A. and M. Levitt, *Theoretical studies of enzymic reactions: Dielectric, electrostatic and steric stabilization of the carbonium ion in the reaction of lysozyme.* Journal of Molecular Biology, 1976. **103**(2): p. 227-249.
166. Field, M.J., P.A. Bash, and M. Karplus, *A combined quantum mechanical and molecular mechanical potential for molecular dynamics simulations.* Journal of Computational Chemistry, 1990. **11**(6): p. 700-733.
167. Neri, M., et al., *Coarse-grained model of proteins incorporating atomistic detail of the active site.* Physical review letters, 2005. **95**(21): p. 218102.
168. Shi, Q., S. Izvekov, and G.A. Voth, *Mixed atomistic and coarse-grained molecular dynamics: simulation of a membrane-bound ion channel.* The Journal of Physical Chemistry B, 2006. **110**(31): p. 15045-15048.
169. Gohlke, H. and M.F. Thorpe, *A natural coarse graining for simulating large biomolecular motion.* Biophysical Journal, 2006. **91**(6): p. 2115-2120.
170. Orsi, M., M.G. Noro, and J.W. Essex, *Dual-resolution molecular dynamics simulation of antimicrobials in biomembranes.* Journal of The Royal Society Interface, 2011. **8**(59): p. 826-841.
171. Han, W. and K. Schulten, *Further Optimization of a Hybrid United-Atom and Coarse-Grained Force Field for Folding Simulations: Improved Backbone Hydration and Interactions between Charged Side Chains.* Journal of Chemical Theory and Computation, 2012. **8**(11): p. 4413-4424.
172. Predeus, A.V., et al., *Conformational Sampling of Peptides in the Presence of Protein Crowders from AA/CG-Multiscale Simulations.* The Journal of Physical Chemistry B, 2012. **116**(29): p. 8610-8620.

173. Riniker, S., A.P. Eichenberger, and W.F. van Gunsteren, *Structural Effects of an Atomic-Level Layer of Water Molecules around Proteins Solvated in Supra-Molecular Coarse-Grained Water.* The Journal of Physical Chemistry B, 2012. **116**(30): p. 8873-8879.
174. Wassenaar, T.A., et al., *Mixing MARTINI: electrostatic coupling in hybrid atomistic–coarse-grained biomolecular simulations.* The Journal of Physical Chemistry B, 2013. **117**(13): p. 3516-3530.
175. Fish, J., *Bridging the scales in nano engineering and science.* Journal of Nanoparticle Research, 2006. **8**(5): p. 577-594.
176. Bouvard, J., et al., *Review of hierarchical multiscale modeling to describe the mechanical behavior of amorphous polymers.* Journal of Engineering Materials and Technology, 2009. **131**(4): p. 041206.
177. Miehe, C. and C. Bayreuther, *On multiscale FE analyses of heterogeneous structures: from homogenization to multigrid solvers.* International Journal for Numerical Methods in Engineering, 2007. **71**(10): p. 1135-1180.
178. Tadmor, E.B., M. Ortiz, and R. Phillips, *Quasicontinuum analysis of defects in solids.* Philosophical magazine A, 1996. **73**(6): p. 1529-1563.
179. Plews, J. and C. Duarte, *Bridging multiple structural scales with a generalized finite element method.* International Journal for Numerical Methods in Engineering, 2015. **102**(3-4): p. 180-201.
180. Weinan, E., *Principles of multiscale modeling*. 2011: Cambridge University Press.
181. Gokhale, A.M. and S. Yang, *Application of image processing for simulation of mechanical response of multi-length scale microstructures of engineering alloys.* Metallurgical and Materials Transactions A, 1999. **30**(9): p. 2369-2381.
182. Shuck, C.E., et al., *X-ray nanotomography and focused-ion-beam sectioning for quantitative three-dimensional analysis of nanocomposites.* Journal of synchrotron radiation, 2016. **23**(4): p. 990-996.
183. Möbus, G. and B.J. Inkson, *Nanoscale tomography in materials science.* Materials Today, 2007. **10**(12): p. 18-25.
184. Groeber, M., et al., *3D reconstruction and characterization of polycrystalline microstructures using a FIB–SEM system.* Materials Characterization, 2006. **57**(4): p. 259-273.
185. Uchic, M.D., et al., *3D microstructural characterization of nickel superalloys via serial-sectioning using a dual beam FIB-SEM.* Scripta Materialia, 2006. **55**(1): p. 23-28.
186. Wilson, J.R., et al., *Measurement of three-dimensional microstructure in a LiCoO 2 positive electrode.* Journal of Power Sources, 2011. **196**(7): p. 3443-3447.
187. Wang, Z., *Non-equilibrim Statistical Physics,"Introduction to Statistical Physics"*. 1965, Higher Education Press) p41 (in Chinese)[王 1965 非平衡态的统计理论 "统计物理学导论"(高等教育出版社) 第 41].
188. Jiang, D.Q. and M. Qian, *Mathematical Theory of Nonequilibrium Steady States: On the Frontier of Probability and Dynamical Systems*. 2004: Springer.
189. Barenblatt, G., *Scaling, Cambridge Texts in Applied Mathematics.* Cambridge: CLIP, 2003.
190. Ansini, N., A. Braides, and V. Valente, *Multiscale analysis by Γ-convergence of a one-dimensional nonlocal functional related to a shell-membrane transition.* SIAM journal on mathematical analysis, 2006. **38**(3): p. 944-976.

191. Otsubo, Y., *Elastic percolation in suspensions flocculated by polymer bridging.* Langmuir, 1990. **6**(1): p. 114-118.
192. Fu, R., Q. Long, and C. Lung, *Interpretation of porosity effect on strength of highly porous ceramics.* Scripta metallurgica et materialia, 1991. **25**(7): p. 1583-1585.
193. Hu, C., B.D. Youn, and J. Chung, *A multiscale framework with extended Kalman filter for lithium-ion battery SOC and capacity estimation.* Applied Energy, 2012. **92**: p. 694-704.
194. Xiong, R., et al., *A data-driven multi-scale extended Kalman filtering based parameter and state estimation approach of lithium-ion olymer battery in electric vehicles.* Applied Energy, 2014. **113**: p. 463-476.
195. Farkas, Z., et al., *Improvement of accuracy of multi-scale models of Li-ion batteries by applying operator splitting techniques.* Journal of Computational and Applied Mathematics, 2017. **310**: p. 59-79.
196. Hua, Y., et al., *A multi time-scale state-of-charge and state-of-health estimation framework using nonlinear predictive filter for lithium-ion battery pack with passive balance control.* Journal of Power Sources, 2015. **280**: p. 293-312.
197. Röder, F., R. Braatz, and U. Krewer, *Multi-scale modeling of solid electrolyte interface formation in lithium-ion batteries.* Computer Aided Chemical Engineering, 2016. **38**: p. 157.
198. Mortazavi, B., et al., *Graphene or h-BN paraffin composite structures for the thermal management of Li-ion batteries: A multiscale investigation.* Applied Energy, 2017. **202**: p. 323-334.
199. Xiao, X., W. Wu, and X. Huang, *A multi-scale approach for the stress analysis of polymeric separators in a lithium-ion battery.* Journal of Power Sources, 2010. **195**(22): p. 7649-7660.
200. Hellwig, C., S. Sörgel, and W.G. Bessler, *A multi-scale electrochemical and thermal model of a LiFePO4 battery.* Ecs Transactions, 2011. **35**(32): p. 215-228.
201. Richardson, G., G. Denuault, and C. Please, *Multiscale modelling and analysis of lithium-ion battery charge and discharge.* Journal of Engineering Mathematics, 2012. **72**(1): p. 41-72.
202. Wang, C.Y. and V. Srinivasan, *Computational battery dynamics (CBD)—electrochemical/thermal coupled modeling and multi-scale modeling.* Journal of Power Sources, 2002. **110**(2): p. 364-376.
203. Du, W., et al., *A surrogate-based multi-scale model for mass transport and electrochemical kinetics in lithium-ion battery electrodes.* Journal of the Electrochemical Society, 2014. **161**(8): p. E3086-E3096.
204. Röder, F., R.D. Braatz, and U. Krewer, *Multi-Scale Simulation of Heterogeneous Surface Film Growth Mechanisms in Lithium-Ion Batteries.* Journal of The Electrochemical Society, 2017. **164**(11): p. E3335-E3344.
205. Zielke, L., et al., *Three-Phase Multiscale Modeling of a LiCoO2 Cathode: Combining the Advantages of FIB–SEM Imaging and X-Ray Tomography.* Advanced Energy Materials, 2015. **5**(5).
206. Bai, B., et al., *Multi-scale method of Nano(Micro)-CT study on microscopic pore structure of tight sandstone of Yanchang Formation, Ordos Basin.* Petroleum Exploration and Development, 2013. **40**(3): p. 354-358.
207. Nanda, J., et al. *Multiscale Imaging and Spectroscopy on a Lithium-Ion Pouch Cell: Experiments and Modelling*. in *Meeting Abstracts*. 2017. The Electrochemical Society.

208. Lee, S., A.M. Sastry, and J. Park, *Study on microstructures of electrodes in lithium-ion batteries using variational multi-scale enrichment.* Journal of Power Sources, 2016. **315**: p. 96-110.
209. Delacourt, C. and M. Safari, *Mathematical Modeling of Aging of Li-Ion Batteries*, in *Physical Multiscale Modeling and Numerical Simulation of Electrochemical Devices for Energy Conversion and Storage: From Theory to Engineering to Practice*, A.A. Franco, M.L. Doublet, and W.G. Bessler, Editors. 2016, Springer London: London. p. 151-190.
210. Behrou, R. and K. Maute, *Multiscale Modeling of Non-Local Damage Evolution in Lithium-Ion Batteries.* ECS Transactions, 2017. **77**(11): p. 1163-1177.
211. Kim, D., et al., *Phase Separation and d Electronic Orbitals on Cyclic Degradation in Li–Mn–O Compounds: First-Principles Multiscale Modeling and Experimental Observations.* ACS applied materials & interfaces, 2016. **8**(26): p. 16631-16639.
212. Moroni, R., et al., *Multi-scale correlative tomography of a Li-ion battery composite cathode.* Scientific reports, 2016. **6**: p. 30109.
213. Gelb, J., et al., *Multi-scale 3D investigations of a commercial 18650 Li-ion battery with correlative electron-and X-ray microscopy.* Journal of Power Sources, 2017. **357**: p. 77-86.
214. Abada, S., et al. *Modeling of Thermal Runaway-Induced Li-Ion Battery Failure Integrating Multiphysics and Multiscale Approaches As Well As Ageing Interaction*. in *Meeting Abstracts*. 2016. The Electrochemical Society.
215. Pan, J., *Understanding electrical conduction in lithium ion batteries through multi-scale modeling.* 2016.
216. Yin, Y., et al., *Impact of Li2O2 Particle Size on Li–O2 Battery Charge Process: Insights from a Multiscale Modeling Perspective.* The journal of physical chemistry letters, 2016. **7**(19): p. 3897-3902.
217. Madani, S.S., M.J. Swierczynski, and S.K. Kær. *The discharge behavior of lithium-ion batteries using the Dual-Potential Multi-Scale Multi-Dimensional (MSMD) Battery Model*. in *Ecological Vehicles and Renewable Energies (EVER), 2017 Twelfth International Conference on*. 2017. IEEE.
218. Bai, Y., et al., *Statistical mesomechanics of solid, linking coupled multiple space and time scales.* Applied Mechanics Reviews, 2005. **58**(6): p. 372-388.
219. Xia, M.-f., et al., *Sample-specific behavior in failure models of disordered media.* Communications in theoretical physics, 1996. **25**(1): p. 49.
220. Zhang, S. and C. Oskay, *Variational multiscale enrichment method with mixed boundary conditions for elasto-viscoplastic problems.* Computational Mechanics, 2015. **55**(4): p. 771-787.
221. Mote, C., *Global-local finite element.* International Journal for Numerical Methods in Engineering, 1971. **3**(4): p. 565-574.
222. Fish, J. and S. Markolefas, *Adaptive global–local refinement strategy based on the interior error estimates of the h-method.* International Journal for Numerical Methods in Engineering, 1994. **37**(5): p. 827-838.
223. Gendre, L., et al., *Non-intrusive and exact global/local techniques for structural problems with local plasticity.* Computational Mechanics, 2009. **44**(2): p. 233-245.
224. Mao, K. and C. Sun, *A refined global-local finite element analysis method.* International journal for numerical methods in engineering, 1991. **32**(1): p. 29-43.

225. Noor, A.K., *Global-local methodologies and their application to nonlinear analysis.* Finite Elements in Analysis and Design, 1986. **2**(4): p. 333-346.
226. Duarte, C.A. and D.-J. Kim, *Analysis and applications of a generalized finite element method with global–local enrichment functions.* Computer Methods in Applied Mechanics and Engineering, 2008. **197**(6): p. 487-504.
227. Fish, J., *The s-version of the finite element method.* Computers & Structures, 1992. **43**(3): p. 539-547.
228. Markovic, D. and A. Ibrahimbegovic, *On micro–macro interface conditions for micro scale based FEM for inelastic behavior of heterogeneous materials.* Computer Methods in Applied Mechanics and Engineering, 2004. **193**(48): p. 5503-5523.
229. Hughes, T.J., *Multiscale phenomena: Green's functions, the Dirichlet-to-Neumann formulation, subgrid scale models, bubbles and the origins of stabilized methods.* Computer methods in applied mechanics and engineering, 1995. **127**(1-4): p. 387-401.
230. Hughes, T.J., et al., *The variational multiscale method—a paradigm for computational mechanics.* Computer methods in applied mechanics and engineering, 1998. **166**(1-2): p. 3-24.
231. Garikipati, K. and T. Hughes, *A variational multiscale approach to strain localization–formulation for multidimensional problems.* Computer Methods in Applied Mechanics and Engineering, 2000. **188**(1): p. 39-60.
232. Hughes, T.J. and G. Sangalli, *Variational multiscale analysis: the fine-scale Green's function, projection, optimization, localization, and stabilized methods.* SIAM Journal on Numerical Analysis, 2007. **45**(2): p. 539-557.
233. Arbogast, T., *Implementation of a locally conservative numerical subgrid upscaling scheme for two-phase Darcy flow.* Computational Geosciences, 2002. **6**(3-4): p. 453-481.
234. Arbogast, T., *Analysis of a two-scale, locally conservative subgrid upscaling for elliptic problems.* SIAM Journal on Numerical Analysis, 2004. **42**(2): p. 576-598.
235. Oskay, C., *Variational multiscale enrichment for modeling coupled mechano-diffusion problems.* International Journal for Numerical Methods in Engineering, 2012. **89**(6): p. 686-705.
236. Oskay, C., *Variational multiscale enrichment method with mixed boundary conditions for modeling diffusion and deformation problems.* Computer Methods in Applied Mechanics and Engineering, 2013. **264**: p. 178-190.
237. Juanes, R. and F.-X. Dub, *A locally conservative variational multiscale method for the simulation of porous media flow with multiscale source terms.* Computational Geosciences, 2008. **12**(3): p. 273-295.
238. Garikipati, K., *Variational multiscale methods to embed the macromechanical continuum formulation with fine-scale strain gradient theories.* International journal for numerical methods in engineering, 2003. **57**(9): p. 1283-1298.
239. Masud, A. and K. Xia, *A variational multiscale method for inelasticity: Application to superelasticity in shape memory alloys.* Computer methods in applied mechanics and engineering, 2006. **195**(33): p. 4512-4531.
240. Yeon, J.-H. and S.-K. Youn, *Variational multiscale analysis of elastoplastic deformation using meshfree approximation.* International Journal of Solids and Structures, 2008. **45**(17): p. 4709-4724.

241. Crouch, R. and C. Oskay, *Symmetric mesomechanical model for failure analysis of heterogeneous materials.* International Journal for Multiscale Computational Engineering, 2010. **8**(5).
242. Oskay, C. and J. Fish, *Eigendeformation-based reduced order homogenization for failure analysis of heterogeneous materials.* Computer Methods in Applied Mechanics and Engineering, 2007. **196**(7): p. 1216-1243.

Chapter 3. Variational Multiscale Modeling of LIB

3.1 Introduction

The subject of energy is a major factor in engineering and designers in all engineering fields are moving toward a developing a model that utilizes energy from renewable sources or reduces energy utilization [1, 2]. In a world with increasing energy demands, energy storage systems play an important role. Batteries are one of the main energy storage systems that help in meeting energy needs of the modern world. The broad application of battery systems in small and portable devices such as smartphones, laptops, and smartwatches has been extended to large systems such as electrical vehicles [3, 4], power electronic systems [5], and aircrafts [6]. Therefore, the study of LIBs is of significant importance. Due to the expensive nature of experimental studies, multiple efforts were put into modeling and numerical investigation of LIBs for studying battery performance or design optimizations. Electrochemical modeling [7-15] and equivalent circuit modeling [16-22] are examples of such modeling efforts in LIB studies.

Since LIBs are systems that have important ongoing physico-chemical phenomena at different length scales, it is important to consider the effects of multiple scales of such physical systems in developing a mathematical model. There have been efforts in considering the occurring physical phenomena in multiple scales of LIB [23-25]. One important phenomenon that affects LIB performance and life cycle is SEI layer growth which happens at the interface of battery electrode and electrolyte. Therefore, models that can present an exact model of that region are of significant importance in LIB studies. Since a LIB solid electrode is comprised of multiple particles that the shapes and sizes of which are not uniform (see Figure 3.1 [26]), it is hard to model its exact structure. Furthermore, there are different phases (solid, liquid, and gas) and modeling the exact interaction between them requires a time consuming molecular dynamics simulation. Therefore, making a more accurate model that at least resolves the heterogeneous structure of the electrode/electrolyte interface is a step forward in the more realistic modeling of LIB.

Resolving the microscale heterogeneity of LIB has been the point of interest to researchers. The previous research attempted to accomplish a model for LIB microstructural heterogeneity by employing imaging techniques such as tomography and SEM imaging to resolve the non-uniform microstructure domain [26-28]. Although information obtained from microstructural images is accurate, employing a multiscale method that is not dependent on expensive and advanced equipment is more desirable. Additionally, having a fully resolved microscopic domain increases the cost of computational analysis. Multiple methods have been proposed to model multiscale phenomena in different physical systems. The bridging scale method [29-31], multigrid method [32, 33], domain decomposition [34, 35], and heterogeneous multiscale method (HMM) [36-38] are some the proposed multiscale analysis approaches in modeling and numerical studies. While these approaches have proved to be powerful tools of modeling, each has its disadvantages. For example, in bridging scale method resolving the difference in spatial and temporal scales between different scales is the challenging factor while HMM relies on scale separation techniques which have their mathematical complexity [39]. Hence, a better understanding of a complex system can be obtained by employing a more straightforward approach in multiscale modeling, which can offer a more realistic demonstration of the actual physical system.

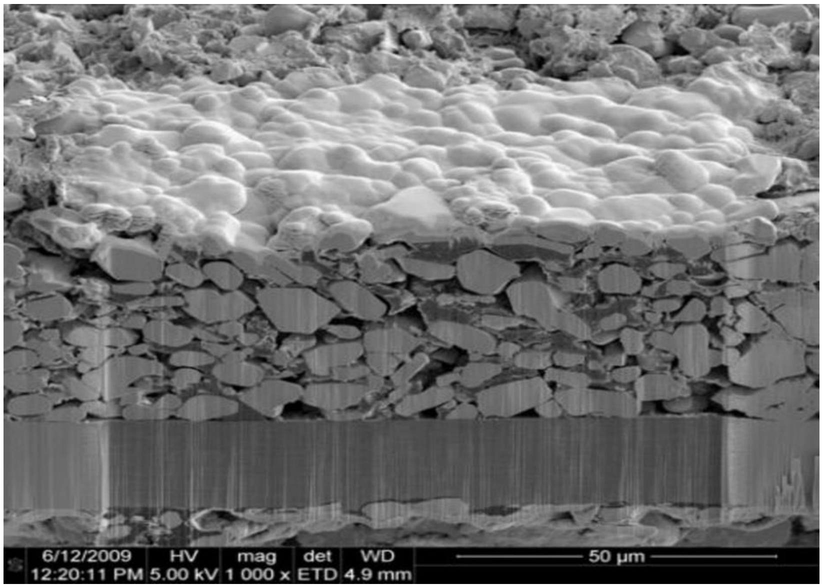


Figure 3.1. SEM image of a LIB cathode [26]

The variational multiscale method (VMM) is a multiscale method of analysis which is based on well-established concepts of finite element method (FEM). The VMM does not employ scale separation techniques in incorporating the microstructure effects into the total response of the system. As reported by Wei, Zheng, Chen, & Xia [40], this method of multiscale modeling has a better computational efficiency compared with the other methods of modeling. The main idea of the VMM is to decompose the solution of the problem into two parts: micro/fine- scale and macro/coarse- scale. The microscale response is obtained semi-analytically via variational projection where the macroscale response is solved numerically. The governing equations of a LIB system that was developed in Newman's research group are presented in this chapter. Then by employing the variational principle, a weak form of solid-state mass transfer equation is obtained. By decomposing the solution of the mass transfer equation into micro- and macro- scale solutions, the weak form equations are separated for each scale of the system. Then, by utilizing Green's function and by the help of basis functions, a solution for microscale is obtained, and the obtained result will be substituted and incorporated into the macroscale equation. Therefore, by solving the macroscale equation, a solution which accounts for the microscale response of the system will be obtained. Details of this methodology are presented in the next section.

3.2 Methods

3.2.1 LIB Electrochemical Modeling

The governing equations for the multiscale analysis of charge transfer in a LIB system are based on Newman's work [41]. The Butler-Volmer equation describes the reaction rate of intercalation. Charge conservation and species conservation govern the cell potentials (solid: $\emptyset_s$; liquid: $\emptyset_e$) and Li-ion concertation (solid: c_s; liquid phase: c_e), respectively. A list of symbols is provided in the appendix.

In detail, mass balance equations are considered in both electrode and electrolyte. Fick's second law explains mass transfer in the solid phase through diffusion:

$$\frac{\partial c_s}{\partial t} = \mathrm{D}_s^{eff} \cdot \frac{\partial^2 c_s}{\partial r^2} \tag{3.1}$$

in which D_s^{eff} is the effective diffusion coefficient and c_s represents concentration of Li-ion in the solid phase. For the flow of ions in the electrolyte, the mass balance equation is derived based on concentrated solution theory as given below:

$$\frac{\partial c_e}{\partial t} = D_e^{eff} \Delta c_e + \frac{i_e(1-t_+)}{F} \tag{3.2}$$

with

$$D_e^{eff} = D\frac{c_T}{c_o}\left(1 + \frac{dln\gamma_\pm}{dlnm}\right) \tag{3.3}$$

c_e is the ion concentration in the solution, and D is the diffusion coefficient based on thermodynamic driving force. The free movement of Li-ion in the electrolyte is caused by its concentration gradient. It is obvious that the gradient in the concentration of Li-ion is the driving force for ion flux which facilitates ion movement in the electrolyte. The dominant flow regime in the liquid phase is migration as convection is usually neglected; for details see [42]. The current in the solution phase, i_e, is given by Ohm's law as follow:

$$i_e = -\sigma_e^{eff} \nabla\emptyset_e + \frac{2RT}{F}(1-t_+)\sigma_e^{eff} \nabla ln c_e \tag{3.4}$$

As stated by [41], the potential in the binary electrolyte is measured by a reference electrode that goes under a half cell reaction and the potential gradient, $\nabla\emptyset_e$, is then measured with respect to another reference electrode of the same kind at a fixed position. The potential gradient helps the flow of ions in the solution and the conductive solid phase. In equation [3.4], R is the universal gas constant, T is temperature, and F is Faraday's constant. The effective conductivity of the electrolyte denoted by σ_e^{eff}.

The electrode-electrolyte interface chemical reaction rate depends on concentration and potential. In this regard, the Butler-Volmer equation is used to determine the relationship between current and surface overpotential:

$$i_n = j_n F = i_0 \left[exp\left(\frac{\alpha_a F(\emptyset_s - \emptyset_e - U - R_{SEI} F j_n)}{RT}\right) - exp\left(\frac{\alpha_c F(\emptyset_s - \emptyset_e - U - R_{SEI} F j_n)}{RT}\right)\right] \tag{3.5}$$

where i_n is the transfer current normal to the surface of active material, j_n is the transfer flux normal to the surface of active material, i_0 is the exchange current density, U is the equilibrium potential difference between electrode and electrolyte, and surface over potential is given by $\emptyset_s - \emptyset_e - U - R_{SEI} F j_n$, R_{SEI} is the resistance of the solid electrolyte interface (SEI) layer, and $\emptyset_s$ is the potential in solid phase which is derived from Ohm's law:

$$i_s = -\sigma_s^{eff} \nabla \emptyset_s \tag{3.6}$$

from which we can derive the charge balance equation in the solid phase:

$$-\nabla.\left(\sigma_s^{eff} \nabla \emptyset_s\right) = 0 \tag{3.7}$$

where σ_s^{eff} is electrode effective conductivity. The exchange current density is a function of reaction rate constants, transfer coefficients, and Li-ion concentrations as it is given below:

$$i_0 = F(k_a)^{\alpha_c}(k_c)^{\alpha_a} c_e^{\alpha_a}(c_t - c_s)^{\alpha_c} c_s^{\alpha_a} \tag{3.8}$$

in which, k_a and k_c are rate constants for anodic and cathodic direction of the chemical reaction, α_c and α_a are anodic and cathodic transfer coefficient, and c_t is the maximum concentration of Li-ion in the electrode.

3.2.2 Stabilized Methods and Multiscale Modeling

The first stabilized method was Streamline Upwind Petrov-Galerkin (SUPG) method which was introduced by Hughes and Brooks [43] for incompressible flows. The SUPG method treated the instabilities of the Galerkin method for convection dominated flows by augmenting the Galerkin method formulation with residual-based terms without introducing any inconsistencies to the solution.

The SUPG for compressible flows was introduced in 1982 [44], with more detailed versions published later [45, 46]. The details of the development of SUPG for compressible flows are summarized in a review paper by Hughes, Scovazzi, & Tezduyar [47]. Another stabilized method called pressure stabilizing Petrov-Galerkin (PSPG) was introduced later for incompressible flows in the scheme of residual-based methods [48]. In this method, interpolation techniques were employed to find interpolating functions for the problem variables, such as pressure, that lead the way to finite element analysis of incompressible flows [48]. Further development of stabilized methods that are based on the inclusion of residual-based terms resulted in a combination of SUPG and PSPG, the SUPS stabilization [49].

Further development of stabilized methods emerged through the introduction of interface tracking and capturing techniques [50-55]. Deforming spatial domain stabilized space-time (DSD/SST) formulation can be mentioned as an interface tracking technique, which was introduced in 1992 [50, 52, 53]. Hughes [56] developed the basic theory of variational multiscale method. Furthermore, Bazilevs, Takizawa, & Tezduyar [48] suggested that understanding the theoretical background of stabilized methods can be achieved by two approaches: Galerkin finite element method with augmented function spaces and variational multiscale method. Hughes [56] derived an equivalency between the two methods to demonstrate the valid identification of stabilized methods as multiscale modeling techniques. This equivalency [56] is presented in the following:

Consider the following abstract problem:

$$\mathcal{L}u = f, in\ \Omega \tag{3.9}$$

$$u = 0, on\ \partial\Omega \tag{3.10}$$

Find $u \in V$ such that $a(u, v) = F(v), v \in V$. V is a Hilbert space, $a(.,.)$ is a bilinear and $F(.)$ a linear form on V. Knowing $a(u, v) = (\mathcal{L}u, v), F(v) = (f, v)$, and $(u, v) = \int uvd\Omega$. Applying the Galerkin approximation on the variational form of the problem and discretizing the problem domain into finite-dimensional subspace V_h, we obtain:

$$a(u_h, v_h) = F(v_h), u_h \& v_h \in V_h \tag{3.11}$$

Employing augmented formulation, the subspace V_h is enlarged and enriched to improve the approximation and avoid inconsistencies that would arise due to computational process instabilities [56]. Let us denote the V_h before enlargement by V_h^R, while $(.)_R$ and $(.)^h$ represent variables in the VMM and Galerkin with augmented spaces, respectively. Considering the new notation, the problem is defined as:

$$a(u_R, v_R) = F(v_R), u_R \& v_R \in V_R^h \tag{3.12}$$

Considering V_U^b as a closed subspace of the already defined Hilbert space such that

$$V_R^h \cap V_U^b = \{0\} \tag{3.13}$$

the augmented space can be defined as:

$$V_h = V_R^h \oplus V_U^b \tag{3.14}$$

The goal is first to find the effect of V_U^b on V_R^h, and then write the variational problem exclusively for V_R^h. From (3.14) we can obtain:

$$v_h = v_R \oplus v_U \in V_R^h \oplus V_U^b \tag{3.15}$$

Therefore following the decomposition in (3.15), the variational problem can be written as:

$$a(u_R + u_U, v_R) = F(v_R), v_R \in V_R^h \tag{3.16}$$

$$a(u_R + u_U, v_U) = F(v_U), v_U \in V_U^b \tag{3.17}$$

By using the bilinear property of $a(.,.)$, (3.17) can be written as:

$$a(u_U, v_U) = F(v_U) - a(u_R, v_U), v_U \in V_U^b \tag{3.18}$$

The solution of (3.18) can be obtained in the following form:

$$u_U = M(\mathcal{L}u_R - f) \tag{3.19}$$

And M is a linear operator (projector operator) from $H^{-1}(\Omega)$ to $H_0^1(\Omega)$.

Incorporating (3.19) into (3.16), the problem is only written in terms of u_R:

$$a(u_R, v_R) + a(M(\mathcal{L}u_R - f), v_R) = (f, v_R), v_R \in V_R^h \tag{3.20}$$

In following the VMM approach, $v_h = v_R + v_U \in V_R^h \oplus V_U$, where V_U is the space containing the microscale domain and is defined as: $V_U = \oplus\, H_0^1(elem)$ [56] (elem is an abbreviation for element and here denotes single element domain). Therefore, $v_U = \sum_{elem} v_{U,elem}\, , v_{U.elem} \in H_0^1(elem)$ and the variational problem can be written as:

$$a(u_R + u_U, v_R) = F(v_R), v_R \in V_R^h \tag{3.21}$$

$$a(u_R + u_{U,elem}, v_{U,elem}) = F\big(v_{U,elem}\big)_{elem}, v_{U,elem} \in H_0^1(elem) \tag{3.22}$$

Exploiting the bilinear form of $a(.,.)$:

$$a\big(u_{U,elem}, v_{U,elem}\big) = F\big(v_{U,elem}\big)_{elem} - a\big(u_R, v_{U,elem}\big)_{elem}, v_{U,elem} \in H_0^1(elem) \tag{3.23}$$

or

$$\mathcal{L}u_{U,elem} = f - \mathcal{L}u_R, on\ element\ domain \tag{3.24}$$

$$u = 0, on\ element\ boundaries \tag{3.25}$$

Therefore, a solution for the unresolved scale can be obtained in the following form:

$$u_{U,elem} = M_{elem}(\mathcal{L}u_R - f) \tag{3.26}$$

And M is a linear operator from $H^{-1}(elem)$ onto $H_0^1(elem)$. Substituting (3.26) into the (3.20):

$$a(u_R, v_R) + \sum_{elem} a(M_{elem}(\mathcal{L}u_R - f), v_R)_{elem} = (f, v_R), v_R \in V_R^h \tag{3.27}$$

Now by following the Galerkin method with augmented function spaces, $v_h = v_R + v_B \in V_R^h \oplus V^b$ where $V^b = \oplus_{elem} B_{elem}$ is the space that augments the functions space V_R^h and B_{elem} is a subspace of $H_0^1(elem)$. The decomposition of v_B over the elements can be demonstrated as:

$$v_B = \sum_{elem} v_{B,elem}\, , v_{B,elem} \in B_{elem} \tag{3.28}$$

Therefore, the variational problem can be written as:

$$a(u_R + u_B, v_R) = F(v_R), v_R \in V_R^h \tag{3.29}$$

$$a(u_R + u_{B,elem}, v_{B,elem}) = F\left(v_{B,elem}\right)_{elem}, v_{B,elem} \in B_{elem} \tag{3.30}$$

(3.30) can be written as:

$$a(u_{B,elem}, v_{B,elem})_{elem} = F(v_{B,elem})_{elem} - a(u_R, v_{B,elem}), v_{B,elem} \in B_{elem} \tag{3.31}$$

Requiring that the augmenting function space, B_{elem}, holds for any test functions $v_{B,elem}$ throughout the whole element domains of $H_0^1(elem)$, a function $u_{B,elem} \in H_0^1(elem)$ is identified for each $u_R \in V_R^h$. The function $u_{B,elem}$ is the solution of the following variational problem:

$$a(u_{B,elem}, v)_{elem} = F(v)_{elem} - a(u_R, v)_{elem}, v \in H_0^1(elem) \tag{3.32}$$

Similar to the VMM, a linear operator M_{elem} can be defined ($M_{elem}: from\ H^{-1}(elem) to\ H_0^1(elem)$) and:

$$u_{B,elem} = M_{elem}(F(v)_{elem} - a(u_R, v)_{elem}) = M_{elem}(\mathcal{L}u_R - f) \tag{3.33}$$

Comparing the approximation for the unresolved scale between the two methods ((3.26) and (3.33)), the equivalency between these methods can be noted. Both methods result in the same equation for the original problem while taking into account the effect of the unresolved scales. In the next section, the process of applying the VMM to a LIB system is presented.

3.2.3 Variational Multiscale Modeling

The details of the developed variational multiscale model are demonstrated in this section. The model is developed based on fundamentals of FEM in which function spaces and corresponding basis functions are employed in the development and solution of the model. In this model, the micro- and macro- scales are decoupled from each other by first decomposing the problem domain into micro- and macro- scales. The decomposition process and application of VMM is presented in detail as it is applied to a response field (e.g. $c_{Lithium}$) and consider it in two different scales; as shown in Figure 3.2. The governing equations will be decomposed into two separate PDEs accordingly: one is associated with the response filed in the macroscale and the other is the governing equation of the microscale. One of the main characteristics of the VMM is that the notion of scale separation is not used in this method and the problem domain is decomposed into coarse/macro- and fine/micro- scales without the complexities associated with scale separation process. Therefore, two solutions will be obtained for the two decomposed scales. The fine-scale subdomain was chosen to be a part of the problem domain where an important physicochemical phenomenal is likely to occur. The solution to the microscale problem is then obtained by the help of Green's function and is incorporated into the problem for macroscale. Considering integrals as distributions (i.e. weak formulation; average of functions over certain areas of the computational domain), we can perform integration operation on the function that represents the solution to the problem, regardless of existence of discontinuity points in the domain. Hence, one of the main advantages of the developed model is that it resolves the heterogeneities of microscale without considering the minor details (such as discontinuity points) but rather our focus is invested in the distribution of the solution over the problem domain (and certain subdomain), which reduces the computational costs of the numerical analysis. This is of significant importance, especially for cases that the effect of ongoing microscale phenomena is more significant than the minor details of the microscale. Employing Green's function, the microscale problem can be solved. The response from the rest of the computational domain will be calculated by obtaining a solution that is idealized and solved at the macroscale.

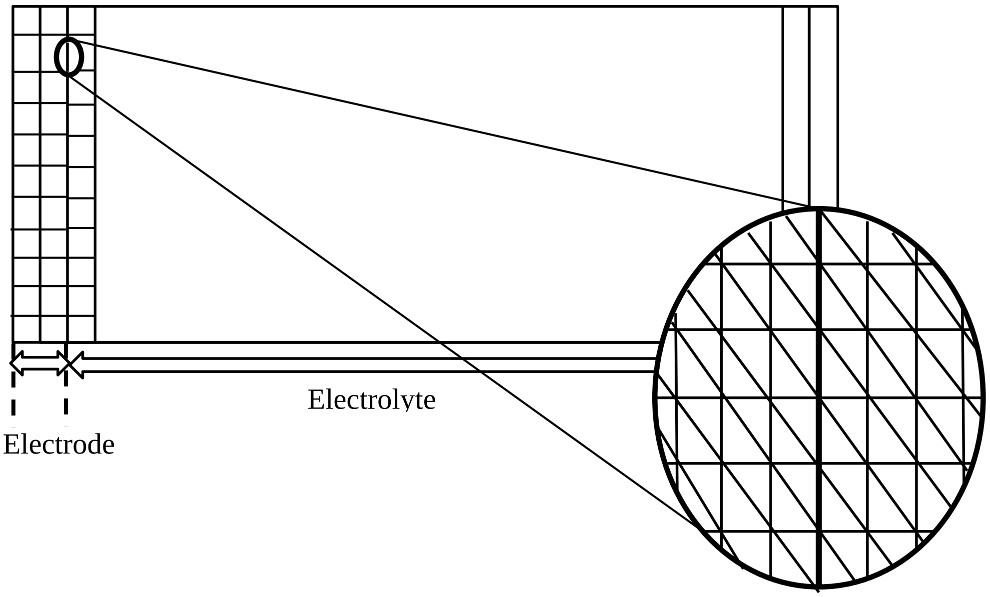


Figure 3.2. Schematic diagram of decomposing battery domain for application of VMM in LIB simulation

The VMM is applied to the mass balance equations for the electrode and electrolyte. The variational form of the equations is derived from the notion of test functions. For 1D analysis of the diffusion problem, the test functions are defined as:

$$v = v(x), v \in V \tag{3.34}$$

where V is the functions space for test functions and is defined as a normed Hilbert space:

$$V = H_0^1(\Omega) \tag{3.35}$$

with the associated norm $\|.\|$ and Ω is the problem domain.

Let us introduce some of the mathematical notations before proceeding further. $(.,.)$ denotes the scalar product in the normed Hilbert space such that:

$$(u\,,v)_{\Omega} = \int uv\,d\Omega \tag{3.36}$$

and $a(.\,,.)$ represents a bilinear form as:

$$a(u\,,v)_{\Omega} = \int \mathcal{L}uv\,d\Omega \tag{3.37}$$

where $\mathcal{L}$ is the differential operator that's been applied on the problem dependent variable, in this case, u.

Now we proceed by decomposing variables into micro- and macro- scale ones. Let $u \epsilon V$ and by decomposing the vector space as following:

$$V = \overline{V} \oplus \tilde{V} \tag{3.38}$$

field variables and test functions are decomposed as:

$$c_s = \overline{c_s} + \widetilde{c_s} \tag{3.39}$$

$$c_e = \overline{c_e} + \widetilde{c_e} \tag{3.40}$$

$$v = \overline{v} + \tilde{v} \tag{3.41}$$

$\overline{V}$ is the macro- and $\tilde{V}$ is the micro- scale solution space. For indicating macro- and micro- scale variables, the overbar and prime signs are used respectively. Test functions are taking a zero value where there is a known value of the dependent variable in any part of the problem domain. By multiplying test functions to the mass balance equations, the variational form (weak formulation) of the equations are derived as follow:

$$\int \frac{\partial c_s}{\partial t} v\,d\Omega - \int D\,\frac{\partial^2 c_s}{\partial x^2} v d\Omega = 0$$

$$=> (\dot{c}_s, v) + a(c_s, v) = 0 \tag{3.42}$$

$$\int \frac{\partial c_e}{\partial t} v\,d\Omega - \int D\,\frac{\partial^2 c_e}{\partial x^2} v d\Omega = \int \underbrace{\frac{i_e(1-t_+)}{F}}_{f} v d\Omega$$

$$=> (\dot{c}_e, v) + a(c_e, v) = (f, v) \tag{3.43}$$

Substituting the decomposed variables, (3.39) – (3.41), into the variational form of the governing equations the following is obtained:

$$(\dot{c}_s, \tilde{v} + \overline{v}) + a(\widetilde{c_s} + \overline{c_s}, \tilde{v} + \overline{v}) = 0 \tag{3.44}$$

$$(\dot{c}_e, \tilde{v} + \overline{v}) + a(\widetilde{c_e} + \overline{c_e}, \tilde{v} + \overline{v}) = (f, \tilde{v} + \overline{v}) \tag{3.45}$$

with further simplifications we have:

$$(\dot{c}_s, \overline{v}) + a(\widetilde{c_s}, \overline{v}) + a(\overline{c_s}, \overline{v}) = 0 \tag{3.46}$$

$$(\dot{c}_s, \tilde{v}) + a(\widetilde{c_s}, \tilde{v}) + a(\overline{c_s}, \tilde{v}) = 0 \tag{3.47}$$

$$(\dot{c}_e, \overline{v}) + a(\widetilde{c_e}, \overline{v}) + a(\overline{c_e}, \overline{v}) = (f, \overline{v}) \tag{3.48}$$

$$(\dot{c_e}, \tilde{v}) + a(\widetilde{c_e}, \tilde{v}) + a(\overline{c_e}, \tilde{v}) = (f, \tilde{v}) \tag{3.49}$$

Since there is no difference between the time steps in the micro- and macro- domain of the problem, the Li-ion concentration is dependent on the spatial rather than time variable. Therefore, no decomposition is required for $\dot{c_s}$ and $\dot{c_e}$. c_s is decomposed because Li-ion concentration is present in both of the micro- and the macro- scale of the problem.

The microscale equations (3.47) and (3.49) can be rewritten as below:

$$\mathcal{L}\widetilde{c_s} = -\mathcal{L}\overline{c_s} \tag{3.50}$$

$$\mathcal{L}\widetilde{c_e} = f - \mathcal{L}\overline{c_e} \tag{3.51}$$

The goal of applying the VMM is to approximate the microscale response in certain areas of the problem domain where it is known ***a priori*** that important physicochemical phenomena are likely to occur. All integrals are in the sense of distributions. Refer to [57, 58] for details, in other words; the objective is to approximate the microscale solution over a specific part of the domain rather than deriving the solution in every single point of the microscale domain. Approximation of microscale solution is accomplished by having Dirac delta functions at the right-hand side of the equation for the microscale problem. The microscale problem then yields a solution in the form of Green's function. The obtained Green's function, in this case, should not be mistaken with the classical form of the Green's function as it is defined according to the constraints of the microscale function space, $\tilde{V}$.

Therefore, the microscale equations can be solved by introducing microscale Green's function, $\tilde{g}$. For the microscale Green's function, we have:

$$\mathcal{L}^{*}\tilde{g}(x, x') = \delta(x - x') \tag{3.52}$$

where $\mathcal{L}^{*}$ is the adjoint operator of $\mathcal{L}$. Considering homogenous Dirichlet boundary condition for microscale field variables, $\widetilde{c_s}$ and $\widetilde{c_e}$, the microscale Green's function takes zero value at the boundaries as well:

$$\tilde{g}(x, x') = 0 \qquad on\ \partial\Omega \tag{3.53}$$

The microscale field variables now can be obtained by the following:

$$\widetilde{c_s}(x') = \int \tilde{g}(x, x')(-\mathcal{L}\overline{c_s})\, d\Omega \tag{3.54}$$

$$\widetilde{c_e}(x') = \int \tilde{g}(x, x')(f - \mathcal{L}\overline{c_e})\, d\Omega \tag{3.55}$$

The obtained microscale solutions can be more simplified by introducing the microscale Green's operator, $\tilde{\mathcal{G}}$, which is represented by the microscale Green's function. Therefore, we have:

$$\widetilde{c_s} = \tilde{\mathcal{G}}(-\mathcal{L}\overline{c_s}) \tag{3.56}$$

$$\widetilde{c_e} = \tilde{\mathcal{G}}(f - \mathcal{L}\overline{c_e}) \tag{3.57}$$

Substituting (3.56) and (3.57) into the (3.47) and (3.49), the exact equations for $\overline{c_s}$ and $\overline{c_e}$ are obtained:

$$(\dot{c}_s, \overline{v}) + a\big(\tilde{\mathcal{G}}(-\mathcal{L}\overline{c_s}), \overline{v}\big) + a(\overline{c_s}, \overline{v}) = 0 \tag{3.58}$$

$$(\dot{c}_e, \overline{v}) + a\big(\tilde{\mathcal{G}}(f - \mathcal{L}\overline{c_e}), \overline{v}\big) + a(\overline{c_e}, \overline{v}) = (f, \overline{v}) \tag{3.59}$$

Next step is finding a relation for the microscale Green's operator, $\tilde{\mathcal{G}}$. $\tilde{\mathcal{G}}$ is obtained by the relation given below [59]:

$$\tilde{\mathcal{G}} = \mathcal{G} - \mathcal{G}\mu^T[\mu\mathcal{G}\mu^T]^{-1}\mu\mathcal{G} \tag{3.60}$$

in which $\mathcal{G}$ is the classical Green's function, and μ is a set of basis functions defined for the adjoint operator of a linear projection operator defined as a projection from the problem function space to the macroscale problem space:

$$\mathcal{P}: V \to \overline{V} \tag{3.61}$$

Assuming the dimension of $\overline{V}$ is N, the following can be obtained [59]:

$$\begin{aligned} &(\mu_i\,, v) = 0 \qquad\qquad \forall i = 1, \dots, N \\ &=> \int \mu_i v \, d\Omega = 0 \end{aligned} \tag{3.62}$$

which supports the previous statement claiming μ_i are the basis functions for the image of adjoint operator of $\mathcal{P}$. Therefore [59],

$$\tilde{\mathcal{G}}\mu_i = 0 \tag{3.63}$$

$$\begin{aligned} &\big(\mu_i\,, \tilde{\mathcal{G}}v\big) = 0 \\ &=> \int \tilde{g}(x\,, x')\mu_i(x')dx' = 0 \end{aligned} \tag{3.64}$$

Satisfying (3.56), we set $\mu_i(x) = \delta(x - x_i)$ and from (3.58) the following is obtained:

$$\tilde{g}\big(x_{i,nodal}\,, x'\big) = 0 \tag{3.65}$$

The obtained relation for $\tilde{g}$ indicates that if x_i is a nodal point of the discretized area, then $\tilde{g}(x_i\,, x') = 0$. In other words, if x' and x belong to the same element of the discretization, the microscale response is obtained and the effect of the microscale is localized [59]. In mathematical form: if $x' > x_i$ or $x' < x_{i-1}$ then $\mathcal{L}^*\tilde{g} = 0$ and if $x_{i-1} < x' < x_i$ then $\mathcal{L}^*\tilde{g} = \delta$. This way, the elements in the microscale are decoupled from each other which simplifies the complexities of a multiscale analysis. Consequently, the microscale problem is separated element by element and the following is obtained from (3.44) and (3.45):

$$\mathcal{L}\tilde{c_s} = -\mathcal{L}\overline{c_s} \qquad \mathit{for\ element}\ (x_{i-1}\,, x_i) :\ \tilde{c_s}|_{x_{i,\ nodal}} = 0 \tag{3.66}$$

$$\mathcal{L}\tilde{c_e} = f - \mathcal{L}\overline{c_e} \qquad \mathit{for\ element}\ (x_{i-1}\,, x_i) :\ \tilde{c_e}|_{x_{i,\ nodal}} = 0 \tag{3.67}$$

Besides the boundary conditions stated in (3.66) and (3.67), we require the microscale solution to become zero in areas of the domain where it coincides with its macroscale counterpart:

$$\tilde{c_s} = 0 \qquad \mathit{on\ overlapping\ line\ between}\ \partial\tilde{\Omega} \mathit{and}\ \partial\overline{\Omega} \tag{3.68}$$

$$\tilde{c_e} = 0 \qquad \mathit{on\ overlapping\ line\ between}\ \partial\tilde{\Omega} \mathit{and}\ \partial\overline{\Omega} \tag{3.69}$$

The boundary of the micro- and macro- scale domain are denoted by $\partial\tilde{\Omega}$ and $\partial\overline{\Omega}$ respectively. Employing integration by parts, the following bilinear forms are obtained from (3.42) and (3.43):

$$\int \frac{\partial c_s}{\partial t} v \, d\Omega - \int D \, c_s \frac{d^2 v}{dx^2} d\Omega = D\left(\frac{\partial c_s}{\partial x} v|_{\partial\Omega} - c_s \frac{dv}{dx}|_{\partial\Omega}\right) \tag{3.70}$$

$$\begin{aligned}\int \frac{\partial c_e}{\partial t} v \, d\Omega - \int D \, c_e \frac{d^2 v}{dx^2} d\Omega \\ = \underbrace{\int \frac{i_e(1-t_+)}{F}}_{f} v \, d\Omega + D\left(\frac{\partial c_e}{\partial x} v|_{\partial\Omega} - c_e \frac{dv}{dx}|_{\partial\Omega}\right)\end{aligned} \tag{3.71}$$

where superscript e indicates element-wise evaluation of the field variable, and $(\mathcal{L}c_{\cdot}^{e}, v)_{\partial\Omega}$ represents the concomitant of the operator $\mathcal{L}$ which is resulted from integration by parts. Writing the obtained weak formulation relations in an abstract form we have:

$$(\dot{c_s}, \overline{v}) + \left(\tilde{\mathcal{G}}(-\mathcal{L}\overline{c_s}), \mathcal{L}^*\overline{v}\right) + (\overline{c_s}, \mathcal{L}^*\overline{v}) = \left(\mathcal{L}\widetilde{c_s^e}, \overline{v}\right)_{\partial\Omega} + \left(\mathcal{L}\overline{c_s^e}, \overline{v}\right)_{\partial\Omega} \tag{3.72}$$

$$\begin{aligned}(\dot{c_e}, \overline{v}) + \left(\tilde{\mathcal{G}}(f - \mathcal{L}\overline{c_e}), \mathcal{L}^*\overline{v}\right) + (\overline{c_e}, \mathcal{L}^*\overline{v}) \\ = (f, \overline{v}) + \left(\mathcal{L}\widetilde{c_e^e}, \overline{v}\right)_{\partial\Omega} + \left(\mathcal{L}\overline{c_e^e}, \overline{v}\right)_{\partial\Omega}\end{aligned} \tag{3.73}$$

By substituting the relation for $\widetilde{c_s}$ and $\widetilde{c_e}$ into the equations for $\overline{c_s}$ and $\overline{c_e}$ (Eqs. (3.58) and (3.59)), and employing typical FEM basis functions ($\overline{v}$), the macroscale solution of the problem will be obtained. This solution has the microscale solution incorporated into it, therefore reflects the response of a system which has ongoing microscale phenomena.

3.3 Conclusion

A review and development of multiscale modeling approach for developing a multiscale model for a LIB system were presented in this chapter. The precise development of methodology can be further incorporated in modeling efforts for the computational study of LIBs. By the help of Green's functions, the effect of microscale on macroscale problem of the battery is taken into account. Incorporation of microscale effects on the macroscale problem is of significant importance since applying VMM helps to examine multiscale phenomena without considering the exact microscale phenomena. In other words, applying VMM does not lead to solving the microscale equation for each element and nodal value. The focus in this method of modeling is rather on modifying the macroscale governing equation by integrating the effects of the microscale domain of the problem.

3.4 Appendix

Symbol	Name	Symbol	Name
c	Concentration ($mol\ m^{-3}$)	U	Equilibrium potential difference between electrode and electrolyte (V)
c_t	Maximum concentration of Li-ion in the electrode ($mol\ m^{-3}$)	v	Test function
c_T	Total concentration of salt and solvent ($mol\ m^{-3}$)	V	Functions space (solution and test function)
D	Diffusion coefficient ($m^2\ s^{-1}$)	Greek symbols	
D^{eff}	Effective Li diffusion coefficient ($m^2\ s^{-1}$)	α	Transfer coefficient
F	Faraday's constant, 96,48 ($C\ mol^{-1}$)	$\gamma_{\pm}$	Mean molal activity coefficient
g	Green's function	σ^{eff}	Effective conductivity ($S\ m^{-1}$)
$\mathcal{G}$	Green's Operator	$\emptyset$	Potential (V)
H	Normed Hilbert space	Ω	Problem domain
i	Current density (Am^{-2})	$\delta(x-.)$	Dirac delta function
i_0	Exchange current density (Am^{-2})	μ	Basis function for the adjoint operator of $\mathcal{P}$
i_n	Transfer current normal to the surface of active material (Am^{-2})	Subscripts	
j_n	Transfer flux normal to the surface of active material ($mol\ s^{-1}m^{-2}$)	a	Anodic
k	Reaction rate coefficient ($m\ s^{-1}$)	c	Cathodic
$\mathcal{L}$	Differential operator of the mass balance equation	e	Liquid phase
m	Molality (mol/kg)	s	Solid phase
$\mathcal{P}$	Linear projection onto the macroscale space	o	Property measured with respect to initial condition
R	Gas constant ($J\ mol^{-1}K^{-1}$)	Superscripts	
R_{SEI}	SEI resistance ($\Omega\ m^2$)	e	Property evaluated at element scale
t	Time (s)	$\sim$	Property at microscale
T	Temperature (K)	$\bar{}$	Property at macroscale
t_+	Li transference number	$*$	Adjoint operator

Table 3.1. List of symbols

3.5 References

1. Momeni, A.F., et al., *Effect of Prestressing Wire Indentation Type on the Development Length and Flexural Capacity of Pretensioned Concrete Crossties.* 2015(56451): p. V001T01A026.

2. Momeni, A.F., et al., *Effect of Concrete Release Strength on the Development Length and Flexural Capacity of Members Made With Different Prestressing Strands.* 2016(49675): p. V001T01A017.
3. Jiang, J. and C. Zhang, *Fundamentals and Application of Lithium-ion Batteries in Electric Drive Vehicles*. 2015: Wiley.
4. Pesaran, A.A., *Lithium Ion Batteries in Electric Drive Vehicles*. 2016.
5. Buller, S., et al. *Impedance-based simulation models of supercapacitors and Li-ion batteries for power electronic applications*. in *38th IAS Annual Meeting on Conference Record of the Industry Applications Conference, 2003.* 2003.
6. Kim, I.-S., *The novel state of charge estimation method for lithium battery using sliding mode observer.* Journal of Power Sources, 2006. **163**(1): p. 584-590.
7. Schmidt, A.P., et al., *Experiment-driven electrochemical modeling and systematic parameterization for a lithium-ion battery cell.* Journal of Power Sources, 2010. **195**(15): p. 5071-5080.
8. Tippmann, S., et al., *Low-temperature charging of lithium-ion cells part I: Electrochemical modeling and experimental investigation of degradation behavior.* Journal of Power Sources, 2014. **252**: p. 305-316.
9. Ploehn, H.J., P. Ramadass, and R.E. White, *Solvent diffusion model for aging of lithium-ion battery cells.* Journal of The Electrochemical Society, 2004. **151**(3): p. A456-A462.
10. Ramadesigan, V., et al., *Efficient reformulation of solid-phase diffusion in physics-based lithium-ion battery models.* Journal of The Electrochemical Society, 2010. **157**(7): p. A854-A860.
11. Safari, M. and C. Delacourt, *Mathematical modeling of lithium iron phosphate electrode: galvanostatic charge/discharge and path dependence.* Journal of The Electrochemical Society, 2011. **158**(2): p. A63-A73.
12. Gordon, I.J., et al., *Electrochemical Impedance Spectroscopy response study of a commercial graphite-based negative electrode for Li-ion batteries as function of the cell state of charge and ageing.* Electrochimica Acta, 2017. **223**: p. 63-73.
13. Zhang, C., et al., *Coupling of Mechanical Behavior of Lithium Ion Cells to Electrochemical-Thermal (ECT) Models for Battery Crush*. 2016, NREL (National Renewable Energy Laboratory (NREL), Golden, CO (United States)).
14. Bahiraei, F., et al., *A pseudo 3D electrochemical-thermal modeling and analysis of a lithium-ion battery for electric vehicle thermal management applications.* Applied Thermal Engineering, 2017.
15. Ghalkhani, M., et al., *Electrochemical–Thermal Model of Pouch-type Lithium-ion Batteries.* Electrochimica Acta, 2017.
16. Widanage, W., et al., *Design and use of multisine signals for Li-ion battery equivalent circuit modelling. Part 2: Model estimation.* Journal of Power Sources, 2016. **324**: p. 61-69.
17. Zhong, F., et al., *An SOC estimation approach based on adaptive sliding mode observer and fractional order equivalent circuit model for lithium-ion batteries.* Communications in Nonlinear Science and Numerical Simulation, 2015. **24**(1): p. 127-144.
18. Feng, T., et al., *Online identification of lithium-ion battery parameters based on an improved equivalent-circuit model and its implementation on battery state-of-power prediction.* Journal of Power Sources, 2015. **281**: p. 192-203.

19. Nejad, S., D. Gladwin, and D. Stone, *A systematic review of lumped-parameter equivalent circuit models for real-time estimation of lithium-ion battery states.* Journal of Power Sources, 2016. **316**: p. 183-196.
20. Hu, X., et al., *Charging time and loss optimization for LiNMC and LiFePO 4 batteries based on equivalent circuit models.* Journal of Power Sources, 2013. **239**: p. 449-457.
21. Xavier, M.A. and M.S. Trimboli, *Lithium-ion battery cell-level control using constrained model predictive control and equivalent circuit models.* Journal of Power Sources, 2015. **285**: p. 374-384.
22. Li, Y., et al. *An equivalent circuit model of li-ion battery based on electrochemical principles used in grid-connected energy storage applications*. in *Future Energy Electronics Conference and ECCE Asia (IFEEC 2017-ECCE Asia), 2017 IEEE 3rd International*. 2017. IEEE.
23. Franco, A.A., *Multiscale modelling and numerical simulation of rechargeable lithium ion batteries: concepts, methods and challenges.* Rsc Advances, 2013. **3**(32): p. 13027-13058.
24. Stamps, M., J.W. Eischen, and H.-Y.S. Huang, *Particle-and crack-size dependency of lithium-ion battery materials LiFePO4.* AIMS Mater. Sci, 2016. **3**(1): p. 190.
25. Latz, A. and J. Zausch, *Multiscale modeling of lithium ion batteries: thermal aspects.* Beilstein journal of nanotechnology, 2015. **6**: p. 987.
26. Stephenson, D.E., et al., *Modeling 3D microstructure and ion transport in porous Li-ion battery electrodes.* Journal of The Electrochemical Society, 2011. **158**(7): p. A781-A789.
27. Cooper, S.J., et al., *Image based modelling of microstructural heterogeneity in LiFePO4 electrodes for Li-ion batteries.* Journal of Power Sources, 2014. **247**: p. 1033-1039.
28. Hutzenlaub, T., et al., *Three-dimensional electrochemical Li-ion battery modelling featuring a focused ion-beam/scanning electron microscopy based three-phase reconstruction of a LiCoO2 cathode.* Electrochimica Acta, 2014. **115**: p. 131-139.
29. Pour, B.H., *Multiscale Modelling of Molecules and Continuum Mechanics Using Bridging Scale Method.* 2016.
30. Qian, D. and S. Chirputkar, *Bridging scale simulation of lattice fracture using enriched space‐time Finite Element Method.* International Journal for Numerical Methods in Engineering, 2014. **97**(11): p. 819-850.
31. Castelnau, O., et al. *Multiscale Modelling of the Effective Viscoplastic Behavior of Mg2SiO4 Wadsleyite and Ringwoodite: Bridging Atomic and Polycrystal Scale*. in *AGU Fall Meeting Abstracts*. 2016.
32. Bu, W., et al., *Finite element multigrid method for multi-term time fractional advection diffusion equations.* International Journal of Modeling, Simulation, and Scientific Computing, 2015. **6**(01): p. 1540001.
33. Falgout, R., et al., *Parallel time integration with multigrid reduction for a compressible fluid dynamics application.* Journal of Computational Physics, 2014.
34. He, X., et al., *A Domain Decomposition Method for the Steady-State Navier--Stokes--Darcy Model with Beavers--Joseph Interface Condition.* SIAM Journal on Scientific Computing, 2015. **37**(5): p. S264-S290.
35. Vay, J.-L., I. Haber, and B.B. Godfrey, *A domain decomposition method for pseudo-spectral electromagnetic simulations of plasmas.* Journal of Computational Physics, 2013. **243**: p. 260-268.

36. Alyaev, S., E. Keilegavlen, and J.M. Nordbotten, *Analysis of control volume heterogeneous multiscale methods for single phase flow in porous media.* Multiscale Modeling & Simulation, 2014. **12**(1): p. 335-363.
37. Arjmand, D. and O. Runborg, *Analysis of heterogeneous multiscale methods for long time wave propagation problems.* Multiscale Modeling & Simulation, 2014. **12**(3): p. 1135-1166.
38. Abdulle, A. and O. Budác, *An adaptive finite element heterogeneous multiscale method for Stokes flow in porous media.* Multiscale Modeling & Simulation, 2015. **13**(1): p. 256-290.
39. Weinan, E. and B. Engquist, *The heterognous multiscale methods.* Communications in Mathematical Sciences, 2003. **1**(1): p. 87-132.
40. Wei, G.-W., et al., *Variational multiscale models for charge transport.* SIAM Review, 2012. **54**(4): p. 699-754.
41. Thomas, K.E., J. Newman, and R.M. Darling, *Mathematical modeling of lithium batteries*, in *Advances in lithium-ion batteries*. 2002, Springer. p. 345-392.
42. Pollard, R. and J. Newman, *Mathematical Modeling of the Lithium‐Aluminum, Iron Sulfide Battery I. Galvanostatic Discharge Behavior.* Journal of The Electrochemical Society, 1981. **128**(3): p. 491-502.
43. Hughes, T. and A. Brooks, *A multidimensional upwinding scheme with no crosswind diffusion, Hughes.* Finite Element Methods for Convection Dominated Flows, 1979. **34**.
44. Tezduyar, T. and T. J. R. Hughes, *Development of Time-Accurate Finite Element Techniques for First-Order Hyperbolic Systems with Particular Emphasis on the Compressible Euler Equations*. 1982.
45. Tezduyar, T. and T. Hughes. *Finite element formulations for convection dominated flows with particular emphasis on the compressible Euler equations*. in *Proceedings of AIAA 21st aerospace sciences meeting, AIAA Paper*. 1983.
46. Hughes, T.J. and T. Tezduyar, *Finite element methods for first-order hyperbolic systems with particular emphasis on the compressible Euler equations.* Computer methods in applied mechanics and engineering, 1984. **45**(1-3): p. 217-284.
47. Hughes, T.J.R., G. Scovazzi, and T.E. Tezduyar, *Stabilized Methods for Compressible Flows.* Journal of Scientific Computing, 2010. **43**(3): p. 343-368.
48. Bazilevs, Y., K. Takizawa, and T.E. Tezduyar, *New directions and challenging computations in fluid dynamics modeling with stabilized and multiscale methods*. 2015, World Scientific.
49. Bazilevs, Y., K. Takizawa, and T.E. Tezduyar, *Computational Fluid-Structure Interaction: Methods and Applications*. 2013: Wiley.
50. Tezduyar, T.E., *Stabilized finite element formulations for incompressible flow computations.* Advances in applied mechanics, 1991. **28**: p. 1-44.
51. Tezduyar, T.E., *Computation of moving boundaries and interfaces and stabilization parameters*. International Journal for Numerical Methods in Fluids, 2003. **43**(5): p. 555-575.
52. Tezduyar, T.E., M. Behr, and J. Liou, *A new strategy for finite element computations involving moving boundaries and interfaces—The deforming-spatial-domain/space-time procedure: I. The concept and the preliminary numerical tests.* Computer Methods in Applied Mechanics and Engineering, 1992. **94**(3): p. 339-351.
53. Tezduyar, T.E., et al., *A new strategy for finite element computations involving moving boundaries and interfaces—the deforming-spatial-domain/space-time procedure: II.*

Computation of free-surface flows, two-liquid flows, and flows with drifting cylinders. Computer methods in applied mechanics and engineering, 1992. **94**(3): p. 353-371.
54. Tezduyar, T.E., *Finite element methods for fluid dynamics with moving boundaries and interfaces, chapter 17.* Encyclopedia of Computational Mechanics, 2004.
55. Tezduyar, T.E. and S. Sathe, *Modelling of fluid–structure interactions with the space–time finite elements: solution techniques.* International Journal for Numerical Methods in Fluids, 2007. **54**(6-8): p. 855-900.
56. Hughes, T.J., *Multiscale phenomena: Green's functions, the Dirichlet-to-Neumann formulation, subgrid scale models, bubbles and the origins of stabilized methods.* Computer methods in applied mechanics and engineering, 1995. **127**(1-4): p. 387-401.
57. Strichartz, R.S., *A guide to distribution theory and Fourier transforms*. 1994: CRC Press.
58. Lützen, J., *The prehistory of the theory of distributions*. 1982: Springer-Verlag.
59. Hughes, T.J. and G. Sangalli, *Variational multiscale analysis: the fine-scale Green's function, projection, optimization, localization, and stabilized methods.* SIAM Journal on Numerical Analysis, 2007. **45**(2): p. 539-557.

Chapter 4. Conclusion and Scientific Contribution

4.1 Conclusion

4.1.1 Summary

Part I of this thesis simplifies the concept of a newly developed mathematical modeling method and can be served as a guide to future efforts in applying the variational multiscale method for the analysis of the different physical system. The framework of this method has been thoroughly developed, and the important aspects of this method of modeling have been presented. The most important aspect of this method has been identified as solving the equation for microscale domain of the problem with the help of element-wise Green's functions. This feature of the VMM can facilitate numerical procedure as it is not concerned with the exact structure or the nature of the phenomena at the microscale, and therefore, reduces the cost of numerical analysis.

4.1.2 Variational Multiscale Modeling of LIB

VMM formulation of a LIB has been accomplished and presented in this work. Necessary steps in applying VMM to the governing equation of the system have been presented. The following conclusions can be drawn from the presented multiscale model:

1. The effects of the unresolved scale of the problem are reflected in the governing equation for the resolved scale without introducing a high number of degrees of freedom and therefore, preventing the numerical model from becoming computationally expensive.
2. Numerical solution of the resolved scale of the problem has the effects of the unresolved scale through the explicit incorporation of microscale solution into the macroscale equation.

4.2 Scientific Contributions

The main scientific contributions of part I of this thesis may be listed as follows:

1. This work provided insight into a class of numerical analysis methods which are suitable for examining systems that represent significant physical phenomena at different length scales.
2. A detailed methodology of the VMM and its features (e.g., Green's function, variational projection) has been presented in this work in a step-by-step approach which provides a comprehensive understanding of this method for implementation in numerical analysis of a LIB.

4.3 Future Work Recommendations

1. Considering the exact structure of system's microscale is essential in the multi-dimensional analysis of physical systems. Therefore, application of VMM for 2D and 3D analysis of physical systems should be considered carefully
2. Finding an analytical solution in the implementation of the VMM -which is in determining the Green's function- might turn into a complex problem. Future research should focus on more novel semi-analytical approaches.

PART II. Online Learning in Engineering Education: Theory and Practice

Chapter 1. Introduction

1.1 Motivation

Another important topic in the field of engineering majors are the efforts to improve students' learning and teaching quality. The number of students in colleges and universities in the U.S. is increasing in recent years. As reported by the National Center for Education Statistics (NCES) [1], there is about 5.2 million increase in the number of students enrolling in U.S. colleges and universities while there is also about 0.5 million increase in the number of students attending colleges who are at least 35 years old from 2000 to 2016; see Tables 1.1 and 1.2.

	Actual				Projected	
	2000	2010	2013	2014	2015	2016
Degree-granting postsecondary institutions	15,312	21,019	20,376	20,207	20,264	20,516
Undergraduate	13,155	18,082	17,475	17,293	17,298	17,490
Full-time	7,923	11,457	10,938	10,784	10,801	10,930
Part-time	5,232	6,625	6,536	6,509	6,497	6,561
Male	5,778	7,836	7,660	7,586	7,499	7,528
Female	7,377	10,246	9,815	9,707	9,799	9,962
2-year	5,948	7,684	6,969	6,714	7,114	7,194
4-year	7,207	10,399	10,506	10,578	10,184	10,296
Public	10,539	13,703	13,347	13,245	13,353	13,499
Private	2,616	4,379	4,128	4,048	3,945	3,992
Postbaccalaureate	2,157	2,937	2,901	2,915	2,966	3,025
Full-time	1,087	1,630	1,659	1,670	1,684	1,721
Part-time	1,070	1,307	1,242	1,244	1,282	1,304
Male	944	1,209	1,201	1,211	1,261	1,279
Female	1,213	1,728	1,700	1,703	1,704	1,746

Table 1.1. Enrollment in degree-granting postsecondary institutions (in thousands), from fall 2000 through fall 2016 [1]

					Projected	
	2000	2010	2013	2014	2015	2016
All students	15,312	21,019	20,376	20,207	20,264	20,516
14 to 17 years old	131	202	256	257	251	256
18 and 19 years old	3,258	4,057	3,720	3,694	3,881	3,929
20 and 21 years old	3,005	4,103	4,183	4,074	4,292	4,279
22 to 24 years old	2,600	3,759	3,964	3,990	3,962	3,974
25 to 29 years old	2,044	3,254	3,050	3,016	2,955	3,066
30 to 34 years old	1,333	1,805	1,606	1,552	1,471	1,506
35 years old and over	2,942	3,840	3,597	3,625	3,453	3,506

Table 1.2. Total fall enrollment in degree-granting postsecondary institutions (in thousands), from 2000 through 2016 [1]

An increasing number of students led to the introduction of new educational systems, often referred to as online or distance education. The expansion of online learning programs made online learning an integral part of today's educational system [2]. The number of educational institutions offering online programs and students enrolling in online programs is increasing in recent years. According to a report released by Babson Survey Research Group [3], student enrollment in online education increased 3.9 percent in fall 2014 compared to the previous fall. Based on the same report, there is not only an increase in student enrollment in public institutions, but also most of the distance learners are enrolling in public institutions; see Figures 1.1 and 1.2.

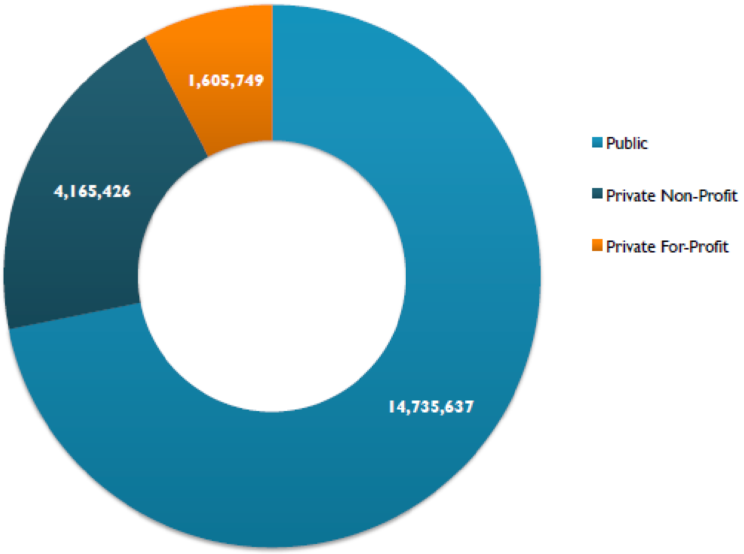


Figure 1.1. Overall higher education enrollment: fall 2014 [3]

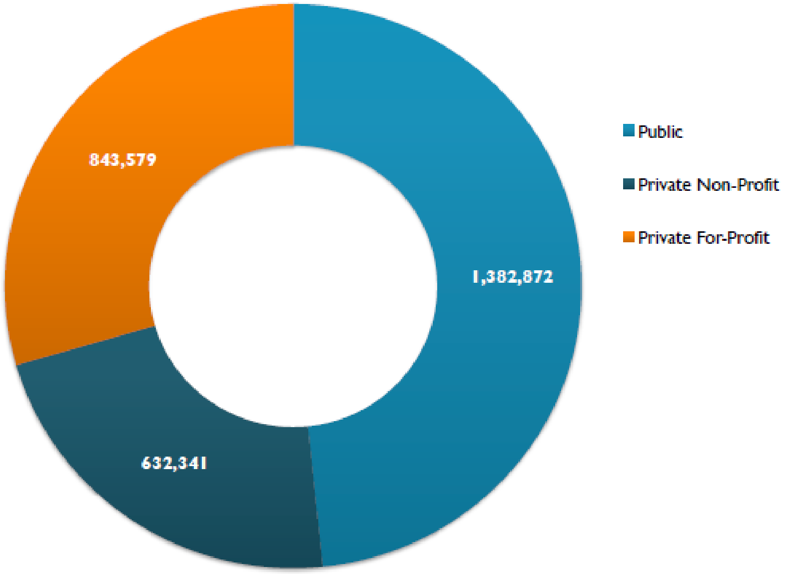


Figure 1.2. Enrollment of students taking distance education courses exclusively: fall 2014 [3]

Distance education has had a continued growth from 2012 to 2014 at a 7% rate [3]. Over that period, the non-profit sector of private institutions reported a 26% growth while the for-profit sector showed a -10% decrease and public institutions had a 9% growth in the number of students enrolled in distance/online programs.

Aside from expanding these programs, one should carefully examine different aspects of incorporating such systems of education to the already in place campus-based programs. This new system of education also introduced new issues in delivering the appropriate content to its targeted group of learners, as students enrolling in online/distance learning programs may feel isolated, and they also do not have the opportunity to collaborate with other students to make progress in their learning [4]. Additionally, there are some other concerns about using online learning in educational institutions, such as students' perception and acceptance of online learning [5], distraction of students by the free entertainment available on the internet [6], better performance of students attending live lectures compared with those who are using internet for education [7], students' resistance to new methods of teaching [8], interactive content production [9], low rates in course completion [10, 11], access issues [12], and issues related to data protection [13].

One of the main issues in implementing online learning into campus-based educational programs is the issue of student engagement and their satisfaction with the online program. With increasing number of students, especially in public universities, it seems inevitable to integrate online education in higher education. Therefore, understanding the limits and shortcomings of online learning helps institutions to improve the learning-teaching quality of their online programs.

1.2 Engineering Education

Having a concrete understanding of physics' and mathematics' fundamental concepts is necessary for engineering students to succeed in their respective academic/career paths. Applications of these concepts in almost every textbook of engineering students make them a key factor in students' academic success. Therefore, there needs to be more emphasis on teaching these fundamental topics to make sure college graduates have a good understanding of fundamental engineering. Furthermore, due to limited time and resources, the development and implementation of new forms of teaching in the traditional curriculum are inevitable. Flipped classrooms, student-centered curriculum, and other types of newly developed teaching methods are all techniques to ensure the delivery of good quality on both ends of an educational institution, which are teaching and learning.

1.3 Research Objectives

Part II of this thesis is focused on the study and implementation of educational methods which improve students' learning and facilitates accomplishing teaching goals in the school of engineering. Thanks to advancements in technology, attending a classroom lecture or accessing a lab session has become easier by the increasing the number of online courses/programs. However, the most important aspect of education, which is, improving the quality of learning, should not be neglected in the attempts for making the education easy to access. The majority of previous research on the topic of technology in the classroom is focused on different ways of technology integration in classroom lectures and the effect it has on students' learning. Therefore, more emphasis should be put on students' satisfaction and enhancing the effectiveness of teaching and learning in online courses. We introduced an effective way for including multimedia in the conventional academic curriculum. Furthermore, we conducted a study by implementing our proposed method in an engineering course to evaluate its effectiveness on the students' learning.

1.4 Thesis Part II Organization

The remaining portion of this part is divided into four chapters. Chapter 2 is a comprehensive literature review of engineering education and online learning practices. In Chapter 3, an introductory step in creating online instructional modules is presented. Enhancing the teaching-learning effectiveness by using the online instructional modules is demonstrated in Chapter 4. Chapter 5 includes a summary of part II, scientific contribution, and suggestions for future research.

1.5 References

1. Snyder, T.D., C. de Brey, and S.A. Dillow, *Digest of Education Statistics 2014, NCES 2016-006.* National Center for Education Statistics, 2016.
2. Harasim, L., *Shift happens: online education as a new paradigm in learning.* The Internet and Higher Education, 2000. **3**(1): p. 41-61.

3. Allen, I.E. and J. Seaman, *Online Report Card: Tracking Online Education in the United States.* Babson Survey Research Group, 2016.
4. Anderson, T., *The Theory and Practice of Online Learning*. 2008: University of Washington Press.
5. Wang, Y.D., *Building student trust in online learning environments.* Distance Education, 2014. **35**(3): p. 345-359.
6. Tsai, C.W., *The effect of online co-regulated learning in the implementation of team-based learning on improving students' involvement.* Higher Education Research & Development, 2015. **34**(6): p. 1270-1280.
7. Figlio, D., M. Rush, and L. Yin, *Is It Live or Is It Internet? Experimental Estimates of the Effects of Online Instruction on Student Learning.* Journal of Labor Economics, 2013. **31**(4): p. 763-784.
8. Murphy, D., R. Walker, and G. Webb, *Online Learning and Teaching with Technology: Case Studies, Experience and Practice*. 2013: Taylor & Francis.
9. Perez-Berenguer, D. and J. Garcia-Molina, *An approach for developing interactive online content.* Red-Revista De Educacion a Distancia, 2016(51): p. 24.
10. de Freitas, S.I., J. Morgan, and D. Gibson, *Will MOOCs transform learning and teaching in higher education? Engagement and course retention in online learning provision.* British Journal of Educational Technology, 2015. **46**(3): p. 455-471.
11. Hew, K.F. and W.S. Cheung, *Students' and instructors' use of massive open online courses (MOOCs): Motivations and challenges.* Educational Research Review, 2014. **12**: p. 45-58.
12. Reedy, A. and H.W. Gulwa, *Online learning and teacher education: The experiences of Indigenous teacher education students.* Learning Communities-International Journal of Learning in Social Contexts, 2016. **20**: p. 40-51.
13. Chou, H.L. and C.H. Chen, *Beyond identifying privacy issues in e-learning settings - Implications for instructional designers.* Computers & Education, 2016. **103**: p. 124-133.

Chapter 2. Literature Review

2.1 Online and Distance Learning

Online and distance learning are gaining attention and have become rather popular in recent years. Comparative studies between online and campus-based learning have been carried out to examine the effectiveness of this new form of education [1-5]. One of the important aspects of online learning is its ability to appropriately deliver content to students and even improve students' learning quality. Therefore, there have been a great number of research focused on developing online learning frameworks and investigating whether they can improve students' learning experience [6-10].

Various online learning models have been proposed in the literature. These models can be categorized into three different categories, as illustrated in Figure 2.1.

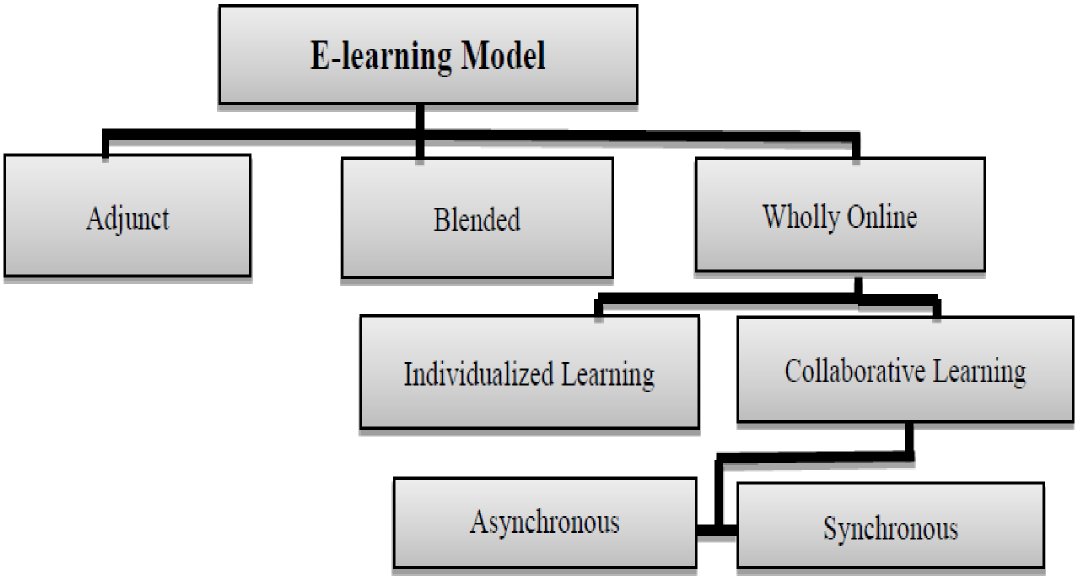


Figure 2.1. Model for incorporation of online learning in educational curriculum [11]

As reported by Volery and Lord [12], there are three success factors in developing an online course: technology, instructor, and student's previous experience with using technology. Additionally, identifying the challenges in developing an online course is an important step in the successful implementation of online learning in today's educational system. Student access to online resources [13], time management [14], lack of feedback from peers and instructors [15], students' perception of online learning programs [16], and challenges of faculty development and quality control [17] have been repeatedly mentioned in the literature as common challenges in the development of online learning programs.

2.2 Technology Integrated Classrooms

Technological advances made it possible for teachers to add new features and ideas to their academic courses and educational institutions to grow and expand their programs [18-22]. With the increasing number of students in engineering majors, the academic sector should be capable of addressing a larger number of educational needs. Integrating technology into education as an attempt to manage the emerging educational needs seems necessary [23-26].

Technology-incorporated classrooms and online courses are examples of technology application in modern day education. However, applying technology in conventional education should be accomplished carefully. There are risks in employing technology in education which need to be considered carefully, as noted by previous research [27-29]. Enhancing the quality of education in these new types of educational services should be the main concern in coordination and expansion of them. As reported in the literature, incorporating technology into traditional classrooms has proven to be effective in improving students' performance [30-34]. It has been pointed out that a strong teacher's presence in online programs to provide feedback to the online course participants encouraged them to perform at a good academic level [35]. Hence, to account for the absence of an instructor in an online environment, it is important to create interactive online courses capable of providing instant helpful feedback to students.

2.3 Online Learning: Background Theories

One of the main discussions in the educational community in recent years is recognizing the effective factor that improves learning, whether it is the delivery method or the instructional design of the content [36, 37]. Further developments in distance education in the modern-day indicated a strong dependency on technology in spite of paper-based learning being previously recognized as the common method in distance education [38, 39]. Despite the dependency of new forms of distance education (e.g., online programs) on technology and the necessity for further technological advances in technology-dependent instruction, the quality of the content that is delivered to students should not be ignored. As noted by Phipps and Merisotis [40], the pedagogy and course design are the more important factors in online programs than the technology used to develop such programs. Challenging activities that help students in gaining knowledge, bridging the new information to the old one, and activating their metacognitive abilities have been recognized as the key factors in designing an online learning program [41]. Additionally, there are reports such as Kozma [37] that show that providing students with the real-life experiences and simulations through the use of technology has an impact on students' learning. However, it is important to note that although the technology helps students' learning, it is not the main cause for learning. If the content is not designed properly, students cannot understand it even if the technology used to deliver the content is utilized to its fullest potential.

As suggested by Rossett [42], online learning has great potential, and it should be implemented in educational practice such that students can contextualize learning, engage with interactive content, and collaborate with one another or the instructor [43]. The development of an online learning program should be based on well-established learning theories to ensure proper design and implementation. There are three main approaches in educational theory identified as three main schools of thought [44], and neither of these approaches should be used as the only background theory for designing online learning materials [45]. A combination of these main schools of thought and newly evolved theories should be used in developing an online course/program [45]. The main three schools of thought in learning theories are:

1) Behaviorist learning theory: As the basis for the design of the first computer learning systems [45], this theory mainly focuses on observable qualities, such as changes in people's particular behaviors [46] and considers this change, which has occurred due to an external process from the environment, as learning [47].
2) Cognitive learning theory: The obvious limitation of the behaviorist theory is its inability to measure what cannot be observed, leading to the proposition of cognitive learning theory. The cognitive theory focuses on brain, memory, and motivation, and considers the learning as an internal process [45, 46]. Furthermore, it suggests that the level of learning depends on multiple internal factors such as level of processing by the learner [48, 49] and the learner's prior knowledge [50].
3) Constructivist learning theory: This theory, which was proposed in the midst of an educational reform in the United States and as a reaction to behaviorism and cognitivism, explains the construction process of meaning by learners; in other words, constructivism views knowledge as the result of the interaction of learners with each other, environment, and their community [46]. Constructivism states that learning is achieved by observation, processing, and personalizing the content into the learner's knowledge [51, 52] and that learners reach the best learning level when they can contextualize the taught content for immediate application [45].

As asserted by Ertmer and Newby [53], the three main schools of thought can be combined with each other to provide a strong theoretical foundation for developing online learning programs. Some of the key features and implications of each of the main learning theories for online learning are demonstrated in the following.

Behaviorists' learning framework for online learning suggests [45]:

- The objective of the online course should be explicitly defined. Defined objective helps learners specifically with self-evaluation.
- Testing to check the level of learners' achievement and provide feedback
- Materials should be appropriately in sequence; e.g., simple to complex, known to unknown, and knowledge to application.
- Feedback must be provided.

Cognitive learning comprises of two parts [45]: The first part is concerned with the structure of the memory and how the information is processed in short-term memory and is transferred to the long-term memory. This part of the theory recommends the inclusion of information maps in online learning materials that demonstrate the major concepts of the course and the relationship between those concepts. Regarding online learning, this part of the cognitive learning theory suggests the following [45]:

- Learners should be allowed to attend to the information to perceive and process them effectively in their working memory. Information is received by sensation before perception and processing can occur. Therefore, effective strategies should be put in place to facilitate the process of sensation for learners. Some examples of these strategies include:
  - Color should be used in presenting the information (e.g., highlighting the important information)
  - Attention should be given to where the information is appearing on the screen (e.g., important information at the center)
- Allowing learners to bridge between the new information and related information that are already perceived. Example of such strategy:
  - Using pre-instructional questions to provide a stimulus for learners to activate their existing knowledge structure (e.g., pre-test)
  - Providing different sets of prerequisite questions so that students with different background can choose their path to review the previous material
- Providing information to learners in appropriate segments to prevent overwhelming presentation of information [54]. Also, presenting the big picture to learners and ask them to generate their information map to facilitate efficient processing in the working memory
- Put in place strategies that allow learners to apply the information in real life

The second part of the cognitive learning theory is focused on [45]: individual differences and learning style. Individual differences can be categorized differently according to previous research [55, 56]. One of the main categories is distinguishing individuals based on their sensing and processing of learning experience (e.g., some learners learn materials that they can relate to in their personal lives and some process the information by following an active experimentation approach rather than conceptualizing the perceived information). Furthermore, cognitive style is identified as an individual difference. Some students can learn more effectively by self-study while others cannot benefit much from self-study approach. This part of the cognitive learning framework suggests [45]:

- Activities for different learning styles should be included in the online learning materials.
- Different forms of information presentation should be utilized (e.g., textual, verbal, visual) as presenting information in different modes helps in better understanding of information compared to single mode presentation [57].
- Students' motivation is an important factor to learning. Following recommendations should be put in practice to motivate students for learning:
  - Include an activity at the beginning of the course to capture students' attention (e.g., pre-tests).

  - Inform students of the benefits they receive by taking the course.
  - Inform the students of the course expectations and outcome
  - Providing a source of encouragement for the students to complete the course.
  - Provide feedback to the students.
- Update students about their performance in the course. Provide them with self-check questions and feedback (e.g., pre- and post-tests).

Constructivist learning theory: students are viewed as active learners. Knowledge is recognized as the learner's interpretation of what is perceived and collected through the learner's senses. Instead of giving knowledge to the learner, the instructor should be the facilitator [45], and the learner should be allowed to construct knowledge [58]. The main emphasis of constructivism is on situated or contextual learning, and it recommends the following points in designing an online learning program [45]:

- High-level processing is guaranteed when the learning process is an active process and students doing meaningful activities.
- Online instructions should be made interactive. Since students receive the information without any filtration, the interactivity of the instruction helps students in personalizing and contextualizing the information as students have control over their learning process [59].
- Group work should be encouraged since it helps the development of constructivist learning [60-62] and students can also learn from each other.
- It should be the student who controls the learning process (with the instructor's interference when necessary).
- Time should be allocated to students to reflect on the taught content. Embedded questions throughout the course can encourage students to process the presented information.
- Providing relative examples helps students in understanding the presented instructional content.

The general belief about online learning programs is the ease of access they provide for learners to enroll in a learning program, but Anderson [63] argues that the temporal freedom which enrollment in online programs provides to the learners is the more important source of motivation for enrollment in online programs. Providing the freedom for students to choose their learning path and pace in learning the instructional content is consistent with the constructivist learning theory that emphasizes on individualization and construction of knowledge [64].

Common forms of interaction in online learning programs have been identified by the work of Anderson [63] and are demonstrated in the following:

- Student-student: Traditionally was not considered as important but deemed valuable by some constructivist theories in investigating and developing multiple perspectives in distance education learners, such as an increase in completion rates [65] and providing a community that allows learners to develop interpersonal skills [66].

- Student-teacher: Asynchronous and synchronous communication using text, audio, and video.
- Student-content: Web-based instruction, such as online learning programs, support passive forms of student-content interactions such as online computer-assisted tutorials and exercises in virtual labs.
- Teacher-content: The focus of this interaction is on content and learning activities creation, which is performed by teachers. Teachers are allowed to monitor and update the content resources and activities steadily to facilitate the process of learning for students.
- Content-content: Content is programmed such that it can update and modify itself through interaction with other contents and resources.

If one of the three main interactions: 1) student-teacher, 2) student-student, and 3) student-content, is highly included in the developed online learning program, high-quality learning can be achieved [63]. Therefore, ensuring a strong presence of one types of the aforementioned main interactions is critical in designing an online course, especially in teaching mathematics which is an important instructional topic in the school of the engineering curriculum.

Teaching mathematics in higher education is of fundamental importance in ensuring engineering students' success in achieving their educational and career goals. Traditional methods in teaching mathematics, usually recognized as non-interactive methods of teaching mathematics [67-69], have long been put in practice without any changes, as some even suggest that these methods did not evolve since times of ancient Egypt [70]. Recently, and by advances in technology, teachers and students show interest in modifying the teaching-learning process [71]. There have been efforts in developing new pedagogical models in reforming the traditional approaches in teaching mathematics to address the needs of all of the students [72-74]. Some of the previous research proposed the use of natural user interfaces (NUI) as supporting teaching tools to provide students a way of interaction with the learning system that is close to their experience in interaction with the real-world [75]. Some of the current trends in teaching mathematics in higher education are:

- Student-centered methods: Although some articles reference the constructivist theory as the implicit base of their work [72, 76], this method is mainly based on the constructivist learning theory [73, 77] and relies heavily on self-construction of knowledge [78]. There are some concerns in the implementation of these methods, as a decline in attitude towards the course topic in a mathematics course was indicated [79] and therefore, further investigation in the application of this method is needed.
- Contextualization of mathematical concepts: The inability for students to apply mathematics to their real-world applications has been identified as one of the reasons for students' failure in mathematics [72]. Therefore, it has been recommended to make mathematical concepts relevant to students' real-world experiences to facilitate their learning process [80, 81]. Contextualization and employing real-world personal

experiences in teaching mathematics has also been considered as an essential factor in student-centered approaches [73].

- Connecting previous mathematical knowledge to newly perceived knowledge: There are a great number of engineering students with significant shortcomings in their previous mathematical knowledge who enter universities, which can cause significant problems in students' learning process of new mathematical topics [78]. There have been efforts to address this issue and models such as predictor-connector-refinement model [82], but further investigations in this area are needed as not all the learning methods proved to be successful (e.g., because of deficiencies in students' knowledge) [78, 82].

In our approach, we employed a cognitive apprenticeship model in teaching mathematics to engineering students enrolled in an introductory engineering mechanics course. The cognitive apprenticeship model which was proposed by Collins [83], asserts that learning mostly occurs through observation, coaching, and more generally speaking, by following methods that resemble apprenticeship methods [84]. The details of this method and its implementation to our study is presented in Chapter 4 of this part of the thesis.

2.4 Online Interactive Instructional Modules

New methods of teaching have emerged and been put into practice recently in the field of educational research. These methods include, but are not limited to: flipped classrooms, design thinking, self-learning, gamification, social media integration into the classroom, and online learning modules. Multiple efforts have been put into the study and implementation of such methods. For example, multiple research and comparative studies were focused on flipped classrooms and the impact they have on student learning [85-87] and engagement [88, 89] in higher education, some researchers focused on design thinking as an innovative method of teaching [90-94], self-regulated learning has also been thoroughly investigated [95-98] and even incorporated into the flipped classroom concept [99]. In addition, gamification has been studied by different groups of researchers [100-102] and some were focused on the drawbacks and possible ways to successfully implement this method [103, 104], while social media in education has been the subject of investigation for multiple papers [105-107] and its potentials and obstacles have been studied [108, 109]. Furthermore, online learning modules have gained attention from researchers across different disciplines [110-115]. Student engagement has been mentioned as one of the most important aspects of teaching methods in almost all of the newly proposed instructional approaches. As recognized by Herrington, Oliver, & Reeves [116], student engagement is paramount to learning success. Hence, making online learning modules as interactive as possible should be the goal of developing an online course. Additionally, more interactive modules can also neutralize the negative effect of online programs on students, which is the lack of feedback from the instructor or peers.

Instructional video modules have been implemented in online programs as one of the methods of content delivery [38, 63, 117, 118]. Challenges and weaknesses of employing online videos as an instructional resource have been the subject of research for some published research reports. Disadvantages and challenges include but are not limited to: a drop in students' level of engagement because of lengthy videos [119] (also see Figure 2.2 [120]), accessibility [121], content delivery [122], student engagement [123], and streaming quality [124]. However, the benefits of using videos in education outscore the negative impacts that videos might have on the quality of education.

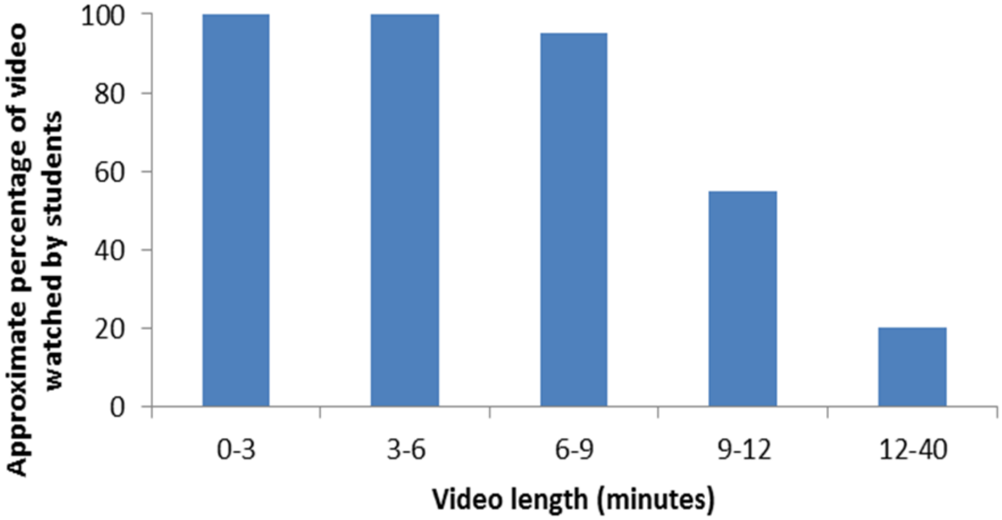


Figure 2.2. Student engagement with streaming videos [120]

Although in some cases it is reported that students' success is not attributed to the media usage in online learning [125], multiple studies have reported the contribution of online video modules in student's success and performance improvement. The significant positive impact of instructional videos on students' achievement [126], significant learning improvement as a result of using online videos [127, 128], enhancing students' communication and critical thinking skills by using videos [129, 130], improvement in understanding content of the instructional topic [131], and promoting active viewing approaches [132] are some of the main advantages of using video as an instructional resource in today's education.

2.5 Conclusion

Hence, a study on identifying important aspects of producing interactive instructional videos will be presented in this part of the thesis. Important characteristics that need to be incorporated into an instructional video to make it interactive and engaging are identified. In the end, an educational study on the application of the developed instructional videos in an engineering course is demonstrated. Results indicated that after using the videos in the form of an interactive instructional module, the students improved significantly in their post-test scores compared to their pre-test scores.

2.6 References

1. Curry, M.G., *Does Course Format Impact Student Learning Outcomes? A Causal-Comparative Study of Online, Hybrid, and Face-to-Face Student Learning Outcomes in an Undergraduate Teacher Preparation Course*. 2016: Wilmington University (Delaware).
2. Muirhead, D.K., et al., *A Comparative Study of Blended and Online Learning using the Virtual Microscope for Earth Sciences.* 2017.
3. Prabhu, S., et al., *A Comparative study of textbook learning and online learning among undergraduate medical students.* Research Journal of Pharmaceutical, Biological and Chemical Sciences, 2016. **7**(4): p. 2014-2017.
4. Gulten, G., E. Kulusakli, and S. Aydin, *A Comparative Study on the Motivation and Attitudes of Language Learners of Online Distance and Traditional in-Classroom Education.* Turkish Online Journal of Distance Education, 2016.
5. Bowers, J. and P. Kumar, *Students' perceptions of teaching and social presence: A comparative analysis of face-to-face and online learning environments*, in *Blended Learning: Concepts, Methodologies, Tools, and Applications*. 2017, IGI Global. p. 1532-1550.
6. Arnott, J.A. and S.L. Planey, *Flipped classroom approaches lead to no improvement in learning outcomes or student perceptions.* The FASEB Journal, 2017. **31**(1 Supplement): p. 751.14-751.14.
7. Secret, M., K.J. Bentley, and J.C. Kadolph, *Student Voices Speak Quality Assurance: Continual Improvement in Online Social Work Education.* Journal of Social Work Education, 2016. **52**(1): p. 30-42.
8. McKnight, K., et al., *Teaching in a digital age: How educators use technology to improve student learning.* Journal of research on technology in education, 2016. **48**(3): p. 194-211.
9. Jaggars, S.S., *Choosing between online and face-to-face courses: Community college student voices.* American Journal of Distance Education, 2014. **28**(1): p. 27-38.
10. Othman, M.S. and M.A. Musa, *The improvement of students' academic performance by using social media through collaborative learning in Malaysian higher education.* Asian Social Science, 2014. **10**(8): p. 210.
11. Arkorful, V. and N. Abaidoo, *The role of e-learning, advantages and disadvantages of its adoption in higher education.* International Journal of Instructional Technology and Distance Learning, 2015. **12**(1): p. 29-42.
12. Volery, T. and D. Lord, *Critical success factors in online education.* International journal of educational management, 2000. **14**(5): p. 216-223.
13. van Rooij, S.W. and K. Zirkle, *Balancing pedagogy, student readiness and accessibility: A case study in collaborative online course development.* The Internet and Higher Education, 2016. **28**: p. 1-7.
14. Adekola, J., et al., *Student transitions to blended learning–challenges and solutions (workshop).* 2017.
15. Muuro, M.E., et al., *Students' perceived challenges in an online collaborative learning environment: A case of higher learning institutions in Nairobi, Kenya.* The International Review of Research in Open and Distributed Learning, 2014. **15**(6).
16. Almarabeh, T., et al., *The University of Jordan E-Learning Platform: State, Students' Acceptance and Challenges.* Journal of Software Engineering and Applications, 2014. **7**(12): p. 999.

17. Miller, G., et al., *Leading the e-Learning Transformation of Higher Education: Meeting the Challenges of Technology and Distance Education*. 2013: Stylus Pub., LLC.
18. Berge, Z.L. and M.P. Collins, *Computer mediated communication and the online classroom: distance learning*. 1995: Hampton press Cresskill.
19. Gallagher, S. and G. Garrett, *Disruptive education: Technology-enabled universities.* The United States Studies Centre at the University of Sydney, 2013.
20. Potter, S.L. and A.J. Rockinson-Szapkiw, *Technology integration for instructional improvement: The impact of professional development.* Performance Improvement, 2012. **51**(2): p. 22-27.
21. Rehmat, A.P. and J.M. Bailey, *Technology integration in a science classroom: Preservice teachers' perceptions.* Journal of Science Education and Technology, 2014. **23**(6): p. 744-755.
22. Lopez, O.C. and R.M.S. Pastor, *Internet, technology and applications for university music education of the 21st Century.* Redu-Revista De Docencia Universitaria, 2016. **14**(1): p. 405-421.
23. Saunders, G. and F. Klemming, *Integrating technology into a traditional learning environment: Reasons for and risks of success.* Active learning in higher education, 2003. **4**(1): p. 74-86.
24. Lee, C.Y. and M.J. Chen, *Developing a questionnaire on technology-integrated mathematics instruction: A case study of the AMA training course in Xinjiang and Taiwan.* British Journal of Educational Technology, 2016. **47**(6): p. 1287-1303.
25. Reigeluth, C.M., et al., *Personalized integrated educational system: Technology functions for the learner-centered paradigm of education.* Journal of Educational Computing Research, 2015. **53**(3): p. 459-496.
26. Aslan, S. and C.M. Reigeluth, *Investigating "The Coolest School in America": how technology is used in a learner-centered school.* Etr&D-Educational Technology Research and Development, 2016. **64**(6): p. 1107-1133.
27. Spitzer, M., *Information technology in education: Risks and side effects.* Trends in Neuroscience and Education, 2014. **3**(3): p. 81-85.
28. Raspopovic, M., et al., *The Effects of Integrating Social Learning Environment with Online Learning.* International Review of Research in Open and Distributed Learning, 2017. **18**(1): p. 141-159.
29. Jacobsen, D.M., *Building Different Bridges: Technology Integration, Engaged Student Learning, and New Approaches to Professional Development.* 2001.
30. Alnahdi, G., *Assistive technology in special education and the universal design for learning.* TOJET: The Turkish Online Journal of Educational Technology, 2014. **13**(2).
31. Frank, J.A. and V. Kapila, *Mixed-reality learning environments: Integrating mobile interfaces with laboratory test-beds.* Computers & Education, 2017. **110**: p. 88-104.
32. Kuo, F.-R., et al., *Web-based learning system for developing and assessing clinical diagnostic skills for dermatology residency program.* Educational Technology & Society, 2016. **19**(3): p. 194-207.
33. Sadik, A., *Digital storytelling: a meaningful technology-integrated approach for engaged student learning.* Educational Technology Research and Development, 2008. **56**(4): p. 487-506.
34. Forehand, J.W., B. Miller, and H. Carter, *Integrating Mobile Devices Into the Nursing Classroom.* Teaching and Learning in Nursing, 2017. **12**(1): p. 50-52.

35. Jaggars, S.S. and D. Xu, *How do online course design features influence student performance?* Computers & Education, 2016. **95**: p. 270-284.
36. Clark, R.E., *A summary of disagreements with the "mere vehicles" argument.* Learning from media: Arguments, analysis, and evidence, 2001: p. 125-136.
37. Kozma, R., *Robert Kozma's Counterpoint theory of "learning with media".* Learning from media: Arguments, analysis and evidence, 2001: p. 137-178.
38. Johnson, S.D. and S.R. Aragon, *An instructional strategy framework for online learning environments.* New directions for adult and continuing education, 2003. **2003**(100): p. 31-43.
39. Börje, H., *The role of technology in distance education.* Instructional Science, 1985. **14**(1): p. 87-93.
40. Phipps, R. and J. Merisotis, *What's the difference? A review of contemporary research on the effectiveness of distance learning in higher education.* 1999.
41. Bonk, C.J. and T.H. Reynolds, *Learner-centered Web instruction for higher-order thinking, teamwork, and apprenticeship.* Web-based instruction, 1997. **8**(11): p. 167-78.
42. Rossett, A., *Waking in the night and thinking about e-learning.* The ASTD e-learning handbook, 2002: p. 3-18.
43. Ring, G. and G. Mathieux. *The key components of quality learning*. in *ASTD Techknowledge 2002 Conference, Las Vegas*. 2002.
44. Cruickshank, D.R., D.B. Jenkins, and K.K. Metcalf, *The act of teaching*. 2005: McGraw-Hill Companies.
45. Ally, M., *Foundations of educational theory for online learning.* Theory and practice of online learning, 2004. **2**: p. 15-44.
46. Harasim, L., *Learning theory and online technologies*. 2017: Taylor & Francis.
47. Skinner, B.F., *About behaviorism*. 2011: Vintage.
48. Craik, F.I. and R.S. Lockhart, *Levels of processing: A framework for memory research.* Journal of verbal learning and verbal behavior, 1972. **11**(6): p. 671-684.
49. Craik, F.I. and E. Tulving, *Depth of processing and the retention of words in episodic memory.* Journal of experimental Psychology: general, 1975. **104**(3): p. 268.
50. Ausubel, D.P., J.D. Novak, and H. Hanesian, *Educational psychology: A cognitive view.* 1968.
51. Cooper, P.A., *Paradigm shifts in designed instruction: From behaviorism to cognitivism to constructivism.* Educational technology, 1993. **33**(5): p. 12-19.
52. Wilson, B.G., *Reflections on constructivism and instructional design.* Instructional development paradigms, 1997: p. 63-80.
53. Ertmer, P.A. and T.J. Newby, *Behaviorism, cognitivism, constructivism: Comparing critical features from an instructional design perspective.* Performance improvement quarterly, 1993. **6**(4): p. 50-72.
54. Miller, G.A., *The magical number seven, plus or minus two: some limits on our capacity for processing information.* Psychological review, 1956. **63**(2): p. 81.
55. Kolb, D.A., *Experiential learning: Experience as the source of learning and development*. 2014: FT press.
56. Briggs, K.C., *Myers-Briggs type indicator*. 1976: Consulting Psychologists Press Palo Alto, CA.
57. Paivio, A., *Mental representations: A dual coding approach*. 1990: Oxford University Press.

58. Cunningham, D. and T. Duffy, *Constructivism: Implications for the design and delivery of instruction.* Handbook of research for educational communications and technology, 1996. **51**: p. 170-198.
59. Murphy, K.L. and L. Cifuentes, *Using Web tools, collaborating, and learning online.* Distance Education, 2001. **22**(2): p. 285-305.
60. Hooper, S. and M.J. Hannafin, *The effects of group composition on achievement, interaction, and learning efficiency during computer-based cooperative instruction.* Educational Technology Research and Development, 1991. **39**(3): p. 27-40.
61. Johnson, D.W. and R.T. Johnson, *Cooperation and the use of technology.* Handbook of research for educational communications and technology: A project of the Association for Educational Communications and Technology, 1996: p. 1017-1044.
62. Palloff, R.M. and K. Pratt, *Building learning communities in cyberspace*. Vol. 12. 1999: San Francisco: Jossey-Bass.
63. Anderson, T., *Towards a theory of online learning.* Theory and practice of online learning, 2004. **2**: p. 109-119.
64. Jonassen, D.H., *Evaluating constructivistic learning.* Constructivism and the technology of instruction: A conversation, 1992: p. 137-148.
65. Slavin, R.E., *Cooperative learning: Theory, research, and practice*. 1990: Prentice-Hall.
66. Wenger, E., R.A. McDermott, and W. Snyder, *Cultivating communities of practice: A guide to managing knowledge*. 2002: Harvard Business Press.
67. Alsina, C., *Why the professor must be a stimulating teacher.* 2001). The Teaching and Learning of Mathematics at University Level. An ICMI Study, 2001: p. 3-11.
68. Anku, S.E., *Fostering students' disposition towards mathematics: A case from a Canadian university.* Education, 1996. **116**(4): p. 536-543.
69. Hillel, J., *Trends in curriculum.* The teaching and learning of mathematics at university level: An ICMI study, 2001: p. 59-69.
70. Abaté, C.J. and K.A. Cantone, *An evolutionary approach to mathematics education: Enhancing learning through contextual modification.* Problems, Resources, and Issues in Mathematics Undergraduate Studies, 2005. **15**(2): p. 157-176.
71. Echeverría, M.A.M., et al., *Natural User Interfaces to Teach Math on Higher Education.* Procedia - Social and Behavioral Sciences, 2013. **106**(Supplement C): p. 1883-1889.
72. Chang, J.-M., *A practical approach to inquiry-based learning in linear algebra.* International Journal of Mathematical Education in Science and Technology, 2011. **42**(2): p. 245-259.
73. Mokhtar, M., et al., *Enhancing calculus learning engineering students through problem-based learning.* WSEAS transactions on Advances in Engineering Education, 2010. **7**(8): p. 255-264.
74. Orton, T. and T. Roper, *Science and mathematics: A relationship in need of counselling?* 2000.
75. Wigdor, D. and D. Wixon, *Brave NUI world: designing natural user interfaces for touch and gesture*. 2011: Elsevier.
76. Maull, W. and J. Berry, *A questionnaire to elicit the mathematical concept images of engineering students.* International Journal of Mathematical Education in Science and Technology, 2000. **31**(6): p. 899-917.
77. Roddick, C.D., *Differences in learning outcomes: calculus & mathematica vs. traditional calculus.* Problems, Resources, and Issues in Mathematics Undergraduate Studies, 2001. **11**(2): p. 161-184.

78. Abdulwahed, M., B. Jaworski, and A. Crawford, *Innovative approaches to teaching mathematics in higher education: a review and critique.* 2012.

79. Ward, B.B., et al., *Assessing a mathematical inquiry course: Do students gain an appreciation for mathematics?* Primus, 2010. **20**(3): p. 183-203.

80. Matthews, K.E., P. Adams, and M. Goos, *Putting it into perspective: mathematics in the undergraduate science curriculum.* International Journal of Mathematical Education in Science and Technology, 2009. **40**(7): p. 891-902.

81. Pennell, S., P. Avitabile, and J. White, *An engineering-oriented approach to the introductory differential equations course.* Primus, 2009. **19**(1): p. 88-99.

82. Turner, P.R., *A predictor-corrector process with refinement for first-year calculus transition support.* Primus, 2008. **18**(4): p. 370-393.

83. Collins, A., *Cognitive Apprenticeship: Teaching the Craft of Reading, Writing, and Mathematics. Technical Report No. 403.* 1987.

84. Collins, A., J.S. Brown, and S.E. Newman, *Cognitive apprenticeship: Teaching the craft of reading, writing and mathematics.* Thinking: The Journal of Philosophy for Children, 1988. **8**(1): p. 2-10.

85. Ram, M.P. and A. Sinha. *An Implementation Framework for FLIPPED CLASSROOMS in Higher Education*. in *Proceedings of the Special Collection on eGovernment Innovations in India*. 2017. ACM.

86. Thai, N.T.T., B. De Wever, and M. Valcke, *The impact of a flipped classroom design on learning performance in higher education: Looking for the best "blend" of lectures and guiding questions with feedback.* Computers & Education, 2017. **107**: p. 113-126.

87. McNally, B., et al., *Flipped classroom experiences: student preferences and flip strategy in a higher education context.* Higher Education, 2017. **73**(2): p. 281-298.

88. Davila, Y., et al. *Enhancing engagement in flipped learning across undergraduate science using the flipped teacher and flipped learner framework*. in *Proceedings of The Australian Conference on Science and Mathematics Education (formerly UniServe Science Conference)*. 2017.

89. Cummins, J.C., *College Student Engagement Patterns in Small Group Learning Activities Conducted in Courses Organized using a Flipped Learning Instructional Pedagogy*. 2016.

90. Leonard, S.N., R.N. Fitzgerald, and G. Riordan, *Using developmental evaluation as a design thinking tool for curriculum innovation in professional higher education.* Higher Education Research & Development, 2016. **35**(2): p. 309-321.

91. Yeager, D.S., et al., *Using design thinking to improve psychological interventions: The case of the growth mindset during the transition to high school.* Journal of educational psychology, 2016. **108**(3): p. 374.

92. Wrigley, C. and K. Straker, *Design thinking pedagogy: the educational design ladder.* Innovations in Education and Teaching International, 2017. **54**(4): p. 374-385.

93. van de Grift, T.C. and R. Kroeze, *Design Thinking as a Tool for Interdisciplinary Education in Health Care.* Academic Medicine, 2016. **91**(9): p. 1234-1238.

94. Gottlieb, M., et al., *Applying Design Thinking Principles to Curricular Development in Medical Education.* AEM Education and Training, 2017. **1**(1): p. 21-26.

95. Roth, A., S. Ogrin, and B. Schmitz, *Assessing self-regulated learning in higher education: a systematic literature review of self-report instruments.* Educational Assessment, Evaluation and Accountability, 2016. **28**(3): p. 225-250.

96. King, A., et al., *A Novel Approach to Self-Directed Learning and the Flipped Classroom Method for Residency Didactic Curriculum.* Western Journal of Emergency Medicine, 2016. **17**(4.1).
97. Winne, P., *Self-regulated learning.* SFU Educational Review, 2016. **1**(1).
98. Lucieer, S.M., et al., *Self-regulated learning and academic performance in medical education.* Medical teacher, 2016. **38**(6): p. 585-593.
99. Lai, C.-L. and G.-J. Hwang, *A self-regulated flipped classroom approach to improving students' learning performance in a mathematics course.* Computers & Education, 2016. **100**: p. 126-140.
100. Taspinar, B., W. Schmidt, and H. Schuhbauer, *Gamification in Education.* Procedia Computer Science, 2016. **99**(C): p. 101-116.
101. Martí-Parreño, J., E. Méndez-Ibáñez, and A. Alonso-Arroyo, *The use of gamification in education: a bibliometric and text mining analysis.* Journal of Computer Assisted Learning, 2016. **32**(6): p. 663-676.
102. Jackson, M., *Gamification in Education: A Literature Review*. 2016.
103. Chee, C.-M. and D.H.-T. Wong, *Affluent Gaming Experience Could Fail Gamification in Education: A Review.* IETE Technical Review, 2017: p. 1-5.
104. van Roy, R. and B. Zaman, *Why Gamification Fails in Education-And How to Make it Successful. Introducing 9 Gamification Heuristics based on Self-Determination Theory.* 2017.
105. Greenhow, C. and C. Lewin, *Social media and education: reconceptualizing the boundaries of formal and informal learning.* Learning, Media and Technology, 2016. **41**(1): p. 6-30.
106. Selwyn, N. and E. Stirling, *Social media and education… now the dust has settled.* Learning, Media and Technology, 2016. **41**(1): p. 1-5.
107. Greenhow, C., J. Sonnevend, and C. Agur, *Education and social media: Toward a digital future*. 2016: MIT Press.
108. Manca, S. and M. Ranieri, *Facebook and the others. Potentials and obstacles of social media for teaching in higher education.* Computers & Education, 2016. **95**: p. 216-230.
109. Sobaih, A.E.E., et al., *To use or not to use? Social media in higher education in developing countries.* Computers in Human Behavior, 2016. **58**: p. 296-305.
110. Russell, R.L., P. Luna, and D.E. Chico, *Using Interactive Online Learning Modules in Histology to Improve Long-term Retention and Efficiency of Learning.* The FASEB Journal, 2017. **31**(1 Supplement): p. 584.7-584.7.
111. Baatar, D., E. Ricks, and T. Gest, *Online Learning Modules Based on Spacing and Testing Effects Improve Medical Student Performance on Anatomy Examinations.* The FASEB Journal, 2017. **31**(1 Supplement): p. lb13-lb13.
112. Ens, A., K. Janzen, and M.R. Palmert, *Development of an Online Learning Module to Improve Pediatric Residents' Confidence and Knowledge of the Pubertal Examination.* Journal of Adolescent Health, 2017. **60**(3): p. 292-298.
113. Al Mamun, M.A., G. Lawrie, and T. Wright. *Factors affecting student engagement in self-directed online learning module*. in *Proceedings of The Australian Conference on Science and Mathematics Education (formerly UniServe Science Conference)*. 2017.
114. Williams, T.E., *Effectiveness of online learning modules for exercise professional certification guidelines*. 2016, The University of North Carolina at Chapel Hill.
115. Mwaniki, E.W., et al., *Development of Interactive Online Learning Modules: Lessons from Kenyatta University, Kenya.* 2016.

116. Herrington, J., R. Oliver, and T.C. Reeves, *Patterns of engagement in authentic online learning environments.* Australasian Journal of Educational Technology, 2003. **19**(1).
117. Hartsell, T. and S.C.-Y. Yuen, *Video streaming in online learning.* AACE Journal, 2006. **14**(1): p. 31-43.
118. Twigg, C.A., *Models for online learning.* Educause review, 2003. **38**: p. 28-38.
119. Guo, P.J., J. Kim, and R. Rubin. *How video production affects student engagement: An empirical study of mooc videos*. in *Proceedings of the first ACM conference on Learning@ scale conference*. 2014. ACM.
120. Brame, C., *Effective educational videos.* Vanderbilt University Center for Teaching, 2015.
121. Harper, K.A. and J. DeWaters, *A Quest for website accessibility in higher education institutions.* The Internet and Higher Education, 2008. **11**(3): p. 160-164.
122. Smith, D.W., *Listening to the learner: Graduate teacher education students' preferences for asynchronous content delivery*. Journal of Online Learning and Teaching, 2013. **9**(4): p. 489.
123. Dixson, M.D., *Creating effective student engagement in online courses: What do students find engaging?* Journal of the Scholarship of Teaching and Learning, 2012. **10**(2): p. 1-13.
124. Reisslein, J., P. Seeling, and M. Reisslein, *Video in distance education: ITFS vs. web-streaming: Evaluation of student attitudes.* The Internet and Higher Education, 2005. **8**(1): p. 25-44.
125. Means, B., et al., *Evaluation of evidence-based practices in online learning: A meta-analysis and review of online learning studies.* US Department of Education, 2009.
126. Zhang, D., et al., *Instructional video in e-learning: Assessing the impact of interactive video on learning effectiveness.* Information & Management, 2006. **43**(1): p. 15-27.
127. Lancellotti, M., S. Thomas, and C. Kohli, *Online video modules for improvement in student learning.* Journal of Education for Business, 2016. **91**(1): p. 19-22.
128. Willmot, P., M. Bramhall, and K. Radley, *Using digital video reporting to inspire and engage students.* The Higher Education Academy, 2012: p. 1-7.
129. Artello, K., *What they learned: Using multimedia to engage undergraduates in research.* Innovative Higher Education, 2014. **39**(2): p. 169-179.
130. Oliver, W.M., *Crime, history, and Hollywood: Learning criminal justice history through major motion pictures.* Journal of Criminal Justice Education, 2011. **22**(3): p. 420-439.
131. Brecht, H.D., *Learning from online video lectures.* Journal of Information Technology Education, 2012. **11**(1): p. 227-250.
132. Galbraith, J.D., *Active viewing: and oxymoron in video-based instruction?* Society for, 2004.

Chapter 3. Identifying Important Aspects in Developing Interactive Instructional Videos

3.1 Introduction

The new age education has undergone some significant changes as more students (e.g., distance learners) are emerging who have different educational needs in term of the teaching schedule and format. Additionally, more institutions are expanding access to instructional programs through utilizing online learning [1]. Moreover, the need for having a more efficient curriculum necessitates new effective teaching methods. Hence, many different forms of teaching are emerging recently due to their remarkable advantageous, such as more uniform learning across the class, more productive social interactions in multicultural classes, higher scores on exams and, facilitating learning process [2-9]. Among them, active learning and flipped classroom are receiving more attention.

Bonwell and Eison [10] proposed the idea of active learning and defined it as anything that "involves students in doing things and thinking about the things they are doing." Active learning has been implemented widely. For example, Prince [11] found that active learning has attracted strong supporters among faculty who are seeking for new methods in teaching. Braxton, Milem, & Sullivan [12] stated that students who frequently experience active learning in their classes might also have more time available for participation in collegiate social communities because they feel that they can spend less time on course preparation and study for examinations. Active learning necessitates a student-centered pedagogy that has been the center of interest for many researchers. For example, Jones [13] developed a framework on how to implement the idea of the student-centered classroom in the educational process. Jones stated that the main goal in student-centered classrooms is to engage as many students as possible. He discussed that enthusiasm is not generated solely by a topic but also by students themselves. Helping students discovering more about the topic will lead to making the topic more appealing. Various aspects of student-centered pedagogy have been detailed reviewed in previous studies. For example, Zepke [14] discussed the concept of student engagement and proposed a new paradigm for research on student engagement, Hannafin, and Land [15] focused on applying technology in a student-centered pedagogy to enhance the quality of learning environment. Docherty, Hoy, Topp, & Trinder [16] asserted the effective learning techniques in helping students acquire required skills in the course. It should be noted that one of the most applicable methods for applying student-centered ideas into the classroom is the inclusion of interactive instructional videos. Roshier, Foster, & Jones [17] demonstrated students perception of videos as a teaching resource. Arya, Christ, & Chiu [18] studied the extent to which teacher-educators used videos in their teacher education courses.

The flipped classroom is another innovative idea that is widely accepted in the new age education. Lage, Platt, & Treglia [19] investigated the issue of mismatch between an instructor's teaching style and student's learning style. They outlined a strategy for teaching that is appealing to a broad range of learning styles without violating the typical constraints faced by instructors. They called it inverting the classroom (also known as flipped-classroom) that can effectively engage a wide spectrum of learners. Instructional videos and web-based tutorials have been recognized as one of the most effective teaching formats by Lai and Hwang [20]. Moos and Bonde [21] studied how to teach and implement the idea of flipped classroom effectively. Moreover, Sohrabi, & Iraj [22] identified the issue of students' engagement in learning at flipped classrooms.

It can be concluded that interactive instructional videos are an essential tool in student-centered curriculum and play an important role in delivering content to students in flipped classrooms. In this study, we focus on exploring the method of developing interactive instructional videos that are suitable for the flipped classroom. Many previous studies [23-27] focused on both student engagement as a key factor in designing interactive student-centered curricula and perception of engagement. Hence, we aim to study the applied method of developing interactive videos based on our first-hand experience. We developed these videos in accordance with previous research on student-centered pedagogies. Then, we identified and discussed the limitations of the videos. Lastly, critical challenges in developing online instructional videos were identified for future study.

3.2 Methodology

As Hughes [28] asserted, teacher's interpretation of the value of technology value for supporting instruction is the main factor in developing innovative technology-supported pedagogy. Therefore, we extracted the maximum potential of available technology tools to create interactive instructional videos.

Firstly, a list of teaching topics was prepared. After coming up with a shortlist, a five-level Likert scale was provided for soliciting feedback from different instructors at different departments of the School of Engineering to prioritize the listed items. Then, specific goals to achieve in developing the videos has been set as follow: First goal set to be covering basic concepts of Mathematics and Physics that are of great relevance in fundamental entry-level engineering classes. The second goal was to have videos ready with near perfect quality, both audio and visionary wise. Having as short videos as possible was the final goal.

Regarding making the videos, Camtasia (TechSmith, Okemos, MI) was chosen as the software to record video. We recorded the video and audio separately and then used Camtasia features to synchronize them appropriately. Instead of having already made slides to cover topics, we implemented smart pad as well as handwriting to teach concepts step-by-step. Elmo cameras (Elmo USA, Plainview, NY) was used for recording real time the handwriting off the paper. The resolution of final videos to be shared was set to 1080p. Figure 3.1 shows a screenshot of Camtasia start screen.

Figure 3.1. Camtasia start screen

As shown in Figure 3.2, aside from synchronizing audio and video by using “Clip Speed,” other features of Camtasia have been implemented in developing the videos. Short questions were added to videos by applying “Quizzing…” element of Camtasia. Additionally, since there was more than one part to be covered in each topic and making the videos as short as possible was one of the main goals, a menu for each video was made by employing “Markers” option of Camtasia. “Callouts…” was the other option of Camtasia which implemented in the videos. Callouts are useful when one desires to jump to specific parts of the video.

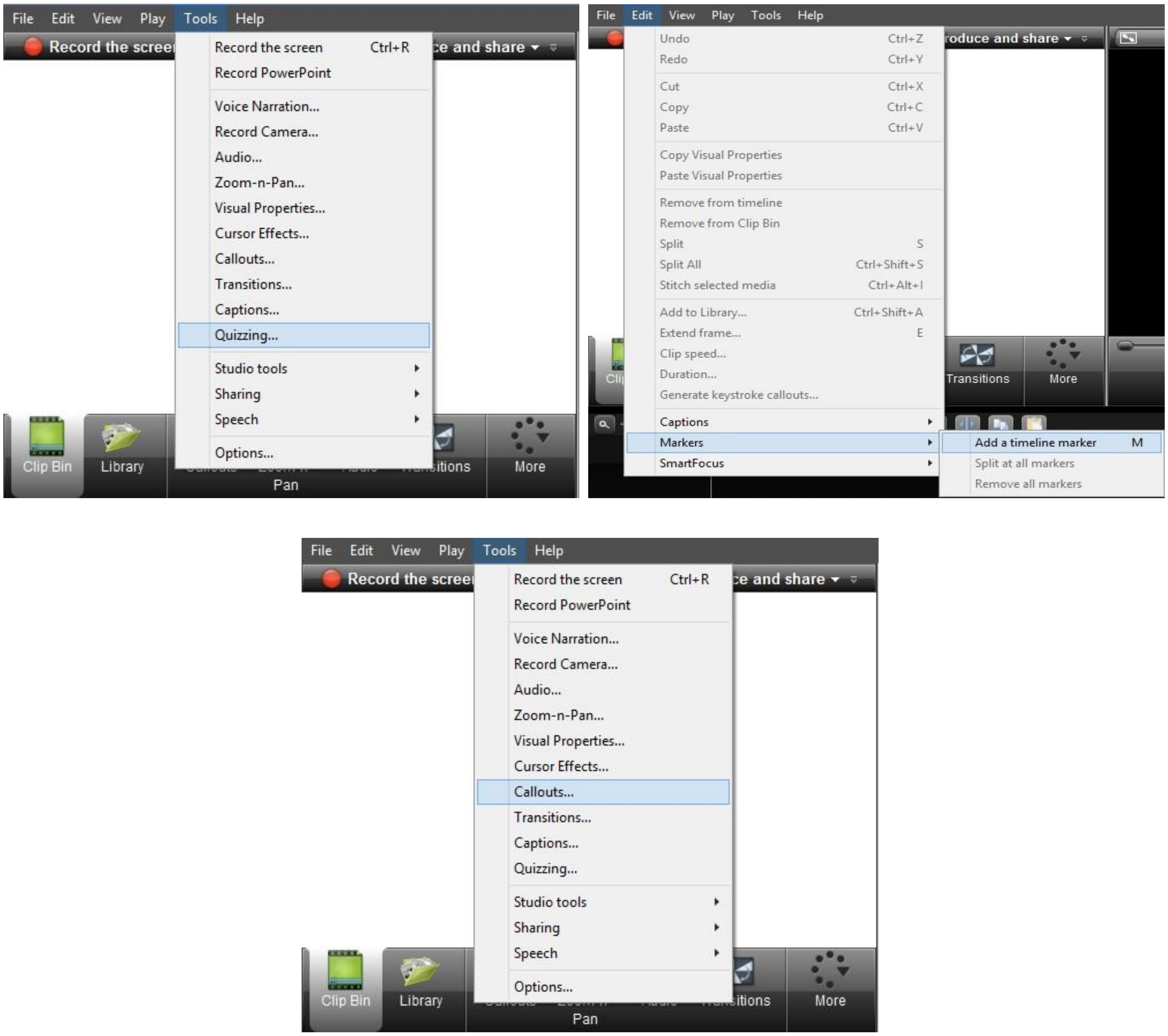


Figure 3.2. Screenshots of quizzing, markers, and callouts features of Camtasia

3.3 Results and Discussion

3.3.1 Videos

Three videos were made to cover the basic concepts of differentiation, integration and vector calculus. Multiple studies show the significance of providing supplementary videos besides regular lecture. For example, Ljubojevic, V. Vaskovic, Stankovic, & J. Vaskovic et al. [29] showed that students acquire a higher level of knowledge when videos are implemented in the lecture. Lemley and Jassemnejad [30] discussed the effectiveness of supplementary videos, and Halupa and Caldwell [31] compared the traditional lectures and Online supplemental videos approach, and reported an improvement in students who were involved in lecture and supplemental videos approach.

As shown in Figure 3.3, the videos were developed to be interactive so that students can choose whichever part they want to review. Hence, students have more control on the course flow and can adjust the teaching speed based on their preference. Employing quizzing tool of Camtasia, questions were added to the video. Students are required to answer the question to proceed to the end of the video. Although they can choose which part of the video they want to watch, if there is a question at the end of the skipped part, they are required to answer it before proceeding to the next part of the video. Another important feature of the videos is the feedback students getting from videos. Chen, Whittinghill, & Kadlowec [32] identified the significance of rapid feedback and its positive effect on student performance. Sarder [33] mentioned positive feedback as one of the strategies which can be implemented to enhance student engagement in online courses. Therefore, by the help of quizzing, videos were designed to provide immediate and positive feedback to students to enhance student engagement. Students receive quick feedback on their perception of the topic. Also by including callouts in the videos, students can readily choose to skip the parts they deem as unnecessary.

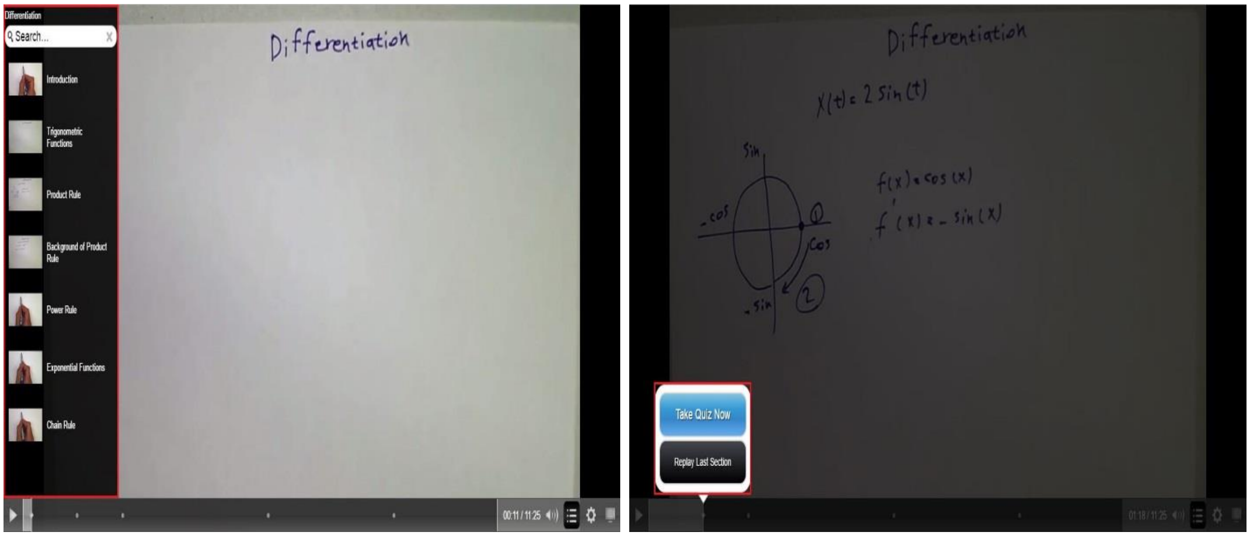


Figure 3.3. Menu and quiz in the video

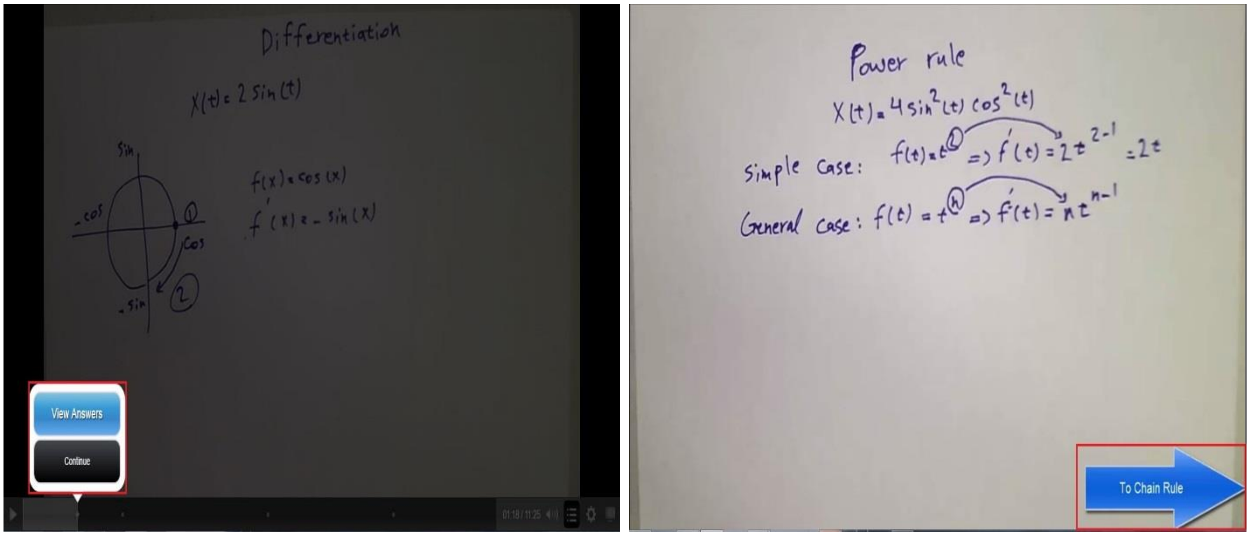


Figure 3.4. Feedback and callout

As shown in Figures 3.3 and 3.4, lecture note was written by hand on a paper and recorded real time. Instead of having PowerPoint slides prepared, a decision was made to write equations and draw figures by hand. Additionally, attempts were made on writing with smartpen on a notebook and writing with a pen on a piece of paper. Comparing smartpen with handwriting on a paper, handwriting option was chosen to be recorded since it provided better quality compared to former one.

3.3.2 Limitations

There are some limitations we noticed during this study. The original idea was to minimize teacher’s lecturing in the course. One major drawback in achieving this goal was lack of available technical resources that are capable of creating such videos. Ideally, creating a video, which provides students with more Q&A conversation, makes the video more interactive. Consequently, learners can be more appealing to engage with these type of videos.

The other limitation we found was about accessibility. All of the videos are transferred to the Blackboard web server and under a specific course. Thus, not all engineering students have access to them, and once the enrolled students finish the course, videos become inaccessible.

Strengthening student engagement is another possible limitation of this work. Since these videos are not part of the course syllabus, motivating students to be properly engaged in watching them is going to be challenging. Furthermore, these videos will be used for a nearly future educational study in the Department of Mechanical Engineering at KU. We are carrying out a further study to address the limitation above.

3.3.3 Future Work

Next step of this work is to implement these videos in an online instructional module and conduct an educational study to evaluate the effects of videos on students' performance. With identifying the above limitations in our study, we would like to make following suggestions for future research:

- Developing more interactive videos by using more versatile technical tools.
- Focus on providing access methods that make videos accessible to a broader range of students than just the ones enrolled in the targeted course.
- Further study of exploring methods of encouraging students for participation in educational studies other than the method of reward and punishment. Students' perception of such studies can be the deciding factor in their willingness for participation.
- Concentrating on incorporating different teaching methods in instructional videos. Finding the proper balance between contents inclusion and duration of a video.

3.4 Conclusion

This study focuses on exploring methods of developing online instructional videos, to be further applied in an educational study or incorporated into a lecture-based course. Our literature review provided insight on important aspects that are of substantial importance in developing interactive instructional videos. Given online courses lack of interactivity, more efforts are needed on developing software and platforms to enable teachers to develop interactive videos. Students' engagement in online activities is a considerable factor in expanding these activities and therefore, needs investigations that are more thorough. Student satisfaction of online courses and the effect of these videos on students learning performance will be the subject of an imminent educational study.

3.5 References

1. Meyer, K.A., *Student Engagement in Online Learning: What Works and Why*. ASHE Higher Education Report, 2014. **40**(6): p. 1-114.
2. Adams, A.J., G.R. Matzke, and K.L. McCall, *A Novel Education and Training Program to Enhance Student Advocacy*. American Journal of Pharmaceutical Education, 2015. **79**(7): p. 5.
3. de Caprariis, P., C. Barman, and P. Magee, *Monitoring the Benefits of Active Learning Exercises in Introductory Survey Courses in Science: an Attempt to Improve the education of Prospective Public School Teachers*. 2012, 2012: p. 11.
4. Kar, S.S., et al., *Student-centred learning in Community Medicine: An experience from Jawaharlal Institute of Postgraduate Medical Education and Research, Puducherry*. National Medical Journal of India, 2014. **27**(5): p. 272-276.

5. Mak, A.S., A. Daly, and M.C. Barker, *Fostering cultural inclusiveness and learning in culturally mixed business classes.* Springerplus, 2014. **3**: p. 12.
6. Elliott, E.R., et al., *Improved Student Learning through a Faculty Learning Community: How Faculty Collaboration Transformed a Large-Enrollment Course from Lecture to Student Centered.* Cbe-Life Sciences Education, 2016. **15**(2): p. 14.
7. O'Connell, R.M., *Adapting Team-Based Learning for Application in the Basic Electric Circuit Theory Sequence.* Ieee Transactions on Education, 2015. **58**(2): p. 90-97.
8. Caviglia-Harris, J., *Flipping the Undergraduate Economics Classroom: Using Online Videos to Enhance Teaching and Learning.* Southern Economic Journal, 2016. **83**(1): p. 321-331.
9. Milman, N.B., *The flipped classroom strategy: What is it and how can it best be used?* Distance Learning, 2012. **9**(3): p. 85-87.
10. Bonwell, C.C. and J.A. Eison, *Active Learning: Creating Excitement in the Classroom. 1991 ASHE-ERIC Higher Education Reports*. 1991: ERIC.
11. Prince, M., *Does Active Learning Work? A Review of the Research.* Journal of Engineering Education, 2004. **93**(3): p. 223-231.
12. Braxton, J.M., J.F. Milem, and A.S. Sullivan, *The Influence of Active Learning on the College Student Departure Process: Toward a Revision of Tinto's Theory.* The Journal of Higher Education, 2000. **71**(5): p. 569-590.
13. Jones, L., *The Student-centered Classroom*. 2007: Cambridge University Press.
14. Zepke, N., *Student engagement research: thinking beyond the mainstream.* Higher Education Research & Development, 2015. **34**(6): p. 1311-1323.
15. HANNAFIN, M.J. and S.M. LAND, *The foundations and assumptions of technology-enhanced student-centered learning environments.* Instructional Science, 1997. **25**(3): p. 167-202.
16. Docherty, C., et al., *eLearning techniques supporting problem based learning in clinical simulation.* International Journal of Medical Informatics, 2005. **74**(7-8): p. 527-533.
17. Roshier, A.L., N. Foster, and M.A. Jones, *Veterinary students' usage and perception of video teaching resources.* Bmc Medical Education, 2011. **11**: p. 13.
18. Arya, P., T. Christ, and M.M. Chiu, *Video use in teacher education: a survey of teacher-educators' practices across disciplines.* Journal of Computing in Higher Education, 2016. **28**(2): p. 261-300.
19. Lage, M.J., G.J. Platt, and M. Treglia, *Inverting the Classroom: A Gateway to Creating an Inclusive Learning Environment.* The Journal of Economic Education, 2000. **31**(1): p. 30-43.
20. Lai, C.-L. and G.-J. Hwang, *A self-regulated flipped classroom approach to improving students' learning performance in a mathematics course.* Computers & Education, 2016. **100**: p. 126-140.
21. Moos, D.C. and C. Bonde, *Flipping the Classroom: Embedding Self-Regulated Learning Prompts in Videos.* Technology, Knowledge and Learning, 2016. **21**(2): p. 225-242.
22. Sohrabi, B. and H. Iraj, *Implementing flipped classroom using digital media: A comparison of two demographically different groups perceptions.* Computers in Human Behavior, 2016. **60**: p. 514-524.
23. McLean, S., et al., *Flipped classrooms and student learning: not just surface gains.* Advances in Physiology Education, 2016. **40**(1): p. 47-55.

24. Heller, R.S., et al., *Student and Faculty Perceptions of Engagement in Engineering.* Journal of Engineering Education, 2010. **99**(3): p. 253-261.
25. Cantrell, P., et al., *The Effects of Engineering Modules on Student Learning in Middle School Science Classrooms.* Journal of Engineering Education, 2006. **95**(4): p. 301-309.
26. Hake, R.R., *Interactive-engagement versus traditional methods: A six-thousand-student survey of mechanics test data for introductory physics courses.* American journal of Physics, 1998. **66**(1): p. 64-74.
27. Foertsch, J., et al., *Reversing the Lecture/Homework Paradigm Using eTEACH® Web-based Streaming Video Software.* Journal of Engineering Education, 2002. **91**(3): p. 267-274.
28. Hughes, J., *The role of teacher knowledge and learning experiences in forming technology-integrated pedagogy.* Journal of technology and teacher education, 2005. **13**(2): p. 277.
29. Ljubojevic, M., et al., *Using supplementary video in multimedia instruction as a teaching tool to increase efficiency of learning and quality of experience.* 2014, 2014. **15**(3).
30. Evan, C.L. and J. Baha, *Use of Supplementary Online Lecture Materials in a Heat Transfer Course*. ASEE Conferences: San Antonio, Texas.
31. Halupa, C.M. and B.W. Caldwell, *A Comparison of a Traditional Lecture-Based and Online Supplemental Video and Lecture-Based Approach in an Engineering Statics Class.* International Journal of Higher Education, 2015. **4**(1): p. 232-240.
32. Chen, J.C., D.C. Whittinghill, and J.A. Kadlowec, *Classes That Click: Fast, Rich Feedback to Enhance Student Learning and Satisfaction.* Journal of Engineering Education, 2010. **99**(2): p. 159-168.
33. Sarder, M.D.B., *Improving Student Engagement in Online Courses*. 2014, ASEE Conferences: Indianapolis, Indiana.

Chapter 4. Enhancing the Teaching–Learning Effectiveness: Creating Online Interactive Instructional Modules

4.1 Introduction

Engineering instructors face a variety of challenges in teaching introductory-level courses. One major challenge is that students frequently lack precursor knowledge of key mathematics and science concepts [1]. Students are generally required to take prerequisite courses in mathematics, physics, and chemistry before beginning their engineering coursework, but retention of knowledge from these prerequisite courses is often low. In order to develop expertise in the engineering field, learners must acquire a deep and well-organized understanding of the domain. This includes knowledge of key concepts (e.g., force, mass) and general principles (e.g., Newton's laws of motion) and awareness of the contextual conditions under which knowledge is useful [2]. Connecting new ideas and concepts to previous knowledge and experience is a key element of developing this expertise [2].

The current study examines the effectiveness of an intervention focused on supplementary online video instruction in an undergraduate statics course. The supplementary videos focused on three key concepts for which students often lack fundamental understanding: differentiation (including the product rule, the power rule, and the chain rule), integration (including the power rule, the quotient rule, and integrals of inverse tangents and natural logarithms), and vector calculus (including unit vectors, dot products, and cross products). The intervention is structured around several key educational principles: ensuring that relevant prior knowledge is accurate and active, integrating testing into study sessions, and allowing for individualized, self-paced learning.

4.1.1 Prior Knowledge

Instructional strategies that promote connections with prior knowledge can promote fuller understanding and deeper learning of new material [e.g., 3, 4]. For example, elaborative interrogation, which activates prior knowledge and encourages students to connect new information with what they already know, can facilitate learning [5, 6]. However, in order to promote learning, prior knowledge must be appropriate, accurate, and sufficient for the task at hand [7].

Students arrive at each course with varying levels of prior knowledge; how to address these differences in prior knowledge is a common challenge for instructors [7]. One approach is to provide remedial instruction for students who lack understanding of key prior concepts. However, it is often not feasible or desirable to provide such instruction during regular class meetings, because there is not sufficient time to cover the material or because students who already understand the material will become bored or disengaged. Thus, the ability to provide out-of-class supplementary instruction to ensure accurate and active prior knowledge is beneficial for both instructors and students.

In the current study, the relevant prior knowledge concepts were fundamental concepts of physics and mathematics that are primary concepts in second year engineering mechanics courses such as Statics and Dynamics. These concepts were differentiation, integration, and vector calculus. Differentiation and integration are recognized as the two most central mathematical concepts in almost all engineering majors. Vector calculus was also selected since the prominent receiver group of the modules were mechanical engineering students, and the Dynamics course is mainly taught using a vector analysis approach.

4.1.2 Benefits of Online Supplementary Instruction

Currently, instructional videos are widely used in both campus-based and online courses [8-12]. The use of such videos in combination with the face-to-face class instruction may be especially beneficial; several meta-analyses have found that hybrid or blended courses, which include both face-to-face and online instruction, are more effective than either traditional in-person courses or fully online courses [13, 14].

Most recent online courses (and related research) adopt the student-centered approach [15-17]. Following a student-centered approach, online instructional materials (e.g., videos) are made as interactive as possible so that the learner controls the flow of the course [18-20].

4.1.2.1 Individualized, Self-Paced Instruction. Students benefit from individual instruction, but most classes do not allow for it [21, 22] and students frequently do not take advantage of opportunities for in-person individual instruction, such as instructor office hours [23, 24]. One common reason students give for their lack of attendance at office hours is that the time and/or location of office hours was not convenient; Griffin et al. [24] found that convenience had a greater impact on student office hour attendance than a number of other factors, such as whether the instructor was perceived as approachable and whether material was explained clearly during class. Online tutoring sessions allow students to access material at a time and place that is convenient for them and thus may increase engagement with these sessions.

One of the main factors contributing to learning effectiveness in online courses, compared to traditional classroom-based courses, is the increased control that learners have over the course flow and content [25-28]. Contrary to popular belief, the major motivation for enrollment in distance education is not physical access, but rather, temporal freedom to move through a course of studies at a pace of the student’s choice [29-33].

4.1.2.2 Presence in Online Instruction. Effective online teaching activities design, facilitate, and direct the cognitive and social process to realize personally meaningful and educationally worthwhile learning outcomes [34]. A sense of presence contributes to the effectiveness of online learning activities.

There are three types of presence in online teaching and learning environments: social, cognitive, and teaching presence. Social presence was defined as “the degree to which a person is perceived as a real person in mediated communication" [35]. A study of the role of social presence has found that interaction among participants is critical in learning and cognitive development [36]. Students with high overall perceptions of social presence performed better regarding perceived learning [36-38]. In the current study, promoting social presence was partly achieved by introducing the instructor within the modules. We encouraged students to share their background with the instructor to help them build a connection with the instructor. Furthermore, all of the participants understood that their opinions on the modules are considered valuable to promote a feeling of relevance to the instructor and course.

Cognitive presence was defined as "the extent to which learners are able to construct and confirm meaning through sustained reflection and discourse in a critical community of inquiry" by Garrison, Anderson, & Archer [39]. Cognitive presence has been identified as the most challenging type of presence to create in online learning environments [40]. To fostering cognitive presence in the current study, we provided prompt feedback to students on their performance in modules quizzes and video embedded questions. Innovative problem-solving techniques were also provided for the students by the instructional videos.

Teaching presence was defined by Anderson, Liam, Garrison, & Archer [41] as the "design, facilitation, and direction of cognitive and social processes for the purpose of realizing personally meaningful and educationally worthwhile learning outcomes". Our modules promoted teaching presence by encouraging independent study among the learners. Additionally, the modules were constructed such that student empowerment was promoted. Students had full control over the pace of progression through the video modules, and therefore, they were given the freedom to address their unique needs based on their aspirations and goals. Information about technology requirement and available resources for technical help was provided to the students to facilitate the utilization of the modules. Furthermore, the instructions and rules of the course were outlined at the beginning of the study.

4.1.2.3 Cognitive Apprenticeship. Cognitive apprenticeship is an instructional model in which expert approaches to thinking and problem solving are made visible [42]. In cognitive apprenticeship approaches to instruction, an expert works through a problem while verbally describing and explaining the underlying cognitive processes in which the expert is engaged. Thus, the learner is able to see correct problem solving modeled while also understanding the decision making and problem solving processes that inform the chosen behaviors or strategies [42, 43].

To make our videos consistent with this model, the verbal explanation of problem solving procedure was synchronized precisely with writing part of the video. Therefore, students were able to follow the solution strategy and steps as they were explained and written down on the paper. In addition, there were references to the already explained concept in solving a problem. This was especially performed to help the students perceive the application of the taught concept in solving a problem.

4.1.3 Integrating Self-Testing into Study Sessions

One benefit of online supplementary instruction is the ability to provide prompt feedback about the accuracy of student's calculations and conclusions. As noted by Anderson [44], to provide motivation and shape the behavior and mental constructs most effectively, detailed feedback should be provided as quickly as possible following the performance of the assessed behavior. For this reason, machine evaluations, such as those provided in online multiple-choice test questions or in simulations, can be very effective learning devices.

A variety of studies have found that integrating self-testing into study sessions promotes better memory and deeper learning. For example, Roediger III and Karpicke [45] found that dividing study time between material review and self-testing was more effective than devoting study time entirely to material review. Subsequent research indicates that recall testing of previously learned information can positively impact not only memory for previously learned information, but also learning of new information [46] and that integrated testing can improve attention to and learning from online lectures [47].

Presence of integrated quizzes also allows for immediate feedback. Prompt feedback helps students to build awareness of what they do and do not know and can prevent the persistence of misconceptions [7]. The instructional videos used in the current intervention included integrated questions that were posed to the viewers at the end of each chapter of the video. After viewing the chapter, students were required to answer the question in order to proceed to the next chapter. The questions were mostly focused on the common mistakes that students would make in applying the concept of that chapter. An immediate feedback was provided to the students which showed whether their answer was wrong or right. Then students were provided with the choice of continuing to the next chapter or replaying the chapter they just watched.

4.2 Methods

4.2.1 Procedure

Participation in the study was voluntary. Informed consent was obtained from each participant included in the study. Extra credit was provided as the benefit of participation to those who completed the study. Figure 4.1 summarizes the overall procedure in this study.

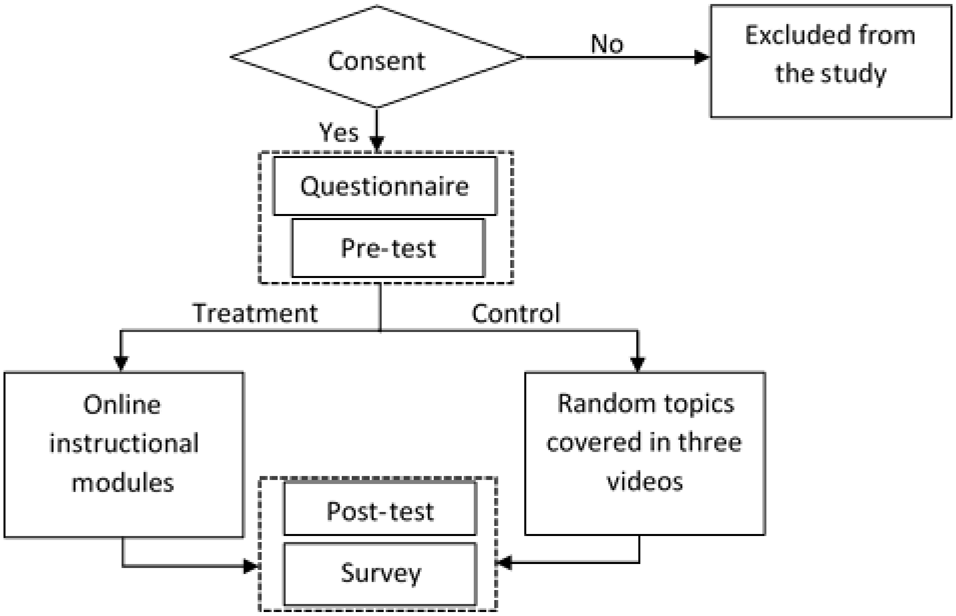


Figure 4.1. Flowchart of the study

Each stage of the study is briefly described as follows:

1. The consent form was distributed to all students in the course. (In classroom)
2. The students choosing to participate in the study returned the filled out consent form and were randomly assigned to either the treatment or control group.
3. A questionnaire was provided and filled out by the study participants. (In classroom)
4. All participants took the pre-test. (In classroom)
5. Links to all the videos and related assignments were provided to participants (treatment and control groups) and they were required to complete all parts of these online instructional modules within a specific 10-day period. All quizzes and videos were provided on the institution’s Learning Management System (Blackboard) website. (Outside classroom)
6. All participants took the Post-tests. (In classroom)
7. A survey form was provided and filled out by all participants.

4.2.2 Participants

Students enrolled in the required Statics course in the fall 2016 semester were invited to participate in this study. Forty-seven students completed the study, with twenty-five in the treatment group and twenty-two in the control group. Group assignments were random and participants did not know if they were members of the experimental or control group as a single-blind experimental design was utilized. Of the participants in the treatment group, 80% were male and 20% female. Of the participants in the control group, 100% were male.

4.2.3 Modules

Our goal was to focus modules on fundamental concepts of physics and mathematics that are utilized in teaching the engineering mechanics courses Statics and Dynamics. To determine the relevant fundamental concepts, we surveyed the faculty members across the School of Engineering who teach engineering mechanics courses. Based on faculty feedback, we focused on three fundamental concepts: differentiation, integration, and vector calculus; and we established the most important parts of each concept. Therefore, we developed three modules, one for each fundamental concept: differentiation, integration, and vector calculus. Each module consisted of: 1) pre-test quiz, 2) instructional video, and 3) post-test quiz. The differentiation, integration, and vector calculus instructional videos were 11, 7, and 18 minutes in length, respectively. Each instructional video had a menu listing chapters, with each chapter focused on a specific concept part and the menu enabling easy navigation between chapters. The chapters were short videos (4 minutes or less). For example, within the vector calculus instructional video, one chapter focused on taking the cross product between two vectors. Within each chapter, first the concept part was explained (e.g., cross product), then a relevant example was elucidated thoroughly to demonstrate the concept part, and finally, a more advanced example problem was presented. Embedded questions were placed at the end of the majority of the chapters, and immediate feedback was provided upon answering these questions. Furthermore, students could either use the menu to navigate to a different chapter or they could use arrow shaped links provided on the screen to continue to the next chapter, replay the previous chapter, or skip to another chapter.

Unlike the treatment group, the control group watched three videos on random topics that were not directly related to the study. These videos were provided to the control group in an attempt to avoid the Hawthorne effect in our study. The Hawthorne effect states that subjects modify their behavior based on their knowledge of an external observer. Although these videos didn’t have any embedded questions, the control group participants were required to watch all three videos to be considered as participants in the study.

4.2.4 Measures

4.2.4.1 Questionnaire: Demographic, Academic, and Social Background Data. All participants completed a questionnaire containing sections for their age, gender, GPA (high school and college), social activity background, and awards and accomplishments information. These data were later assessed to draw a correlation between the participants’ performance and engagement in the online learning environment.

4.2.4.2 Pre- and Post- Quiz. For each module, all participants completed the same quiz pre- and post- an instructional video exposure. Videos were developed according to the process previously described by Moradi, Liu, & Luchies [48]. Each pre- and post- quizzes consisted of five multiple choice questions. The pre- and post- quiz contained the same multiple choice questions with answers provided in a random order. Two examples of quiz questions in each module are:

- $x(t) = \exp(t^2)$ is the displacement of a particle. Find its velocity. (Differentiation module)
- The acceleration of a car, which was initially at rest, is approximated as: $a(t) = \frac{3}{4}t^3$. What would be the velocity of the car at $t = 2$?

Each quiz was designed to assess the participants' knowledge of topics related to the corresponding module and the performance of the student in these quizzes were not used in the data analysis. Furthermore, the quizzes were included in the modules to: 1) provide a pre-study opportunity for the student so he/she would have a better idea about the content of the instructional video before watching it, and 2) help the student to review the material after watching the video. Participants were only provided quiz performance feedback after the post-quiz. Based on their choice of answer, appropriate feedback was provided to them. The feedback either referred to a particular part of the video or reminded a key point which would lead to the correct choice of answer. For example, if the student answered incorrectly the first example question about calculating particle velocity using the displacement function, they would be directed to a specific part of the related instructional video that reviewed using the method of differentiation.

4.2.4.3 Pre- and Post- Test. All participants took the pre-test at the beginning of the study and the post-test at the end of the study, both were administered in the classroom. Both tests consisted of 10 multiple-choice questions focused on the fundamental concepts: differentiation, integration, and vector calculus. The questions were different between the two tests, but they were related to the same concepts in both tests. The questions were designed to assess the students understanding of the concepts, rather than performing computations. The participants' scores from both tests were recorded and included in the data analysis.

4.2.4.4 Survey. After the post-test was complete, each participant filled out a survey. The 5-point Likert scale survey consisted of six statements (Table 4), and participants were asked to provide their opinions on each statement by choosing a number from 1 to 5 (1 = strongly disagree – 5 = strongly agree). The quality and student satisfaction of the modules, and students' control over the pace of learning were the fundamental elements of the survey statements.

4.2.5 Data Analysis

One-sample Kolmogorov-Smirnov test (KS test) was employed to check the normality of data in all statistical analysis. An independent t-test was conducted on the age of participants in both groups to verify that the two groups were similar in age

In order to have a more robust opinion on participants' test results, a statistical analysis was performed. After the normality of the data was checked, a t-test on the test scores was performed.

Mean- and standard deviations of pre- and post-test of both groups were calculated. An independent samples t-test was conducted on the pre-test total score for the two groups to verify that the two groups were not statistically different before the video exposure. A paired samples t-test was conducted within each group across the pre- and post- test score to determine the effect of the video exposure. The significance level of $p \leq 0.05$ was used for all t-tests.

4.3 Results and Discussion

Normality distribution check of data revealed that the collected data was not normally distributed for the following cases: 1) participants' age in both groups, and 2) post-test scores of the treatment group. Although the normal distribution of data is one of the assumptions of the t-test, previous investigations showed that t-test results are reliable in cases with relatively large sample size, $n \geq 30$ [49-51]. A study by Ratcliffe [52] stated increasing sample size to greater than fifteen will make the normality assumption of t-test negligible. Lumley, Diehr, Emerson, & Chen [53] also stated that the findings of Ratcliffe [52] were related to one-tailed t-tests which are more sensitive to non-normality of data. Hence, since the sample size in the current study was greater than 15, and our intention was on reporting the results of two-tailed t-tests, we concluded that performing a t-test on the data was reasonable.

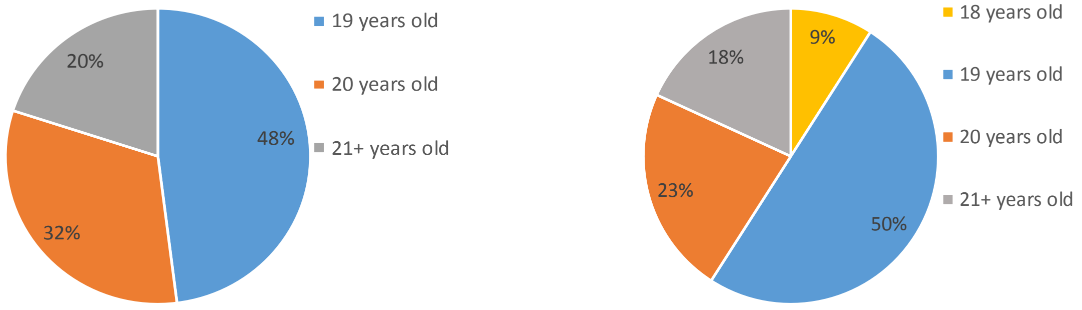
Based on the results of the t-test, the two groups were similar to each other in term of the age of the participants (Table 4.1).

	t-test results
t Stat	0.87
p (T≤t)	0.38*
t Critical	2.01

* Value of p indicates no significant difference between the compared data ($p>0.05$)

Table 4.1. Age of participants in two groups ($\alpha=0.05$)

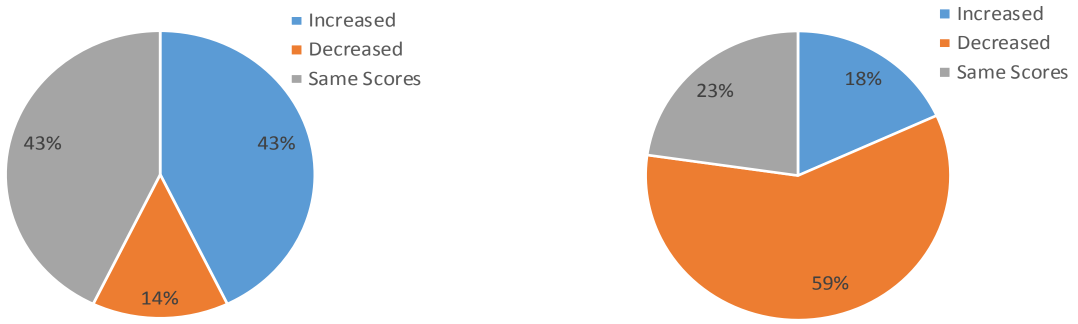
Age distribution of participants in both groups showed that most of the population were 19 years old (Figures 4.2, (a) and (b)), with 20 years old participants as the second biggest age group.



(a) Treatment group *(b) Control group*

Figure 4.2. Participants' age distribution

Performing KS test, all four sets of data for pre- and post- test scores of participants were verified to have a normal distribution. Students' performance in both groups are depicted in Figures 4.3(a) and 4.3(b). As the figures demonstrate, there is a small decrease in test results in the treatment group which is contrary to the control group as the majority of control group dropped in their test score over the two tests. Furthermore, the number of students who performed better and also the rate of increase in the treatment group was more than that of the control group, which is in accordance with previous research [54].



(a) Treatment group *(b) Control group*

Figure 4.3. Participants' performance overall the two tests

Test results indicate that the control group had a better understanding of the targeted topics than the treatment group by 10% in the average of pre-test scores (Table 4.2) and this difference was statistically significant (Table 4.3). Since the treatment group was exposed to online instructional modules, it was expected that they would improve their learning, which is consistent with previous research [55]. For the treatment group, the quiz score was higher by 13% in the post-assessment, compared to the pre-assessment (Table 4.2) and t-test analysis proved that the increase in test scores was significant (Table 4.3). These results suggest that the instructional videos had a significant impact on the treatment group and improved their scores in the post-test compared to the pre-test. Table 4.2 also denotes a 13% increase across the post- vs. pre- test scores in the treatment group, which was expected since the post-quiz assessment was on the topics that were covered in the modules. The control group watched videos unrelated to the quiz, and it was expected that their quiz scores would not change; t-test result demonstrated that the post-quiz score was not significantly different compared to the pre-assessment (Table 4.3).

	Pre-Test		Post-Test	
	Treatment	Control	Treatment	Control
Mean	6.68	7.59	7.52	6.73
Median	6	8	7	7
Standard Deviation	1.80	1.71	1.68	1.86

Table 4.2. Mean, median and standard deviation of test scores

	Age of participants in two groups	Pre-test scores of the two groups	Post- vs. Pre- test scores (treatment group)	Post- vs. Pre- test scores (control group)
t Stat	0.87	-2.55	-3.67	2.02
p (T≤t)	0.38*	0.01**	0.001**	0.06*
t Critical	2.01	2.02	2.06	2.08

* Value of p indicates no significant difference between the compared data ($p>0.05$)

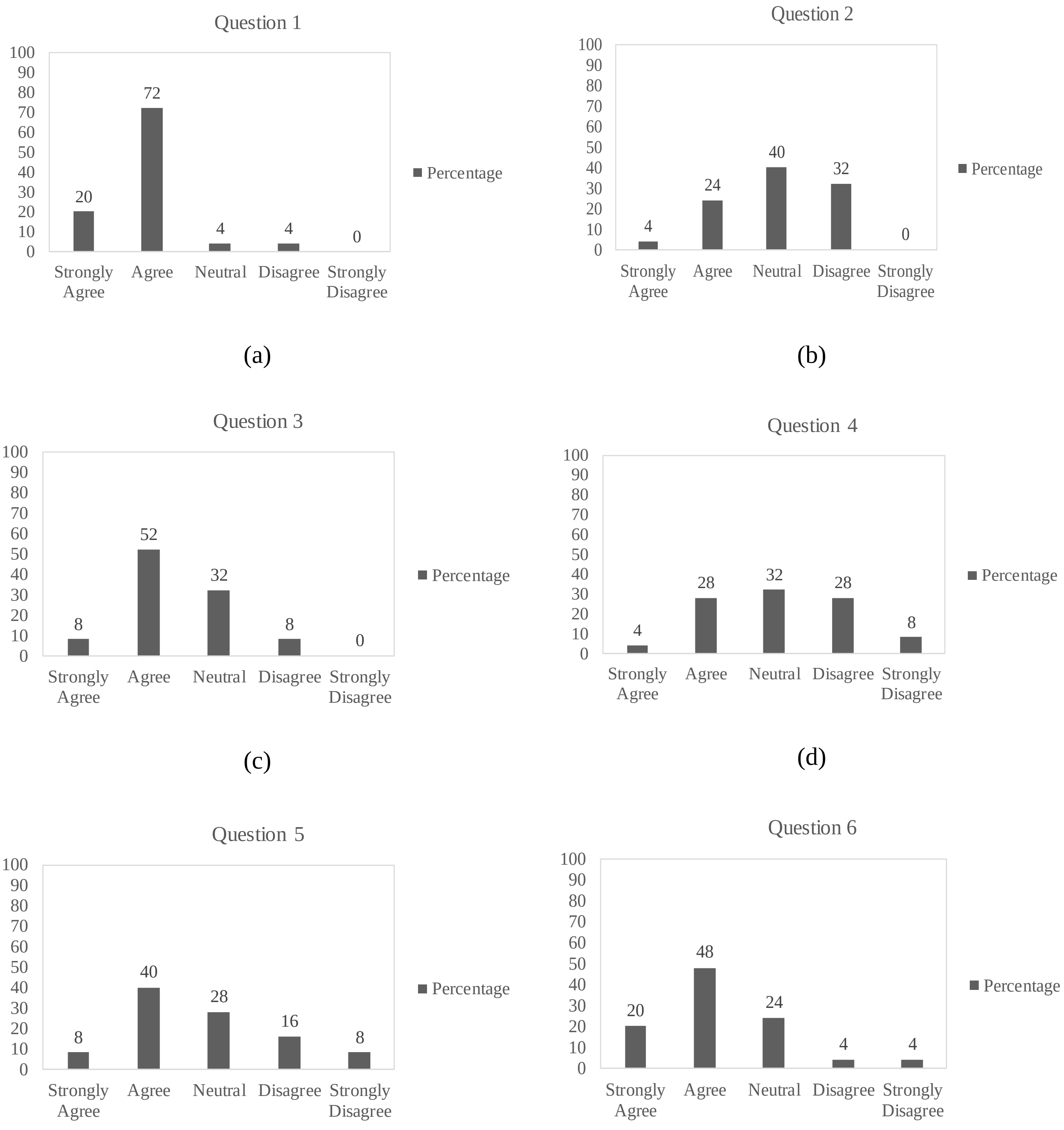
** Value of p indicates significant difference between the compared data ($p\leq0.05$)

Table 4.3. t-test results for the collected data ($\alpha=0.05$)

Table 4.4 represents survey statements and the results of the treatment group survey. Numbers in each column are indicative of the number of the treatment group participants, who gave feedback to each row statement. Percentages of each Likert item corresponding to a survey statement are also illustrated (Figures 4.4, (a)-(f)).

Survey Questions	Mean	STD	Mode
1. Videos were good quality wise (audio, visual, length, buffering)	4.08	0.62	4
2. Having lectures covered in videos was better than in classroom	3	0.84	3
3. Having a quiz helped me in understanding concepts better	3.6	0.74	4
4. I think one of the two quizzes was unnecessary	2.92	1.01	3
5. I felt more engaged to the course, and I had better control over course flow	3.24	1.06	4
6. I recommend using these modules to cover basic concepts	3.76	0.94	4

Table 4.4. Survey results



(a) (b)

(c) (d)

(e) (f)

Figure 4.4. Distribution of survey questions feedback in percentages

Approximately 92% of the treatment group participants were satisfied with the quality of the developed modules, with quality defined as audio, visual, length and buffering (Figure 4.4(a)).

However, one participant was not satisfied with the video quality. The second statement indicates a wider spectrum of opinions. As demonstrated by Figure 4.4(b), only 28% percent of participants preferred videos over classroom lectures, and 72% were either neutral or against having videos rather than lectures. The above relatively low percentage approval rate indicates that although participants were awarded extra credit, there is a high possibility that they didn’t have a bias towards the videos. Therefore, it is reasonable to recognize this experimental study as being unbiased, which is very important when trying to interpret the results and proposing new ideas. Only 8% disagreed with the third statement; see Figure 4.4(c). It suggests that the majority of the students found the modules helpful. According to Figure 4.4(d), approximately 32% percent agreed that either of pre or post-test was unnecessary and 36% percent disagreed with the statement. They were asked to single out which test they think was unnecessary and an equal 50% chose either pre or post-test. Although there is disagreement between participants about the necessity of either pre- or post- test, it is of significant importance to design a pre- and post-assessment process. The pre- and post-test are necessary to evaluate the effectiveness of the implemented teaching method and including them in future studies is strongly recommended. Also, the remaining 32% were neutral on the topic which is another indicative that there is not enough evidence to draw any conclusion on excluding the assessment tools from a study framework.

Almost half of the participants felt that they had more control over the course flow and were engaged in the course, as it is demonstrated in Figure 4.4(e). This percentage is especially important when it comes to reviewing course materials or adjusting the progress of the course based on one’s self-personality since individualized learning has been considered as an important factor in students’ learning in incorporated online learning environments [56]. As some students need extra time to fully understand course materials, using the developed modules helps them gain control over the speed of their learning. This finding is especially important when considering their opinion on the sixth statement. Participants’ feedback on this statement indicates their level of satisfaction of the modules and possibly their engagement in the course and self-education [57, 58]. Figure 4.4(f) shows that 70% of students expressed a positive attitude towards the modules and recommended the use of such modules in the future. This high rate of recommendation from students is a promising figure in activities and policies practicing the use and development of online instructional modules and supports the idea of incorporating these modules into lecture-based classrooms [59]. About 8% were against using modules in the future, which is a considerably smaller percentage compared with 70% approval of the modules. Another important indication of the feedback is that although they did not prefer replacing lectures with videos, they were still satisfied by having access to the videos as an enhancement of the lectures. This means that the students prefer to have a blended course design, where they can have access to both lectures in the classroom and supplemental instructional videos. This result is consistent with previous research that emphasizes the significance of providing students with videos as a supplemental instructional tool [48]. Furthermore, since these modules were provided as a tool for course preparation, the level of the students’ satisfaction is consistent with the findings of a previous study [60].

4.4 Conclusion

The present study focuses on enhancing the effectiveness of online instructional modules of students learning. Since the modules were focused on covering basic concepts of mathematics and physics, developing and extending the use of these modules will significantly reduce the time an instructor needs to spend reviewing these concepts within mechanical engineering mechanics courses. This study shows that students who had access to the modules performed significantly better in their post-test, with their scores improving by 13%.

The students' feedback of the study indicates that they felt more engaged in the course by using the online instructional modules. Participant feedback provides evidence of the advantages of using student-centered classrooms and integrating technology in lecture-based courses. Almost 70% of treatment group recommended using these modules to cover prerequisite course materials. Also, they felt that incorporating quizzes in the videos and having short tests before and after the video helps them in understanding course material. As these features add interactivity to a video, this data shows that online instructional modules are useful in students' learning and preparedness.

Based on the participant feedback, we suggest that online instructional modules are an effective tool when combined with a lecture-based course. However, further research is needed that focuses on the instructors' opinion on the use of online instructional modules. Finally, reviewing basic mathematics and physics concepts should be the core part of the developed online instructional modules in order to address specific needs within the targeted engineering course. One of the main aspects that must be considered in future studies is to assess the effectiveness of such instructional modules on students' performance within the statics course by comparing final grades of the two groups, and also the effect of the modules in downstream courses. The length of similar future studies should be extensive enough that it enables researchers to evaluate the effectiveness of these resources on students' perception of not only their currently enrolled course but also the downstream courses. However, the current study provides evidence that targeted online instructional modules is a strong tool to enhance the engineering students' understanding of mathematics and physics fundamentals.

4.5 References

1. Krause, S., J.C. Decker, and R. Griffin. *Using a materials concept inventory to assess conceptual gain in introductory materials engineering courses*. in *Frontiers in Education, 2003. FIE 2003 33rd Annual*. 2003. IEEE.
2. Litzinger, T., et al., *Engineering education and the development of expertise.* Journal of Engineering Education, 2011. **100**(1): p. 123-150.
3. Cook, M.P., *Visual representations in science education: The influence of prior knowledge and cognitive load theory on instructional design principles.* Science education, 2006. **90**(6): p. 1073-1091.

4. Garfield, J., R. delMas, and B. Chance, *Using students' informal notions of variability to develop an understanding of formal measures of variability.* Thinking with data, 2007: p. 117-147.
5. Martin, V.L. and M. Pressley, *Elaborative-interrogation effects depend on the nature of the question.* Journal of Educational Psychology, 1991. **83**(1): p. 113.
6. Woloshyn, V.E., A. Paivio, and M. Pressley, *Use of elaborative interrogation to help students acquire information consistent with prior knowledge and information inconsistent with prior knowledge.* Journal of Educational Psychology, 1994. **86**(1): p. 79.
7. Ambrose, S.A., et al., *How learning works: 7 research-based principles for smart teaching.* 2010.
8. Bos, N., et al., *The use of recorded lectures in education and the impact on lecture attendance and exam performance.* British Journal of Educational Technology, 2016. **47**(5): p. 906-917.
9. Giannakos, M.N., L. Jaccheri, and J. Krogstie, *Exploring the relationship between video lecture usage patterns and students' attitudes.* British Journal of Educational Technology, 2016. **47**(6): p. 1259-1275.
10. Heitink, M., et al., *Teachers' professional reasoning about their pedagogical use of technology.* Computers & education, 2016. **101**: p. 70-83.
11. Lee, C.-J. and C. Kim, *An implementation study of a TPACK-based instructional design model in a technology integration course.* Educational Technology Research and Development, 2014. **62**(4): p. 437-460.
12. Moreno, R. and L. Ortegano-Layne, *Do classroom exemplars promote the application of principles in teacher education? A comparison of videos, animations, and narratives.* Educational Technology Research and Development, 2008. **56**(4): p. 449-465.
13. Means, B., et al., *Evaluation of evidence-based practices in online learning: A meta-analysis and review of online learning studies.* US Department of Education, 2009.
14. Todd, E.M., et al., *A meta-analytic comparison of face-to-face and online delivery in ethics instruction: the case for a hybrid approach.* Science and Engineering Ethics, 2017: p. 1-36.
15. Fraser, B., *Classroom Learning Environments*, in *Encyclopedia of Science Education*, R. Gunstone, Editor. 2015, Springer Netherlands: Dordrecht. p. 154-157.
16. Gilboy, M.B., S. Heinerichs, and G. Pazzaglia, *Enhancing Student Engagement Using the Flipped Classroom.* Journal of Nutrition Education and Behavior, 2015. **47**(1): p. 109-114.
17. Simon, B., et al. *Student experience in a student-centered peer instruction classroom*. in *Proceedings of the ninth annual international ACM conference on International computing education research*. 2013. ACM.
18. Allen, L.K., R. Eagleson, and S. de Ribaupierre, *Evaluation of an online three-dimensional interactive resource for undergraduate neuroanatomy education.* Anatomical sciences education, 2016. **9**(5): p. 431-439.
19. McLean, S., et al., *Flipped classrooms and student learning: not just surface gains.* Advances in physiology education, 2016. **40**(1): p. 47-55.
20. Windt, K., *Development of online learning modules as an adjunct to skills fairs and lectures to maintain nurses' competency and comfort level when caring for pediatric patients requiring continuous renal replacement therapy (CRRT).* Nephrology Nursing Journal, 2016. **43**(1): p. 39.

21. Chung, G.K., et al., *Towards Individualized Instruction with Technology-Enabled Tools and Methods: An Exploratory Study. CRESST Report 854.* National Center for Research on Evaluation, Standards, and Student Testing (CRESST), 2016.
22. Moores, D.F., *One size does not fit all: Individualized instruction in a standardized educational system.* American Annals of the Deaf, 2013. **158**(1): p. 98-103.
23. Cox, B.E., et al., *Pedagogical signals of faculty approachability: Factors shaping faculty–student interaction outside the classroom.* Research in Higher Education, 2010. **51**(8): p. 767-788.
24. Griffin, W., et al., *Starting the conversation: An exploratory study of factors that influence student office hour use.* College Teaching, 2014. **62**(3): p. 94-99.
25. Adamopoulos, P., *What makes a great MOOC? An interdisciplinary analysis of student retention in online courses.* 2013.
26. Hew, K.F. and W.S. Cheung, *Students' and instructors' use of massive open online courses (MOOCs): Motivations and challenges.* Educational Research Review, 2014. **12**(Supplement C): p. 45-58.
27. Lewis, S., A. Whiteside, and A.G. Dikkers, *Autonomy and responsibility: Online learning as a solution for at-risk high school students.* Journal of Distance Education (Online), 2014. **29**(2): p. 1.
28. Tseng, J.-L. and C. Pai, *Analyzing the Learning Modes of Learners using Time-Management Modules in Self-Paced Learning.* GSTF Journal on Computing (JoC), 2014. **2**(3).
29. Simonson, M., S. Smaldino, and S.M. Zvacek, *Teaching and Learning at a Distance: Foundations of Distance Education, 6th Edition*. 2014: Information Age Publishing.
30. Terras, M.M. and J. Ramsay, *Massive open online courses (MOOCs): Insights and challenges from a psychological perspective.* British Journal of Educational Technology, 2015. **46**(3): p. 472-487.
31. Du, S., et al., *Web‐based distance learning for nurse education: a systematic review.* International nursing review, 2013. **60**(2): p. 167-177.
32. Naidu, S., *Openness and flexibility are the norm, but what are the challenges?* 2017, Taylor & Francis.
33. Anderson, T., *Towards a theory of online learning.* Theory and practice of online learning, 2004. **2**: p. 109-119.
34. Laat, M.D., et al., *Online teaching in networked learning communities: A multi-method approach to studying the role of the teacher.* Instructional Science, 2006. **35**(3): p. 257-286.
35. Gunawardena, C.N., *Social presence theory and implications for interaction and collaborative learning in computer conferences.* International journal of educational telecommunications, 1995. **1**(2): p. 147-166.
36. Richardson, J. and K. Swan, *Examing social presence in online courses in relation to students' perceived learning and satisfaction.* 2003.
37. Zhan, Z. and H. Mei, *Academic self-concept and social presence in face-to-face and online learning: Perceptions and effects on students' learning achievement and satisfaction across environments.* Computers & Education, 2013. **69**(Supplement C): p. 131-138.
38. Zhang, D.J., G. Allon, and J.A. Van Mieghem, *Does Social Interaction Improve Learning Outcomes? Evidence from Field Experiments on Massive Open Online Courses.* Manufacturing & Service Operations Management, 2017.

39. Garrison, D.R., T. Anderson, and W. Archer, *Critical thinking, cognitive presence, and computer conferencing in distance education.* American Journal of distance education, 2001. **15**(1): p. 7-23.
40. Garrison, D.R. and J.B. Arbaugh, *Researching the community of inquiry framework: Review, issues, and future directions.* The Internet and Higher Education, 2007. **10**(3): p. 157-172.
41. Anderson, T., et al., *Assessing teaching presence in a computer conferencing context.* 2001.
42. Collins, A., J.S. Brown, and A. Holum, *Cognitive apprenticeship: Making thinking visible.* American educator, 1991. **15**(3): p. 6-11.
43. Dennen, V.P. and K.J. Burner, *The cognitive apprenticeship model in educational practice.* Handbook of research on educational communications and technology, 2008. **3**: p. 425-439.
44. Anderson, T., *Teaching in an online learning context.* Theory and practice of online learning, 2004. **273**.
45. Roediger III, H.L. and J.D. Karpicke, *The power of testing memory: Basic research and implications for educational practice.* Perspectives on Psychological Science, 2006. **1**(3): p. 181-210.
46. Pastötter, B. and K.-H.T. Bäuml, *Distinct slow and fast cortical theta dynamics in episodic memory retrieval.* Neuroimage, 2014. **94**: p. 155-161.
47. Szpunar, K.K., N.Y. Khan, and D.L. Schacter, *Interpolated memory tests reduce mind wandering and improve learning of online lectures.* Proceedings of the National Academy of Sciences, 2013. **110**(16): p. 6313-6317.
48. Moradi, M., L. Liu, and C. Luchies, *Identifying Important Aspects in Developing Interactive Instructional Videos*, in *2016 American Society for Engineering Education Midwest Section Conference*. 2016, ASEE: Manhattan. p. 1-8.
49. Arnold, S.F., *Mathematical Statistics*. 1990: Prentice-Hall.
50. Casella, G. and R.L. Berger, *Statistical Inference*. 2002: Thomson Learning.
51. Moore, D.S. and G.P. McCabe, *Introduction to the Practice of Statistics*. 1993: Freeman.
52. Ratcliffe, J., *The effect on the t distribution of non-normality in the sampled population.* Applied Statistics, 1968: p. 42-48.
53. Lumley, T., et al., *The importance of the normality assumption in large public health data sets.* Annual review of public health, 2002. **23**(1): p. 151-169.
54. Erbas, A.K., M. Ince, and S. Kaya, *Learning Mathematics with Interactive Whiteboards and Computer-Based Graphing Utility.* Educational Technology & Society, 2015. **18**(2): p. 299-312.
55. Hwang, G.-J. and C.-L. Lai, *Facilitating and Bridging Out-Of-Class and In-Class Learning: An Interactive E-Book-Based Flipped Learning Approach for Math Courses.* 2017.
56. Delialioglu, O. and Z. Yildirim, *Students' perceptions on effective dimensions of interactive learning in a blended learning environment.* Educational Technology & Society, 2007. **10**(2): p. 133-146.
57. Sahin, I. and M.C. Shelley, *Considering Students' Perceptions: The Distance Education Student Satisfaction Model.* Educational Technology & Society, 2008. **11**(3): p. 216-223.
58. Kuo, F.-R., et al., *Web-based learning system for developing and assessing clinical diagnostic skills for dermatology residency program.* Educational Technology & Society, 2016. **19**(3): p. 194-207.

59. Neo, M. and T.-K. Neo, *Engaging students in multimedia-mediated constructivist learning-Students' perceptions*. Educational Technology & Society, 2009. **12**(2): p. 254-266.
60. Montrieux, H., et al., *Blending Face-to-Face Higher Education with Web-Based Lectures: Comparing Different Didactical Application Scenarios*. Educational Technology & Society, 2015. **18**(1): p. 170-182.

Chapter 5. Conclusion and Scientific Contribution

5.1 Conclusion

5.1.1 Summary

Part II of this thesis illustrated new practices in engineering education and provided proof of the effectiveness of one of the important innovations in education, online learning modules. Videos have been recognized as one of the most important tools in delivering content in today’s education. Important factors to be considered in developing interactive instructional videos has been identified and recommended for integration into online education courses. Furthermore, an engineering education study was conducted by providing interactive instructional modules to the students. The effect of these modules on the students’ learning and teaching experience was evaluated by statistical analysis of the collected data and conducting a survey study. The obtained results reflected the positive effect of interactive instructional modules as students with access to the modules demonstrated a significant improvement in their learning.

5.1.2 Identifying Important Aspects in Developing Interactive Instructional Videos

This study focused on developing interactive instructional videos for implementation in lecture-based classrooms. Important aspects of the development and content selection of the videos have been identified and presented to be put into practice across various instructional disciplines. The conclusions of this study may be presented as follow:

1. Comprehensive questionnaires should be provided to faculties in the related field to prepare a complete list of topics to be covered in the instructional videos.
2. The length of the videos should be as short as possible. Splitting the videos into short and separate sections should be considered in cases where recording lengthy videos is unavoidable.
3. Making the videos as interactive as possible so that students can completely control the pace of their learning and consequently, becoming more engaged in the instructional videos.

5.1.3 Enhancing the Teaching–Learning Effectiveness: Creating Online Interactive Instructional Modules

Conducting an engineering education study was the subject of this investigation. Complete process design of an engineering education study was presented in this research. Students were divided into two groups, with only one group having access to the developed online interactive instructional modules. The following are important conclusions from this research effort:

1. Students' high level of satisfaction of the online modules indicates the importance of producing interactive modules.
2. Students with access to the modules improved their test scores significantly compared to their scores before accessing the modules.
3. The majority of participants recommended production and implementation of such modules to cover part of the course materials.

5.2 Scientific Contributions

1. Important aspects in the development of instructional videos were explored and suggested.
2. The main features that can make instructional videos more interactive were identified and incorporated into the videos
3. The effectiveness of online interactive instructional modules in students' learning and teaching experience was presented and confirmed.

5.3 Future Work Recommendations

1. The developed interactive modules still need a supervisor to guide and lead students in using the modules. Producing complete interactive modules which do not need any supervision is highly recommended.
2. The length of educational studies should be extended to a year or even more, to obtain a better understanding of the effect of the developing online modules on students' learning.