Chapter 1

INTRODUCTION

1.1 RESEARCH BACKGROUND

Rechargeable lithium batteries are being used worldwide for consumer electronic application due to their advantages over the conventional liquid-electrolyte batteries. The demand for a high energy, high power density, longer life cycle and lighter battery has produced great interest in the development of an advanced battery system. Buchmann (2001) showed the lithium-ion battery is highly demanded amongst users. Due to this instigation, many researchers and batteries developers need to study, understand and improve the action-reaction behavior in the components of batteries and manufacture better batteries. Mathematical modeling gives this group of people much information in order to understand the reaction and performance behavior inside the electrodes of batteries. Once the materials selection and preparation procedures have been selected, it is essential to proceed with detailed designing of a mathematical model for the battery system in order to produce the optimum battery design and configuration for a specific application. Hence, mathematical models and simulations allow various battery systems to be repeatedly and simultaneously tested. This in return allows great saving of materials and time.

Battery is an electrochemical cell that can be charged electrically to store a static potential for power and released electrical charge when needed. Battery was invented by Count Alessandro Volta in 1800. He discovered that a continuous flow of electrical force was generated when using certain fluids as conductors to promote a chemical reaction between the metals or electrodes and the voltage would increase when voltaic cells were stacked on top of each other. This led to the invention of the first voltaic cell or battery. Table 1.1 summarizes history of battery development and figure 1.1 illustrates the first voltaic cell invented by Volta according to Buchmann (2001).

Table 1.1: History of Battery Development.

History of Battery Development		
Year	**Researcher**	**Chronology**
1600	Gilbert (England)	Establishment electrochemistry study
1791	Galvani (Italy)	Discovery of animal electricity
1800	Volta (Italy)	Invention of the voltaic cell
1802	Cruickshank (England)	First electric battery capable of mass production
1820	Ampere (France)	Electricity through magnetism
1833	Faraday (England)	Announcement of Faraday's Law
1836	Daniell (England)	Invention of Deniell cell
1859	Plante (France)	Invention of the lead acid battery
1868	Leclanche (France)	Invention of Leclanche cell
1888	Gassner (US)	Completion of the dry cell
1899	Jungner (Sweden)	Invention of the nickel-cadmium battery
1901	Edison (US)	Invention of the nickel-iron battery
1932	Shlecht & Ackermann (Germany)	Invention of the sintered pole plate
1947	Neumann (France)	Successfully sealing the nickel-cadmium battery
1960	Union Carbide (US)	Development of primary alkaline battery
1970		Development of valve-regulated lead acid
1990		Commercialization nickel-metal hydride battery
1992	Kordesch (Canada)	Commercialization reusable alkaline battery
1999		Commercialization lithium-ion polymer
2001		Anticipated volume production of proton exchange membrane fuel cell

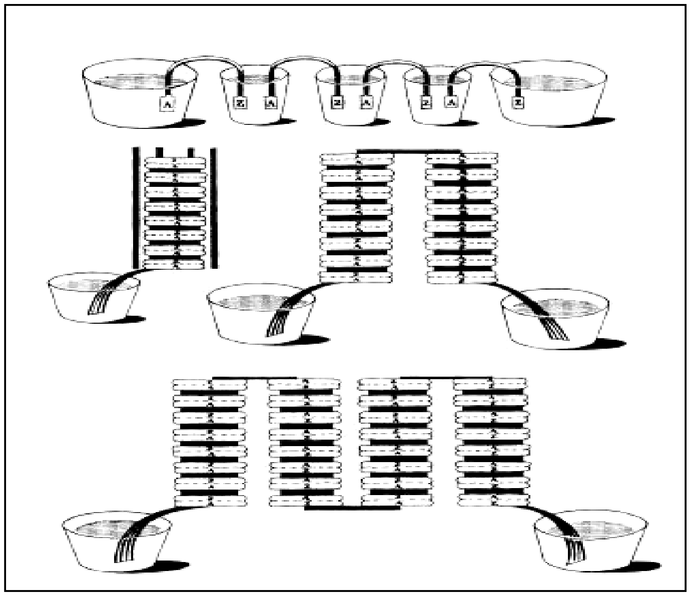

Figure 1.1: Four variations of Volta's electric battery.

Pioneering works related to lithium battery began in year 1912 by G. N. Lewis and the first non-rechargeable lithium battery was introduced and commercialized by M.S. Whittingham in year 1970. In order to invent the rechargeable lithium battery, it was found that there was inherent instability of lithium metal in anode during charging. Due to this instability problem, lithium battery was shifted to non-metallic lithium battery using lithium-ion compound in both anode and cathode. Lithium-ion compound is safer when charging and discharging process despite lithium-ion compound is slightly lower in energy density then lithium metal (Buchmann 2001). The first lithium-ion battery was introduced by the Sony Corporation and was commercialized in 1991. Tarascon and Armand (2001) have clearly explained the historical developments in lithium battery research for the past 40 years, which will be explained further in Chapter 2.

Today, there are many types of commercialized batteries. Sealed Lead Acid (SLA), Nickel-Cadmium (Ni-Cd), Nickel-Metal Hydride (Ni-MH) and Lithium-ion (Li-ion) are the most common secondary (rechargeable) battery that are being used now. Amongst these common batteries, lithium-ion battery is more stable, safe and has the highest energy capacity. Lithium-ion battery also has twice the charge capacity compared to Ni-Cd battery and slow self-discharges. The lithium-ion battery has no memory effect which means lithium-ion batteries do not have to be completely discharged before recharging it (Buchmann 2001; Dahn et al. 2005). In addition, lithium-ion batteries can operate over a wide temperature range, typically from -20^{o}C to +50^{o}C, and can last for hundreds or even thousands of charge/discharge cycles (Solution and Ltd. 2009). These good characteristics make lithium-ion battery popular among individual user, industry and are being used worldwide in ordinary electronic item such as portable computers, cellular phones, remote controls and also as a source of energy to hybrid and electrical vehicles.

Center for Transportation Research Argonne National Laboratory of United States (Gaines and Cuenca 2000; Yang et al. 2008; Abe et al. 2009) and many other researchers have been doing research on the usage of lithium-ion battery for electrical vehicle. Generally, these researches cover battery design, components, materials, production process, costing and fabrication. Table 1.2 shows the comparison among three common commercialized batteries according to General Electronics Battery Co. (2006).

Table 1.2: Comparison among three common commercialize batteries.

Items	Li-ion	Ni-MH	Lead-acid
Working voltage (V)	3.7	1.2	2.0
Gravimetric energy density (Wh/kg)	130 – 200	60 – 90	30 – 40
Volumetric energy density (Wh/L)	340 – 400	200 – 250	130 – 180
Cycle life (cycles)	500	400	300
Capacity self discharge rate (% per month)	5 %	30 %	10 %
Memory effect	None	40 %	None
Energy efficiency ($C_{discharge}$ / C_{charge})	99 %	70 %	75 %
Weight comparison for the same capacity	1	2	4
Size comparison for the same capacity	1	1.8	3.5
Realiability	High	Low	High

The research about lithium-ion battery is not a new realm for researchers or batteries developers. In spite of that, researchers and batteries developers have continued their research in this field in order to produce better lithium-ion batteries. This interesting development of lithium battery has brought me to study in depth because it is the most popular amongst users and also has good characteristics compared to other batteries. Thus, this research will focus on the lithium-ion battery as the research subject.

Figure 1.2: Example of lithium-ion battery that was used in some devices nowadays.

1.2 OBJECTIVE

The first objective of this study is to develop a one-dimensional mathematical model for the lithium-ion battery that will be used to predict the intercalation behavior of lithium-ion in a lithium-ion battery. This is done by comparing latest development in modeling of lithium-ion battery and determining suitable model for this

This work focuses on modeling the lithium-ion concentration profiles inside separator and cathode of the lithium-ion battery. The second objective of this work is to solve the governing equations in the model. There are two approaches that may be used in dealing with this type of equation models. The two approaches are analytical approach and numerical approach. In this study a numerical approach called the Theta formulation under Finite Difference Method (FDM) will be used.

The third objective is to develop the coding for the FDM using Wolfram MATHEMATICA 8 software in order to solve the model equation. This would be a pilot study that uses Mathematica program code to solve diffusion problem in lithium-ion battery.

The fourth objective is to simulate and verify the results from this work with published results. This will be carried out by simulating the solution to the model equation and comparing it to the published results. Then various simulations to the solution of the model will be performed using various conditions and parameter values in order to further understand the concentration profiles of the lithium-ion inside the separator and cathode of lithium-ion battery.

1.3 THESIS ORGANIZATION

This thesis contains six chapters. Chapter 1 is the introduction. The chapter begins with some introduction on the interest and demand towards lithium-ion battery and will discuss on the current research background and objectives of this study.

Chapter 2 is the literature review. This chapter discusses on the basic and general knowledge of lithium-ion battery such as its physical and chemical processes. A reviews on previous studies related to this work is presented in this chapter.

Chapter 3 defines the problem statements of this work. Generally, this chapter discusses the development of the model for the diffusion process in a lithium-ion battery. This chapter starts with the derivation and development of the governing equation for the lithium-ion diffusion process including the initial and boundary conditions that is suitable for this work.

Chapter 4 presents the methodology used in this work. This chapter explains more in depth on the approaches used in this work, specifically on the Finite Difference Method. This chapter also discusses on the derivation of Theta formulation under FDM. Theta formulation allows the FDM to be divided into three familiar schemes under FDM; explicit scheme, implicit scheme and Crank Nicolson scheme. These three schemes are applied to the model discussed in Chapter 3 to obtain solutions to the model equations. Besides that, this chapter also shows the coding use in Wolfram Mathematica 8 to solve the model equations.

The results obtained in Chapter 4 are presented in Chapter 5. This chapter elucidates the best scheme in Theta formulation under FDM using some comparison and statistical test. The best scheme is then used to study the behavior of the lithium-ion battery under various conditions. The conditions that have been considered in this simulation work are discharge current (I), electrode porosity (ε), discharge time (τ) and different combination of separator/cathode thicknesses (L_s/L_c).

Finally, the last chapter (Chapter 6) is the conclusion chapter. This important chapter presents the conclusion of the results that were obtained in this work. This chapter ends with some suggestions for further work.

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