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Simplified Lithium-Ion Movement Simulation during Discharge Process

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Abstract. Research of lithium-ion battery (LIB) performance based on simulation has been carried out to calculate and optimize the battery performance parameters such as battery capacity, working potential, and discharge time. The simulation is carried out using electrochemical models, namely the Single Particle Model (SPM). This model's approach comes by observing the lithium diffusion process between the spherical electrode particles through a separator. From the SPM model, a simple mathematical equation has been derived that describes the electrochemical process that occurs inside the battery and also used to calculate the output of battery performance such as battery capacity, discharge time, and battery potential. Calculations are performed quickly on simple software such as Excel without reducing the accuracy of the output. Mathematical equations in the model gives profiles of lithium concentration, electrolyte concentration, and potential at the electrodes, as well as battery working potential compared to the battery capacity. The LIB type with LMO cathode in a pouch-cell was chosen as the initial reference for simulating battery performance. The calculation of the lithium concentration at the electrode gives value of the lithium concentration at the anode to decrease and the lithium concentration at the cathode to increase during the discharge process. The increase in the discharge current parameter in this calculation gives smaller discharge time value and lower battery capacity value (421s and 1.169 $mAh.cm^{-2}$ at 0.01 $mA.cm^{-2}$), while decreasing the discharge current value gives a higher time value. larger and larger rated battery capacity (13,360s and 1.855 $mAh.cm^{-2}$ at 0.0005 $mA.cm^{-2}$

INTRODUCTION

Devices applicated in information, communication and transportation fields are experiencing vast developments and are in accordance with the energy required to run these devices. Now, the energy supply for these devices can be stored in lithium-ion battery. Lithium-ion battery (LIB) opted as first choice of electrical energy storage devices for having several advantages such as high energy density, small size, and can be used repeatedly for long periods of time [1]. For this advantage reason, the demand for batteries in supplying energy for electronic devices is predicted to increase gradually every year [2].

Despite the high-demand prediction of LIB, there are still many developments needed to achieve better quality and quantity performance. Also, low lithium source in the world gives another thing to be concerned to make the lithium content inside the battery able to store energy in longer time and gives better performance even after hundreds of cycles [3]. Laboratory experimental research related to the materials for cathode-anode has been worked and published in many journals. This experimental based research is "trial and error" and there is yet exact composition which gives best performance, or in another word, refers to only one set of battery physical parameter

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data which is claimed to provide optimal battery performance. One way that can be done to complement this research is by modeling battery performance during the usage process [4].

The Single Particle Model (SPM) is one of the electrochemical models used to simulate movements of particles such as lithium-ion inside the cathode-anode-separator interface [5]. This model was derived from the pseudo 2D electrochemistry model (P2D). This SPM model was first published by Zhang et al. in 2000[11]. This model was developed based on 2 main assumptions. First, the electrode is assumed to be a spherical particle where lithium intercalation-deintercalation occurs during the charge-discharge process. Second, variations in electrolyte concentration in the separator are ignored so that the concentration values are assumed to be constant. Battery modeling using SPM has been published in various journals to predict electrochemical processes and LIB battery performance. This model mainly available as mathematical modelling using software which require high performance computer device, such as COMSOL Multiphysics or Matlab [8-10].

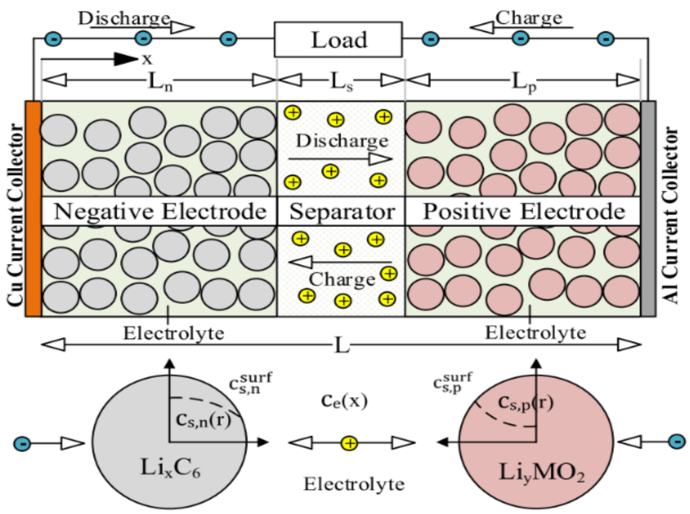


FIGURE 1. Schematic diagram of Pseudo 2D model derived from Single Particle Model (SPM)[13].

The aim of this study is to simplify equation used in modelling using SPM can be used in software which doesn't require high performance computer device like Microsoft Excel, without reducing the overall accuracy of modelling. The advantage of this model lies in its simple modeling, calculation and can be used to calculate various battery performance parameters such as capacity, voltage, usage life, to charge-discharge efficiency.

METHODOLOGY

The selection of the model used to be converted to Excel program refers to the model in a simulation study conducted by Henquin and Aguirre in 2014. The model specifications are summarized in **Table 1**. Parameter identification is carried out by collecting parameter data from a predetermined battery model. These parameters then matched with the variables in the mathematical equation at the main reference. The initial parameter values refer to the parameter data reported in the main reference, and other additional references. The partition diffusion distance parameter on the electrode is determined by manual calculation with the assumption that the partition volume of the electrode is the same.

The Excel worksheet design was carried out by dividing the simulation calculation into several parts, namely the calculation of lithium concentration, electrolyte concentration, overpotential profile, potential drop profile, pure electrode potential profile (the four calculations are for the cathode and anode), and the working potential profile of the battery. For this study, we only focused on calculation of lithium concentration. An example of the worksheet display that has been made is shown. The calculation of the concentration profile of lithium at the electrode is carried out using an equation which states the relationship between lithium concentration and discharge time.

$$C_{s,2}^{i} = C_{s,2}^{i,0} \pm j^{i} \frac{a_{2}^{i}}{v_{S}^{i}} \left[t + \frac{1 - \exp\left(-\frac{4D_{S}^{i}}{\left(\delta_{2}^{i} + \delta_{3}^{i}\right)} \frac{a_{1}^{i}}{v_{S}^{i}} t \right)}{\left(-\frac{4D_{S}^{i}}{\left(\delta_{2}^{i} + \delta_{3}^{i}\right)} \frac{a_{1}^{i}}{v_{S}^{i}} \right)} \right] \quad (1)$$

$$C_{s,1}^{i} = C_{s,1}^{i,0} \pm j^{i} \frac{a_{2}^{i}}{v_{S}^{i}} \left[t - \frac{1 - \exp\left(-\frac{4D_{S}^{i}}{\left(\delta_{2}^{i} + \delta_{3}^{i}\right)} \frac{a_{1}^{i}}{v_{S}^{i}} t \right)}{\left(-\frac{4D_{S}^{i}}{\left(\delta_{2}^{i} + \delta_{3}^{i}\right)} \frac{a_{1}^{i}}{v_{S}^{i}} \right)} \right] \quad (2)$$

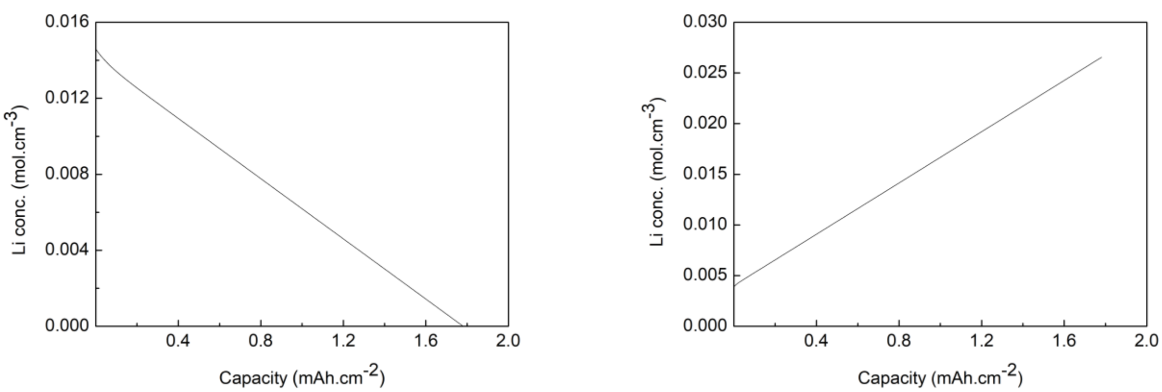
The discharge time of the battery in this simulation is defined as the discharge time when the lithium concentration value on the surface of the anode particles runs out or equal to 0. The t value that has been obtained is then used as a reference for the final state in calculating the output value of the next performance parameter.

TABLE 1. Selection for modelling used in this work.

Battery type	
Cathode material	Manganese Oxide (LMO)
Anode material	Graphite
Electrolyte	$LiPF_6$
Cell type	Pouch cell
Modelling type	
Electrochemical model	SPM – Pseudo 2D model
Software	Excel

RESULTS AND DISCUSSION

The lithium concentration profile at the two electrodes in the battery is plotted to identify the diffusion process that occurs in the battery during the discharge process [7]. In the discharge process, the battery is connected to electronic equipment thus forming a closed circuit. Under these conditions, the lithium particles are being intercalated from the anode of the battery and will lose electrons through the electric circuit to the cathode, while Li^+ ions will move past separator towards the cathode, thereby recapturing the electrons released at the anode and the lithium intercalation process occurs on the cathode surface. This process generates electric current as energy to run various devices electronic.



(a) (b)

FIGURE 2. Lithium concentration profile on the (a) anode; (b) cathode based on simulation result (C_{anode} = 0.015 mol.cm^{-3}, $C_{cathode}$ = 0.004 mol.cm^{-3} , i = 0.0015 mA.cm^{-2})

The phenomenon of lithium concentration change during the process is observed in the simulation results depicted in **Figure 2**. From the picture it is observed that there is a decrease in value concentration of Li on the surface of the anode during the discharge process, and the increase at the cathode. Variation of initial lithium concentration parameter value and discharge currents were also generated similar profile, where the decreasing of Li concentration at the anode and increasing at cathode during discharge. This result is agreed with other scientific publications in other journals discussing the concentration profile of Li in electrode [9,12]. There seems to be a similar trend decrease in the concentration value at the anode and increase in value at the cathode at the value different initial parameters with the literature. Based on this comparison, the Li concentration profile calculation worksheet that has been made has been successfully simulated concentration of Li on the electrode well.

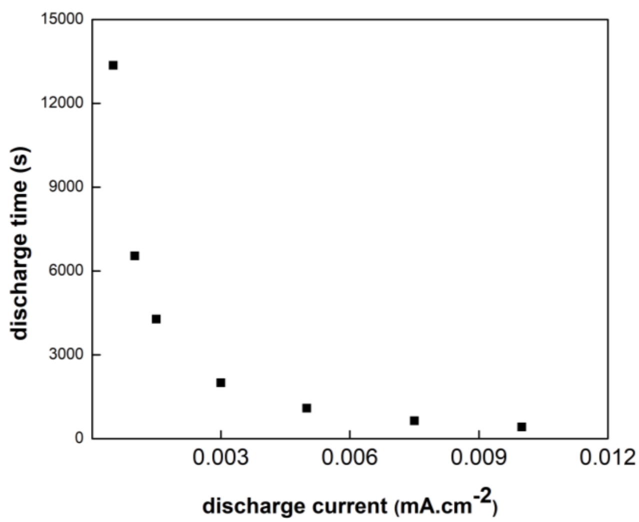


FIGURE 3. Profile of discharge time to discharge rate of the resulted simulation.

The discharge current in the simulation is then varied to simulate the effect on the value of battery capacity and battery discharge time. **Figure 3** shows that an increase in the current value causes the discharge time to become faster. High discharge current provides more energy for Li particles so that they can diffuse faster from the anode to the cathode so that shorter battery usage time. However, this phenomenon causes the value of the battery capacity to be lower, which can be seen in **Figure 4**. The increase in current results in a lower battery capacity. The use of high currents in the discharge process results in conversion other energy in the form of heat in the battery which reduces the energy efficiency of Li particle diffusion. This phenomenon is known as "bloat" in batteries with condition of decreased capacity and the battery becomes easily hotter.

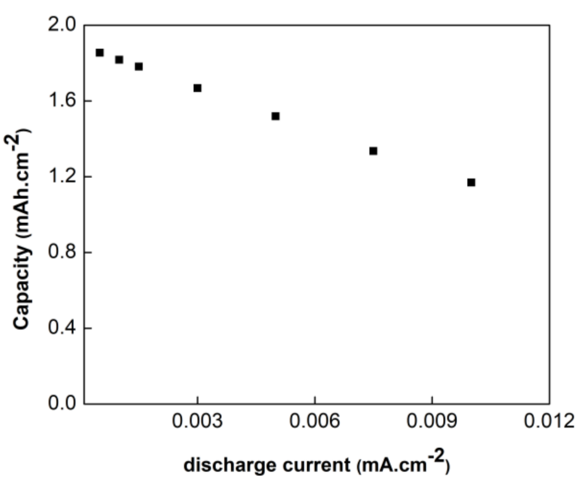


FIGURE 4. Profile of capacity to discharge rate of resulted simulation.

CONCLUSION

In this study, a simulation calculation tools has been successfully created to simulate LIB performance in the form of discharge time, battery capacity, and working potential of battery design parameters, electrode composition, and parameters battery operation. The results of calculations using the initial parameters provide profiles that gives resemblance to the calculations published in other studies addressing the performance of lithium-ion batteries with using different parameters. The simulated lithium concentration profile resulting in values that decrease in the anode component and increase in cathode component, which describes the process of diffusion of lithium ions from the anode to the cathode during the discharge process. This lithium concentration profile as well depending on the amount of lithium intercalated at the anode and cathode before the discharge process is carried out, as well as the discharge current used.

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