Chapter 6

CONCLUSION

6.1 CONCLUSION

The research work is conducted with the objective of obtaining the profile for concentration of lithium-ion battery during discharge process under various conditions. A part of that, the material balance equation governing the lithium-ion concentration in the electrolyte/solution phase of a lithium-ion battery was solved using Theta formulation under Finite Difference Method subject to certain initial and boundary conditions. The Wolfram MATHEMATICA 8 software is used as a tool to solve the material balance equation. The material balance equation governing the lithium-ion concentration in the electrolyte/solution phase of a lithium-ion battery according to Theta formulation for separator is defined as follows

$$-\alpha\frac{k}{h^2}\vartheta_{j+1}^{i+1}+\left(1+2\alpha\frac{k}{h^2}\right)\vartheta_{j+1}^{i+1}-\alpha\frac{k}{h^2}\vartheta_{j-1}^{i+1}=(1-\alpha)\frac{k}{h^2}\vartheta_{j+1}^{i}+\left[1-2(1-\alpha)\frac{k}{h^2}\right]\vartheta_{j+1}^{i}+(1-\alpha)\frac{k}{h^2}\vartheta_{j-1}^{i}$$

---------(6.1)

and for cathode is as follows

$$-\alpha\varepsilon^{1/2}\frac{k}{h^2}\vartheta_{j+1}^{i+1}+\left(1+2\alpha\varepsilon^{1/2}\frac{k}{h^2}\right)\vartheta_{j+1}^{i+1}-\alpha\varepsilon^{1/2}\frac{k}{h^2}\vartheta_{j-1}^{i+1}=$$

$$(1-\alpha)\varepsilon^{1/2}\frac{k}{h^2}\vartheta_{j+1}^{i}+\left[1-2(1-\alpha)\varepsilon^{1/2}\frac{k}{h^2}\right]\vartheta_{j+1}^{i}+(1-\alpha)\varepsilon^{1/2}\frac{k}{h^2}\vartheta_{j-1}^{i}+kJ$$

---------(6.2)

The equations for Theta formulation (equation 6.1 and equation 6.2) provide us three difference schemes that is explicit scheme $(\alpha = 0)$, implicit scheme $(\alpha = 1)$ and Crank Nicolson $(\alpha = 0.5)$ scheme. These three schemes were tested using significant test or known as *t*-test in order to prove there is no significant difference between these three schemes with published analytical result. The *t*-test shows that there are no significant differences (within 95% confidence interval) between these three schemes with published analytical result.

Then, the Root Mean Square Error (RMSE) and Mean Absolute Error (MAE) are used in order to evaluate the effectiveness and accuracy of the profiles of lithium-ion concentration calculated from this work compared to published analytical result. Computational time needed by Wolfram Mathematica 8 software to solve the equation also recorded to identify the fastest schemes based on the same style of computer coding from Theta formulation.

Then using the best scheme from Theta formulation, the profile for lithium-ion concentration in the electrolyte/solution phase of a lithium-ion battery was simulated under various conditions. The conditions that are being considered in this simulation work are discharge current (I), electrode porosity (ε), discharge time (τ) and different combination of separator/cathode thicknesses. These simulations are able to provide information and understanding in the reaction and performance inside the separator and cathode.

From the results of this study, it can be concluded that:

(a) Despite the FDM is one of the methods under numerical approach (generally known as approximation approach) but the result in graphically comparison with published analytical result, RMSE, MAE and significant test shows that FDM has high accuracy towards analytical approach. Hence, FDM can be one of the alternative ways in order to solve the material balance equation governing the lithium-ion concentration in the electrolyte/solution phase of a lithium-ion battery.

(b) According to RMSE, MAE and computational time needed to solve the equation, an implicit scheme is the best scheme in Theta formulation for the material balance equation in this work.

(c) Wolfram MATHEMATICA 8 software is the most efficient and practical as a tool to solve the material balance equation in this work. This is because the Wolfram MATHEMATICA 8 software did not take much time to compute the result. The Wolfram MATHEMATICA 8 software not only able to solve the material balance equation from Theta formulation and present the graphical result but also able to perform the result for statistical test such as significant test (*t*-test), RMSE and MAE.

(d) From the simulation of the concentration profile for lithium-ion in lithium-ion battery, the following results are observed; the lithium-ion deplete slower

- when the discharge current lower
- when the discharge time shorter
- in the higher electrode porosity
- when thickness of cathode is larger than that of separator

Overall, this study has succeeded in achieving two main objectives that is to solve the material balance equation governing the lithium-ion concentration in the electrolyte/solution phase of a lithium-ion battery and to study the behavior of lithium-ion concentration under various conditions. The development of the model for this work have been done in chapter 3, the derivation for Theta formulation are shown in chapter 4 and the result and discussion about the simulation graph are done in chapter 5.

6.2 SUGGESTION FOR FUTURE WORK

The model that has been developed in this work is only considered solution-phase concentration in separator and cathode. Thus the model can be extended in order to study the behavior of full cell, solid-phase part and more including its electrochemical and thermal parts. The Theta formulation can be applied to this new extended model in order to approve the accuracy of Theta formulation towards various battery models. Besides that this study also did not consider the specific material of the anode or cathode. Hence, the model can also be extended to study the effect of the different cathode or separator materials. For example, the $LiFePO_4$ is one of the potential cathode materials that have high demand in the industry now. The Wolfram MATHETMATICA software 8 used in this work as a tool can be developed and applied in MATHEMATICA GUI system to make it more user friendly. Hence, it is suggested that further work should be done to develop Wolfram MATHEMATICA 8 coding in MATHEMATICA GUI for various battery models that will consider full cell model, solid-phase part and more about its electrochemical and thermal parts to make it easy for user to understand the battery performance.