

8-1-2017

## Mathematical Modeling of Charge and Discharge Process in Lithium Ion Batteries Using COMSOL Multiphysics

Azeez A. Barzinjy Mr.

*Department of Physics, College of Education, Salahaddin University-Erbil, Erbil-Iraq*

Kadhim Q. Jabbar Mr.

*Department of Physics, College of Education, Salahaddin University-Erbil, Erbil-Iraq*

Haidar J. Ismael Mr.

*Department of Physics, College of Education, Salahaddin University-Erbil, Erbil-Iraq*

Mohammed A. Hamad Mr.

*Department of Physics, College of Education, Salahaddin University-Erbil, Erbil-Iraq*

Samir M. Hamad Mr.

*Department of Mathematics Soran University, Faculty of Science, Erbil, Iraq*

Follow this and additional works at: <https://polytechnic-journal.epu.edu.iq/home>

### How to Cite This Article

Barzinjy, Azeez A. Mr.; Jabbar, Kadhim Q. Mr.; Ismael, Haidar J. Mr.; Hamad, Mohammed A. Mr.; and Hamad, Samir M. Mr. (2017) "Mathematical Modeling of Charge and Discharge Process in Lithium Ion Batteries Using COMSOL Multiphysics," *Polytechnic Journal*: Vol. 7: Iss. 4, Article 7.

DOI: <https://doi.org/10.25156/ptj.2017.7.4.91>

This Research Article is brought to you for free and open access by Polytechnic Journal. It has been accepted for inclusion in Polytechnic Journal by an authorized editor of Polytechnic Journal. For more information, please contact [karwan.qadir@epu.edu.iq](mailto:karwan.qadir@epu.edu.iq).

---

# Mathematical Modeling of Charge and Discharge Process in Lithium Ion Batteries Using COMSOL Multiphysics

## Abstract

Rechargeable lithium-ion batteries are remarkable nominees for application into new large-scale energy storage requests, such as hybrid and electric vehicles, as a result of their high energy density. We present here a comprehensive dynamic model which is suitable for studying the charge and discharge systems in the Lithium-Ion Battery. The chosen geometry in this study is in one dimension and the model is isothermal. In this case carbon material represents the negative electrode and lithium manganese oxide (LiMn<sub>2</sub>O<sub>4</sub> spinel) indicates the positive electrode. In addition, in the proposed model the diffusion coefficient of Li ions in its solid state and electrolyte, the electrochemical reaction's rate constants, the thermal conductivity of the binary electrolyte rely on the temperature. In this investigation, COMSOL Multiphysics is utilized to investigate Lithium-Ion battery model reliant on dilute electrolyte principle and rapid diffusion of lithium in the electrode fragment. This modeling can offer appreciated understandings into the fundamental defect and ion transport properties of electrode materials at the atomic scale, which are vital for a full appreciative of lithium battery function. Modeling founding for a lithium-ion battery are presented and compared to experimental data. Good agreement exists for both charge and discharge between theory and the outcome of this study for numerous investigational cell configurations. This mathematical model specifies that the battery in its existent design is ohmically restricted.

## Keywords

Li-Ion Batteries; Rechargeable Batteries; LiMn<sub>2</sub>O<sub>4</sub>; Electrochemical Model; COMSOL Multiphysics



---

## Mathematical Modeling of Charge and Discharge Process in Lithium Ion Batteries Using COMSOL Multiphysics

Azeez A. Barzinjy<sup>1,2\*</sup>, Kadhim Q. Jabbar<sup>1</sup>, Haidar J. Ismael<sup>1</sup>

Mohammed A. Hamad<sup>1</sup>, Samir M. Hamad<sup>3</sup>

<sup>1</sup>Department of Physics, College of Education, Salahaddin University-Erbil, Erbil-Iraq.

<sup>2</sup>Department of Physics Education, Faculty of Education, Ishik University, Erbil-Iraq.

<sup>3</sup>Department of Mathematics Soran University, Faculty of Science, Erbil, Iraq.

---

### ABSTRACT

*Rechargeable lithium-ion batteries are remarkable nominees for application into new large-scale energy storage requests, such as hybrid and electric vehicles, as a result of their high energy density.*

*We present here a comprehensive dynamic model which is suitable for studying the charge and discharge systems in the Lithium-Ion Battery. The chosen geometry in this study is in one dimension and the model is isothermal. In this case carbon material represents the negative electrode and lithium manganese oxide (LiMn<sub>2</sub>O<sub>4</sub> spinel) indicates the positive electrode. In addition, in the proposed model the diffusion coefficient of Li ions in its solid state and electrolyte, the electrochemical reaction's rate constants, the thermal conductivity of the binary electrolyte rely on the temperature.*

*In this investigation, COMSOL Multiphysics is utilized to investigate Lithium-Ion battery model reliant on dilute electrolyte principle and rapid diffusion of lithium in the electrode fragment. This modeling can offer appreciated understandings into the fundamental defect and ion transport properties of electrode materials at the atomic scale, which are vital for a full appreciative of lithium battery function. Modeling founding for a lithium-ion battery are presented and compared to experimental data. Good agreement exists for both charge and discharge between theory and the outcome of this study for numerous investigational cell configurations. This mathematical model specifies that the battery in its existent design is ohmically restricted.*

**Key words:** *Li-Ion Batteries; Rechargeable Batteries; LiMn<sub>2</sub>O<sub>4</sub>; Electrochemical Model; COMSOL Multiphysics.*

---

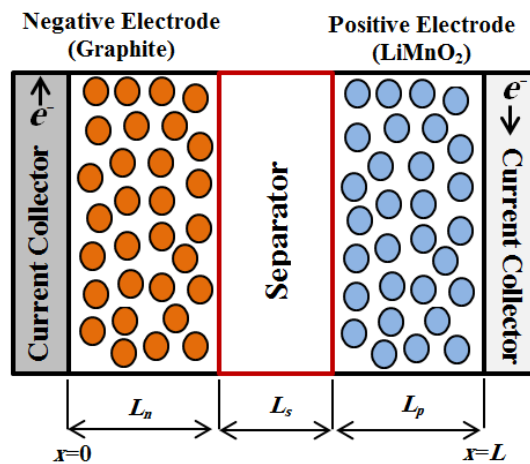
## INTRODUCTION

Batteries have attracted progressively more consideration in recent years. They are now frequently utilized for energy storage in a numeral of electronic devices(Larcher and Tarascon, 2015). Recently rechargeable lithium ion batteries are utilized in cell phones, tablet and laptop computers in addition to in electric or hybrid electric ambitious vehicles(Peiró et al., 2013). The geometrical size and the life time capacity of the batteries differ with the application, because they possess the highest energy density of any rechargeable battery. Even though modern Li battery technologies have been effectively applied into a number of hybrid-electric and fully electric vehicles, there are numerous technological difficulties to overcome before they can be integrated sustainably. The main growth obstacle is a lack of good electrode materials and electrolytes, which can present problems regarding safety, cost and life cycle mainly when scaled up to come across the stresses of powering vehicles. Novelty is therefore essential from materials chemists to produce more effective and sustainable electrode materials (Skylas-Kazacos et al., 2011).

It can be noted that, lithium was first utilized as an anode material in batteries in the 1970's. It is both the most electro-positive and the lightest metal in the periodic table, which facilitates fabrication of cells with high energy density. Initially, lithium cells were primary, and were preferably suited to low power applications which required long functioning times, such as watches, calculators and a selection of small medical devices. Nevertheless, around the same time numerous intercalation materials were discovered, which allowed reversible supplement and extraction of Li ions; this motivated research towards the development of rechargeable lithium batteries (Liang et al., 2012, Cheng et al., 2011).

Similar to all batteries, lithium ion batteries are comprised of two electrodes, the anode and cathode, separated by an electrolyte which needs to be a good ionic conductor but an electronic insulator (Winter and Brodd, 2004).

The anode and cathode possess different chemical potentials, which rely upon the chemistry that occurs at each. A schematic of Li-ion battery operation is provided in **Figure 1**.



**Figure 1.** Diagram of Li-ion cell sandwich consisting of composite negative and positive electrodes and separator (Fu et al., 2015).

To stop a short circuit both electrodes must be separated, thus a thin absorbent material is inserted between them to maintain them apart (Mayo, 1972).

The electrolyte has the vital role of enabling transport of Li ions between the anode and cathode over this absorbent separator. It must be an exceptional ionic conductor but an electronic insulator; otherwise the cell would short circuit.

The electrolyte is normally lithium salt  $\text{LiPF}_6$  liquefied in an organic solvent. Existing electrolytes are thermodynamically steady up to 3.5V; at voltages greater than this the electrolytes decompose through oxidation reactions. Luckily recent electrolytes possess high kinetic steadiness so are capable to work well outside of this steadiness window, at voltages as high as 5.5 V (Subbarao, 2012).

Nevertheless, even though electrolyte decomposition is slow, it still occurs constantly during the lifetime of the cell producing a slow decline in enactment. Preferably we have a desire for electrolytes with much higher thermodynamic steadiness, which do not damage at all, even in very high voltage cells.

Regarding the anode it is significant that the anode material has a low potential *vs.*  $\text{Li/Li}^+$  and that Li ions can be constantly introduced and extracted from the material during cycling. As pointed out before, Li metal was initially utilized as the anode material, but dendritic growth caused by continuous re-plating of its surface during cycling, produced serious safety concerns. This was luckless as Li metal has a higher capacity than any of its possible alternatives, and for this reason investigation into Li metal anodes is still energetic (Lee et al., 2011).

The recent anode material is graphite, which permits lithium to be inserted between the carbon layers (Endo et al., 2000). Graphite possesses many benefits, being inexpensive, readily obtainable and an exceptional electronic conductor. Even though, there has been ongoing investigation efforts focused on developing anodes with higher capacities (Brownson et al., 2011).

The cathode material is at present the obstacle for battery improvement, since cathode materials normally possess much lower capacities than the anodes. Based on the existing researches, there are two main cathode structures which oversee in commercial lithium cells: these are  $\text{LiMO}_2$  (where  $M = \text{V, Cr, Mn, Fe, Co, Ni}$ ) layered and  $\text{LiMn}_2\text{O}_4$  spinel (Molenda and Marzec, 2009). The spinel structure consists of an array of cubic close-packed oxide ions with Mn ions in half of the octahedral sites. The  $\text{Mn}_2\text{O}_4$  outline provides a series of tunnels which pass across in all three dimensions, enabling fast lithium migration (Meng and Arroyo-de Dompablo, 2012). Contrary to the layered materials site disorder is unseen in  $\text{LiMn}_2\text{O}_4$ ; this is caused by its greater structural rigidity which makes its tunnels more selective to the small lithium ions (Meng and Arroyo-de Dompablo, 2012). Lithium can be introduced into the material to an extreme composition of  $\text{Li}_2\text{Mn}_2\text{O}_4$ .

Modeling and simulations are essential tools for quicker sympathetic, design optimization, and design of spontaneous control of batteries and battery systems. They permit for the analysis of an almost limitless number of design parameters and functional conditions to a reasonably small cost.

The utilized simulation in this investigation requires a mathematical model that is sophisticated sufficiently to describe the presented system properly. A general mathematical model has been

settled to simulate the lithium-ion cell (Fuller et al., 1994) although, the challenging of this model against experimental discharge curves has been unfulfilled by the lack of all of the necessary experimental data. Battery developers can utilize the 1D isothermal model to examine the effect of numerous design parameters for instance the optimal materials, sizes, and the particle dimension distribution of the dynamic materials, in this case carbon material in the negative electrode and lithium manganese oxide (LiMn<sub>2</sub>O<sub>4</sub> spinel) in the positive electrode.

## THEORY

As lithium ions travel (**Figure 1**), along with an electrochemical reaction, from the host material in one electrode to the other, numerous procedures associated with mass transport in electrolyte and active material particles, electrochemical reaction, and electron conduction take place. The procedures can all be investigated with the assistance of four key coupled differential equations that have been widely used. These determine the spatial variation of potential and concentration in the solid and electrolyte phase with time or frequency (Meyers et al., 2000).

Three of the equations are solved through the battery domains *i.e.* electrodes, separator, and current collectors, and the one describing mass transport in active material over the thickness of the active material particle (**Figure 1**).

In the last two decades, numerous methods have been described in literature starting with the effort of Doyle based on the theory of porous electrodes (Doyle et al., 1996). This theory is based on an electrochemical explanation of diffusion dynamics and charge transfer kinetics of a battery and can provide a prediction of the electric response of a cell in an intercalation electrode system. This model, perhaps, is suitable for small battery systems.

Doyle *et al.* (Doyle et al., 1996) presented a model for a lithium-ion battery that was applied by considering 1D transport for a galvanostatic current. It was found that the reduced lithium concentration in the composite cathode illustrated the need for higher lithium concentrations.

The subsequent equations express the function of lithium-ion batteries. In these equations LiMO<sub>2</sub> metal oxide indicates cathode materials, whereas graphite is typically used as the anode material (Fu et al., 2015).

Reaction at the positive electrode of Li-Ion cells:



Reaction at the negative electrode of Li-Ion cells:



Summary reaction:



It is significant to define correctly the chemical processes mathematically. The output can be the charging and discharging curves, the concentration profiles of electrolyte during charging and discharging, state of charge characteristic. The mathematical model (Doyle et al., 1996) can be divided into the separator and two composite electrode regions. In the solution phase of each of the composite electrodes the equations are:

$$\varepsilon \frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c) - \frac{i_2 \cdot \nabla t_{\pm}^0}{F} + a j_n (1 - t_{\pm}^0) \quad (4)$$

where  $\varepsilon$  is a porosity,  $c$  is a concentration of salt,  $t$  is a time,  $D$  is a salt diffusion coefficient,  $F$  is a Faraday's constant,  $i_2$  is an exchange current density for the insertion process,  $t_{\pm}^0$  is a maximum concentration in intercalation material,  $a$  is a specific interfacial area and  $j_n$  pore-wall flux across interface.

$$i_2 = -k \nabla \phi_2 + \frac{2kRT}{F} \left( 1 + \frac{\partial \ln f_{\pm}}{\partial \ln c} \right) (1 - t_{\pm}^0) \nabla \ln c \quad (5)$$

Where  $k$  is an electrical conductivity of the electrolyte,  $\phi_2$  is a second electrical potential,  $R$  is a universal gas constant,  $T$  is an absolute temperature,  $f_{\pm}$  is an activity coefficient of the salt, and  $t_{\pm}^0$  is transference number of the species.

$$a j_n = \frac{1}{F} \nabla \cdot i_2 \quad (6)$$

In the solid phase of the composite electrodes

$$i_1 = -\sigma \nabla \phi_1 \quad (7)$$

Where  $\sigma$  is an electrical conductivity of the solid matrix and  $\phi_1$  is a first electrical potential.

$$\frac{\partial c_s}{\partial t} = D_s \left[ \frac{\partial^2 c_s}{\partial r^2} + \frac{2}{r} \frac{\partial c_s}{\partial r} \right] \quad (8)$$

Where  $c_s$  is a concentration of lithium in solid phase,  $D_s$  is a diffusion coefficient of lithium in the solid matrix and  $r$  is a distance normal to surface of cathode material.

These two phases are related through the boundary condition

$$j_n = -D_s \frac{\partial c_s}{\partial r} \text{ at } r = R_s \quad (9)$$

where  $R_s$  is a radius of cathode material, as well as a Butler-Volmer kinetics expression

$$j_n = k(c)^{1/2} (c_t - c_s)^{1/2} (c_s)^{1/2} \left\{ e^{\left(\frac{F}{2RT}(\eta-U)\right)} - e^{\left(-\frac{F}{2RT}(\eta-U)\right)} \right\} \quad (10)$$

where  $U$  is an open-circuit potential, and the electrode potential  $\eta$  is defined as:

$$\eta = \phi_1 - \phi_2 \quad (11)$$

Where  $\phi_1$  and  $\phi_2$  are electrical potentials of the solid electrode particle and electrolyte, respectively and the reaction rate parameter  $k$  represents the product of the forward and backward rate constants, each raised up to a power contingent on the transfer coefficients, for the charge-transfer reaction at the electrode surface. This parameter is related to the exchange current density through:

$$i_o = Fk(c)^{1/2} (c_t - c_s)^{1/2} (c_s)^{1/2} \quad (12)$$

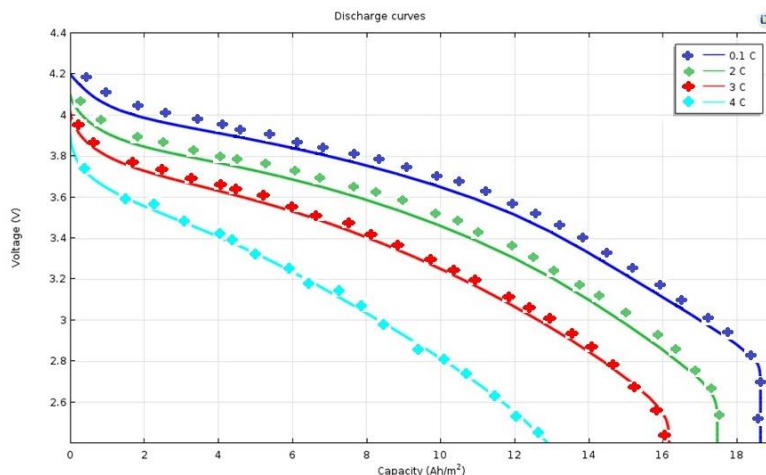
Where  $i_o$  is the exchange current density,  $c_t$  and  $c_s$  are the concentration of lithium in solution and solid phase. In the separator region equations (4) and (5) apply with  $j_n = 0$  and  $\varepsilon = 1$ . These equations are linearized and solved all together in Ref. (Baker et al., 1991). There are two independent variables ( $x$  and  $t$ ) and six dependent variables ( $c$ ,  $c_s$ ,  $\phi_1$ ,  $\phi_2$ ,  $i_2$  and  $j_n$ ). Extra details

of the equations and boundary conditions solved, along with the details of the solution processes, can be found in (Baker et al., 1991).

## RESULTS AND DISCUSSION

As soon as the electrodes are connected through an external circuit, the redox reactions at the electrodes proceed spontaneously. Electrons flow from the anode, round the external circuit to the cathode; alongside an equivalent number of Li ions are transported across the electrolyte before inserting into the cathode, thus keeping the charge balance (Santhanagopalan et al., 2014). Charging the cell requires applying a higher external potential in the opposite direction, forcing the inverse process.

In **Figure 2** the cell potential is assumed as a function of the capacity of discharges at different rates. The markers are experimental data; the solid lines are simulation results. The capacity at 0.1 C, Columb, which reaches the maximum capacity for this cell, is 18.5 Ah/m<sup>2</sup>. Butler-Volmer kinetics equations, namely equation 10 and 11, are utilized to study the discharge curves given in **Figure 2** at 0.1, 2, 3, and 4C. The discharge time for 0.1C is 2000s. Similar trend obtained by Vyroubal *et al.* (Vyroubal et al., 2014) in their study regarding the concentration profiles of electrolyte during charging and discharging in Li ion batteries. The experimental data were taken from a cell that was about five cycles into its life where the behavior of the cell (*i.e.*, capacity) fundamentally had become constant. Since the cell is negative-electrode restricted on discharge at low rates, the cell capacity is determined by the primary state of charge of the negative electrode.



**Figure 2.** Cell potential vs. attainable capacity for cell at various discharge rates.

The demonstrated cell voltage could well describe the measured cell voltage for a Li-ion battery, by fitting of the cell parameters related to local and current-collector resistances. The fitted and measured cell voltages are presented in **Figure 3**. To plot **Figure 3** across 8000 s the authors utilized the data in **Figure 2** only 0.1C discharge process has been chosen since this discharge rate gave the highest cell potential. The calculated contributions to the polarization are also demonstrated. Presumably, the mass transport limitations are hence contributed to the polarization observed in **Figure 3** during that period of the limited cycle. This behavior agrees well with the results obtained by Ji *et al.* (Ji et al., 2013). They showed that in similar optimization of cell design considerations and material properties for 1 C rate discharge. Ji *et al.* indicates that the enactment restrictions are found to be Li<sup>+</sup> diffusion in the electrolyte and solid-



state Li diffusion in graphite particles, rather than charge-transfer kinetic or ohmic resistance. Our simulation gives an understanding in the dynamics of the procedures and in possible limitations but is not enough to tell the significance of the separate procedures in terms of polarization.

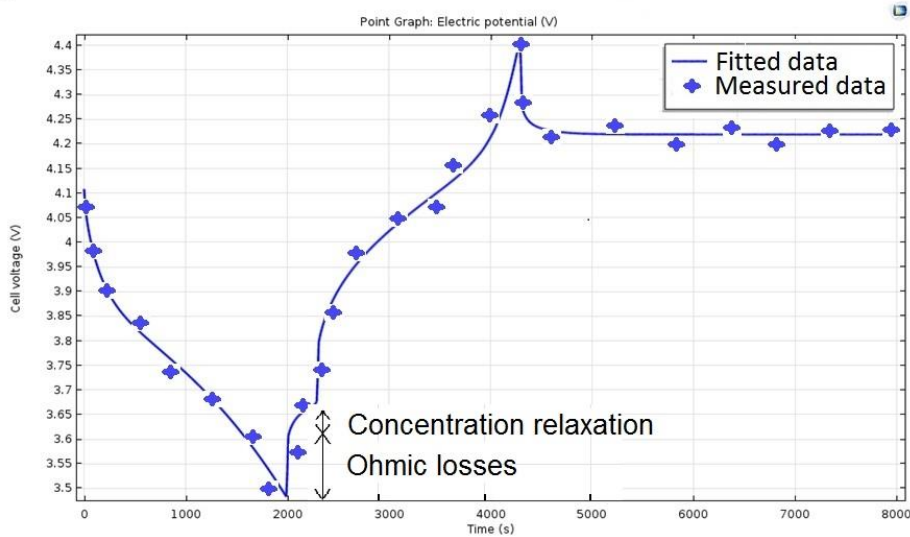


Figure 3. The cell voltage during 0.1C discharge process.

Throughout both discharge and charge process, the cell voltage displays ohmic losses of nearly 100 mV and a concentration over-potential of around 50 mV. These losses are obviously noticeable in **Figure 3** when the current is set to 0, where one can perceive an instant relaxation of the voltage as a result of the relaxation of ohmic losses followed by a slower relaxation of the concentration over-potential.

The intended polarizations in the cell throughout the limited cycles are presented in **Figure 3** between the cell voltage and equilibrium cell voltage. The contributions vary with time. In the beginning the polarization is dominated by the contact resistance, the ohmic potential fall in the electrolyte and the activation over-potential. The contact resistance is constant at the given current, whereas the ohmic potential drop rises to some extent with time during each current step as the reaction zone moves deeper into the electrodes towards the current collector. The activation over-potential is relatively constant with time throughout each current step. On the other hand, the two diffusion polarizations display enormous variation with time.

The simulations were also performed with the current load profile with a constant current density of  $i = \pm 16 \text{ A/m}^2$  as seen in **Figure 4**. The relaxation periods of 250s between charging and discharging pulses can be seen also in **Figure 4**. Melcher *et al.* (Melcher et al., 2016) showed relaxation periods of 250s between charging and discharging pulses, with a complete current cycle lasts 500 s and 1000 s. In spite of the fact that the advantages of this model in the spatial resolution are not used in this work, it is the intention of the authors to consider covering a wider range of time *i.e.* 8000s.

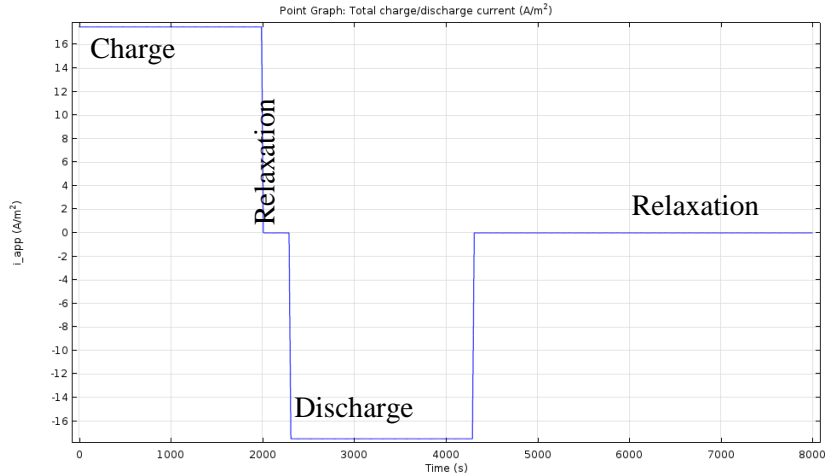


Figure 4. First 8000 s of the current load profile with relaxation times of 250 s between charging and discharging pulses.

The concentration of Li-ion in the electrolyte, illustrated in **Figure 5**, varies locally for most time steps. This is a significance of limitations in mass transport affected by the current in the electrolyte being only partly carried by the Li-ion and being hindered by diffusion. During the periods of non-zero current the concentration profiles build up. In contrast, once the current is switched off, both the concentration profiles and cell voltage relax towards equilibrium. A similar process takes place in the active material. In a comparable attempt Yu *et al.* (Yu et al., 2013) using  $\text{LiFePO}_4$  showed, experimentally, that the slope of the lithium-ion concentration rises with increasing electrode thickness as the transport of the lithium ions in the electrolyte phase turn out to be limited in the thick electrodes.

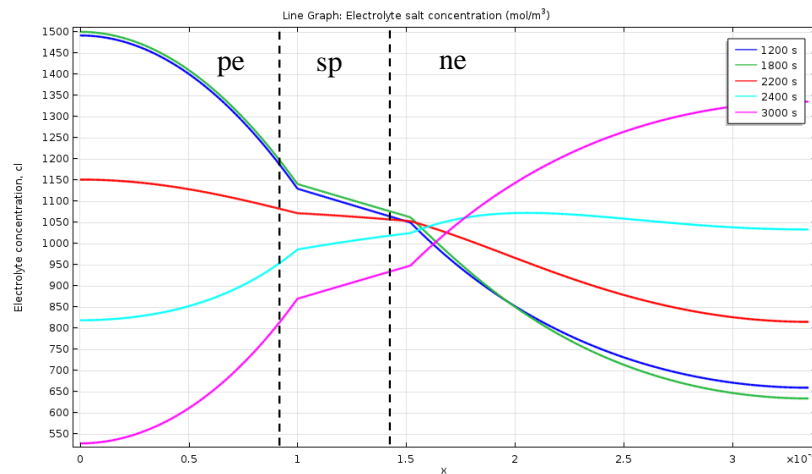


Figure 5. Electrolyte concentration profiles at various time during charge and discharge process.

**Figure 5** shows electrolyte concentration profile in the innermost layer of the battery at various time during charge and discharge process. It can be noted that, the presented data in **Figure 5** agrees well with the experimental results (Doyle et al., 1996). The low lithium-ion concentration in the cathode, beside the high concentration in the anode, detected in the thick electrodes leads to extra voltage drops that reduced the discharge capacity.

## CONCLUSION

To sum up, it was our major interest in this study to effectively simulate  $\text{LiMn}_2\text{O}_4$  cathode with the lithium-ion battery interface. Associated with the real battery discharge curves, the simulated discharge results not only show similar curves, but also explain the Li distribution in the active material particle phase and electrolyte phase. This illustration describes that Li concentration increases throughout discharge at the cathode. The  $\text{LiMn}_2\text{O}_4$ /graphite lithium-ion batteries with these electrode proposal parameters were perceived to possess area explicit discharge capacities  $\sim 18.5 \text{ Ah/m}^2$  using a 0.1 C current rate. Moreover, the model joins a side-reaction term in the constant-current constant-voltage battery test. This term causes a slow battery voltage decrease throughout charge and discharge. This conclusion is appear to agree well with the experimental data in terms of discharge process, but variations are essential meanwhile the charge process in the experiment displays dissimilar tendency associated with the model.

## ACKNOWLEDGEMENTS

The authors would like to express their acknowledgement to the Salahaddin University for supporting them with available tools. If anyone who needs the details regarding COMSOL model please contact the corresponding author for any additional help.

## REFERENCES

1. BAKER, D. R., VERBRUGGE, M. W. & NEWMAN, J. 1991. A transformation for the treatment of diffusion and migration. Application to stationary disk and hemisphere electrodes. *Journal of electroanalytical chemistry and interfacial electrochemistry*, 314, 23-44.
2. BROWNSON, D. A., KAMPOURIS, D. K. & BANKS, C. E. 2011. An overview of graphene in energy production and storage applications. *Journal of Power Sources*, 196, 4873-4885.
3. CHENG, F., LIANG, J., TAO, Z. & CHEN, J. 2011. Functional materials for rechargeable batteries. *Advanced Materials*, 23, 1695-1715.
4. DOYLE, M., NEWMAN, J., GOZDZ, A. S., SCHMUTZ, C. N. & TARASCON, J. M. 1996. Comparison of modeling predictions with experimental data from plastic lithium ion cells. *Journal of the Electrochemical Society*, 143, 1890-1903.
5. ENDO, M., KIM, C., NISHIMURA, K., FUJINO, T. & MIYASHITA, K. 2000. Recent development of carbon materials for Li ion batteries. *Carbon*, 38, 183-197.
6. FU, R., CHOE, S.-Y., AGUBRA, V. & FERGUS, J. 2015. Development of a physics-based degradation model for lithium ion polymer batteries considering side reactions. *Journal of Power Sources*, 278, 506-521.
7. FULLER, T. F., DOYLE, M. & NEWMAN, J. 1994. Simulation and optimization of the dual lithium ion insertion cell. *Journal of the Electrochemical Society*, 141, 1-10.
8. JI, Y., ZHANG, Y. & WANG, C.-Y. 2013. Li-ion cell operation at low temperatures. *Journal of The Electrochemical Society*, 160, A636-A649.
9. LARCHER, D. & TARASCON, J.-M. 2015. Towards greener and more sustainable batteries for electrical energy storage. *Nature chemistry*, 7, 19-29.
10. LEE, J. S., TAI KIM, S., CAO, R., CHOI, N. S., LIU, M., LEE, K. T. & CHO, J. 2011. Metal-air batteries with high energy density: Li-air versus Zn-air. *Advanced Energy Materials*, 1, 34-50.

11. LIANG, Y., TAO, Z. & CHEN, J. 2012. Organic electrode materials for rechargeable lithium batteries. *Advanced Energy Materials*, 2, 742-769.
12. MAYO, A. M. 1972. Fuel cell battery. Google Patents.
13. MELCHER, A., ZIEBERT, C., ROHDE, M. & SEIFERT, H. J. 2016. Modeling and simulation the thermal runaway behavior of cylindrical li-ion cells—Computing of critical parameter. *Energies*, 9, 292.
14. MENG, Y. S. & ARROYO-DE DOMPABLO, M. E. 2012. Recent advances in first principles computational research of cathode materials for lithium-ion batteries. *Accounts of chemical research*, 46, 1171-1180.
15. MEYERS, J. P., DOYLE, M., DARLING, R. M. & NEWMAN, J. 2000. The impedance response of a porous electrode composed of intercalation particles. *Journal of The Electrochemical Society*, 147, 2930-2940.
16. MOLEND, J. & MARZEC, J. 2009. FUNCTIONAL CATHODE MATERIALS FOR Li-ION BATTERIES—PART III: POTENTIAL CATHODE MATERIALS  $\text{Li}_x\text{Ni}_{1-yz}\text{Co}_y\text{Mn}_z\text{O}_2$  AND  $\text{LiMn}_2\text{O}_4$ . *Functional Materials Letters*, 2, 1-7.
17. PEIRÓ, L. T., MÉNDEZ, G. V. & AYRES, R. U. 2013. Lithium: sources, production, uses, and recovery outlook. *Jom*, 65, 986-996.
18. SANTHANAGOPALAN, S., SMITH, K., NEUBAUER, J., KIM, G.-H., PESARAN, A. & KEYSER, M. 2014. *Design and Analysis of Large Lithium-Ion Battery Systems*, Artech House.
19. SKYLLAS-KAZACOS, M., CHAKRABARTI, M., HAJIMOLANA, S., MJALLI, F. & SALEEM, M. 2011. Progress in flow battery research and development. *Journal of The Electrochemical Society*, 158, R55-R79.
20. SUBBARAO, E. 2012. *Solid Electrolytes and Their Applications*, Springer US.
21. VYROUBAL, P., MAXA, J. & KAZDA, T. 2014. Simulation of the Behavior of the Lithium Ion Battery. *Advances in Military Technology*, 9.
22. WINTER, M. & BRODD, R. J. 2004. What are batteries, fuel cells, and supercapacitors? *Chemical reviews*, 104, 4245-4270.
23. YU, S., KIM, S., KIM, T. Y., NAM, J. H. & CHO, W. I. 2013. Model Prediction and Experiments for the Electrode Design Optimization of  $\text{LiFePO}_4$ /Graphite Electrodes in High Capacity Lithium-ion Batteries. *Bull. Korean Chem. Soc*, 34, 79-88.