COMSOL Modelling for Li-ion Battery Diagnostics

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Abstract: Li-ion battery is being used as power source for various applications such as stationary applications, auto-motives, hybrid power systems for residential use and for commercial grid scale. Smart battery diagnostics is essential for creating a better control over the energy storage system and cycle life of a Li-ion battery. It is especially required for real time applications, where more power and energy demand together with an extended lifetime is critical. In this paper, under battery diagnostics, the parameters of Li-ion battery ageing are evaluated using a non-invasive magnetic field technique. A P2D based model has been designed using COMSOL Multiphysics that evaluates the magnetic field response of Li-ion battery on various domains of a battery.

Keywords: Li-ion, Diagnostics, Ageing, COMSOL Multiphysics, Magnetic field.

1. Introduction

Li-ion battery is a preferred choice for power source especially for green energy vehicles (EVs/HEVs) and other automotive applications. The performance and cycle life of Li-ion batteries are gradually becoming important as the applications are shifting from small-scale consumer electronics to dynamic power applications (EVs, HEVs) [1]. Performance loss over time is an existing problem. Extensive research is going on around battery diagnostics to understand the ageing mechanisms.

Li-ion battery is a complex system to understand, and the process of its diagnosis is even more complicated. During the battery diagnostics, following parameters can be monitored such as capacity loss, impedance rise, potential change, state of charge (SoC) and state of health (SoH). This paper is an attempt to investigate a relationship between magnetic field probing [2, 3] and above parameters to predict ageing of a battery. The relationship can later lead to a model that can predict real time ageing in a battery.

2. Magnetic field probing (MFP) method

Despite differences in chemistry, all Li-ion batteries work in the same basic ways. Energy is released when lithium ions diffuse towards the positive electrode. Thus, as the battery discharges, the negative electrode will contain fewer lithium ions. This change in composition of Li-ions can be exploited to directly assess of energy the battery contains. We can expect following behaviour of battery components under the influence of magnetic field:

- Li^+ is a paramagnetic ion that affects the magnetic field. Therefore, a concentration change of Li-ions at the anode during charging and discharging will certainly change the existing external magnetic field.
- Carbon is a diamagnetic substance its presence will minimize the magnetic field. Lithium and carbon are predominant chemistry that present at the negative electrode and that affects the net magnetic field.
- During a battery cycle $LiMn_2O_4$ converts to Mn_2O_4, which alters the valence of the manganese ion from Mn^{+3} to Mn^{+4}. The valence change of manganese affects its magnetic properties, which in turn affect the values of MFP [4].

3. Use of COMSOL Multiphysics

3.1 Model geometry

A lithium manganese oxide ($LiMn_2O_4$) battery is chosen as a case study for this work. This is a simple model based upon battery and fuel cells physics. Magnetic field equations are integrated with it from AC/DC physics. The model has been designed using COMSOL Multiphysics simulation tool. The designed 2-D Li-ion battery model consists of the following three domains:

Table 1: Geometry domains with materials

Material	Domain
Negative Electrode (Li_xC_6)	1
Separator with electrolyte (1:2 EC : DMC/ $LiPF_6$)	2
Positive electrode ($Li_xMn_2O_4$)	3
Magnetic field	1-3

Current feeder and current collector are applied to boundaries 1 and 10 respectively.

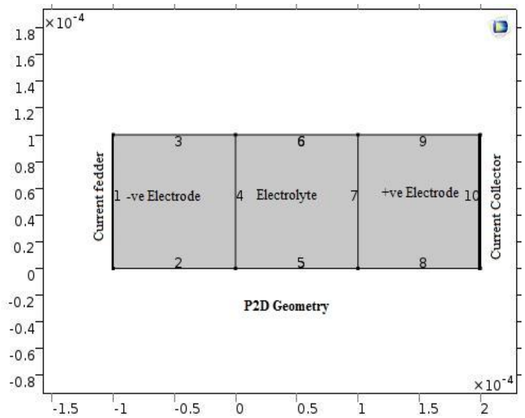

Figure 1. A 2-D cross sectional geometry of the model

3.2 Governing equations

The physical and electrical properties of all the domain materials have been derived from the material library of COMSOL Multiphysics. The electrode reactions have been modelled based on model presented by J. Newmen et.al.[5] Boundary conditions are based on Butler-Volmer kinetic equation, which are given by the expression:

Battery electrode/electrolyte equations:

$$\frac{\partial C_1}{\partial t} + \nabla . N_l = R_l$$

$$\nabla . i_l = Q_l$$

$$\nabla . i_s = Q_s , i_s = -\sigma_s \nabla \phi_s$$

$$i_l = -\sigma_l \nabla \phi_l + \frac{2\sigma_l RT}{F}\left(1 + \frac{\partial nf}{\partial \ln C_1}\right)(1 - t_+)\nabla \ln C_1$$

$$N_l = -D_l \nabla C_1 + \frac{i_l t_+}{F}\phi$$

Symbols used:
Φ_l=phil, Φ_s=phis,
C_1 = cl (electrolyte concentration),
i_l = electrolyte current density,
σ_s = electrical conductivity,
σ_l = electrolyte conductivity,
D_l = electrolyte salt diffusivity,
t_+ = transport number

Magnetic field equations:

$$\sigma \frac{\partial A}{\partial t} + \nabla \times \left(\mu_0^{-1}\mu_r^{-1}B\right) - \sigma V \times B = J_e$$

$$\sigma \frac{\partial A}{\partial t} + \nabla \times H = J_e$$

$$B = \nabla \times A$$

Symbols used:
σ = electrical conductivity
B = magnetic flux density
H = magnetic field
J_e = external current density
A = magnetic vector potential

Table 2 is a summary table for parameter configuration. The initial concentration of lithium ion in the negative electrode is 14870 mol/m^3 and in the positive electrode is 3900 mol/m^3. Few parameters are also borrowed from researched papers [6, 7].

Table 2: Some of the parameters used:

Name	Description	Values
rp_neg	Particle radius Negative	12.5e-6[m]
rp_pos	Particle radius Positive	8e-6[m]
epss_pos	Solid phase vol-fraction Positive	0.297
epsl_pos	Electrolyte phase vol-fraction Positive	0.444
epss_neg	Solid phase vol-fraction Negative	0.471
epsl_neg	Electrolyte phase vol-fraction Negative	0.357
cs0_neg	Initial Negative State of Charge	14870[mol/m^3]
cs0_pos	Initial Positive State of Charge	3900[mol/m^3]
mf.H0x	App. Magnetic field, x component	100[A/m]
mf.H0y	App. Magnetic field, y component	100[A/m]

3.3 Physics used

At this stage, we have used two physics coupled to design a 2-D model (P2D) in COMSOL Multiphysics. Table 3 summarizes the physics used for the model.

Table 3: Physics coupled

	Li-ion Battery	Magnetic field
Physics	1	2

3.4 Meshing

Extra fine meshing is used under physics controlled option with following properties:

Table 4: Meshing properties

Property	Value
Minimum element quality	0.7575
Average element quality	0.9659
Triangular elements	3298
Edge elements	430
Vertex elements	17

4. Model Results

During Battery diagnosis, following simulation results provide behaviour of battery ageing under the influence of the applied magnetic field. All the results are analyzed at boundary number 8 as shown in figure 1.

The designed model has a maximum voltage of 4.25V related to 100% SoC while a discharge cut-off voltage is 3.45V related to 0% SoC. For discharging the battery the inward electrode current density ($i_{n,s}$) is set to -17.5 [A/m^2].

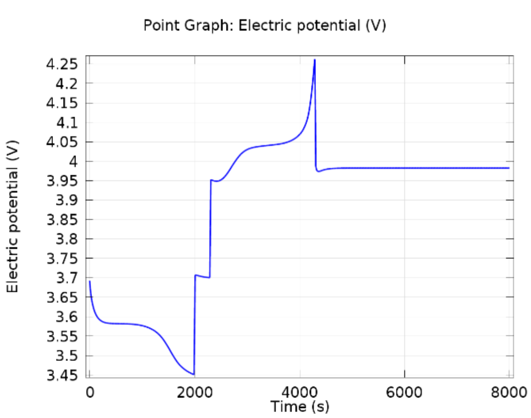

Figure 2. Discharging and charging cycles with relaxation time.

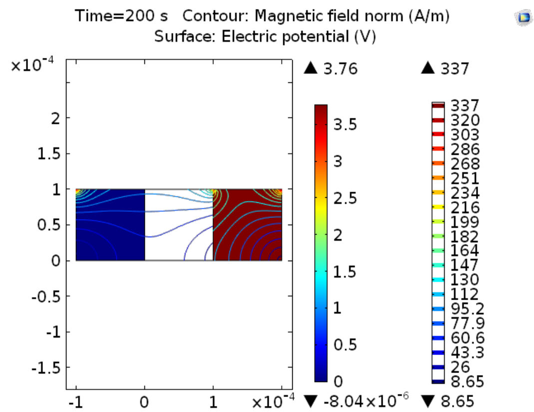

Figure 3. Surface view Electric potential with magnetic field.

During the discharging and charging process, the current collector and current feeder are in contact with positive and negative electrodes respectively. Discharging time is 2000 second. Initially, the battery is charged and in the experiment, it gets discharge for 2000 second followed by a relaxation time of 300 second. Then it gets charge for 2000 second again. All results are investigated for applied magnetic field (H_0) of 100 [A/m].

Figure 3 shows a surface view of electric potential range 0 volt to 3.7 volt for all domains and magnetic field range 8.86 A/m to 337 A/m in all domains at 200 second during discharging. Figures 4 (a, b) show the magnetic field response with respect to electric potential in domain 1 (positive electrode) at boundary 8. As stated in section 2, Li-ion concentration increases the

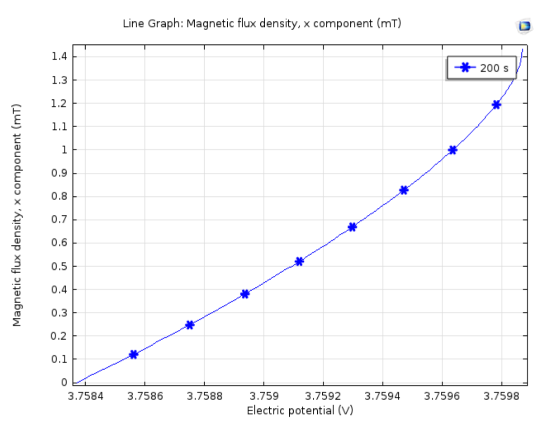

Figure 4(a). Electric potential (V) of Li-ion battery Vs. Magnetic flux density norm (mT) during charging.

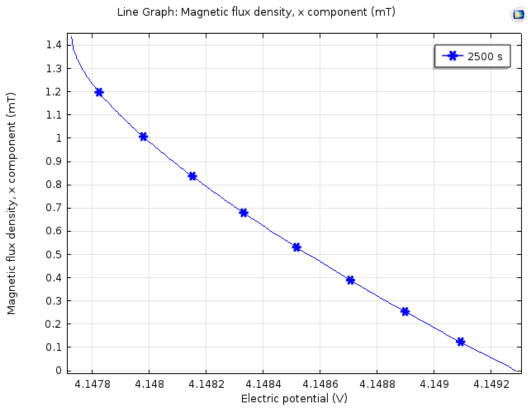

Figure 4(b). Electric potential (V) of Li-ion battery Vs. Magnetic flux density norm (mT) during charging.

magnetic field, which can be verified in the figures 4, 5 Figure 4 (a, b) show the behavior of battery electric potential with applied magnetic field.

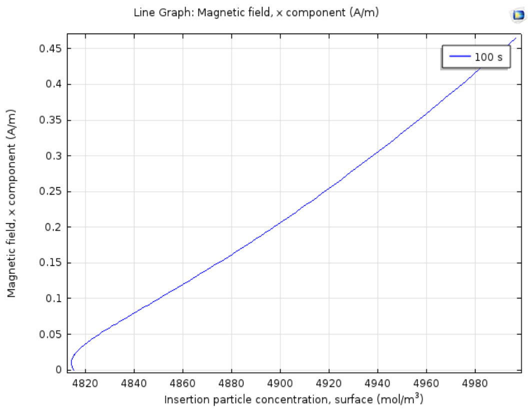

Figure 5. Magnetic field Vs. insertion particles concentration.

Figure 5 shows that magnetic flux density increases as insertion particles concentration increases. These results are the initial results towards addressing the battery ageing analysis.

During battery diagnosis, we will also investigate the impact of magnetic field on other ageing parameters like:

- The effect of MFR (Magnetic Field Response) with respect to the capacity of the Li-ion battery
- MFR with respect to change in internal impedance of the Li-ion battery
- MFR with respect to charging/discharging behaviour of the Li-ion battery

4. Conclusions

Results indicate that COMSOL Multiphysics model is able to simulate the response of applied magnetic field on battery domains to diagnose and calculate the battery aging. This model will be helpful to design a prototype for real time aging prediction for Li-ion Battery.

5. References

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