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OPTIMISATION OF LI-ION BATTERY DESIGN PARAMETERS

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ABSTRACT

Demand for energy storage facilities and non-fossil fuel powered vehicle has furthered the research into Li-ion batteries. In this work, an electrochemical Lithium-ion battery model was built taking into account the electrochemical reactions is presented. The mathematical model is validated against experimental data for LCO cell operating under 1 C electrical load at room temperature. Electrode thickness and the porosity of the positive electrode were varied to determine the influence on the battery capacity..

Keywords: Li-ion battery, simulation, electrode thickness

1. INTRODUCTION

The sprint for alternative sources of energy and green technologies is happening worldwide, mainly as a result of global warming and forecast depletion of limited fossil fuel. Additional, this race has been boosted by environmentally informed buyers willing to spend extra to reduce the impact on the planet. The main concern is the reduction of CO_2 generated from the transport industry to the power plants. Among the alternative sources include the biofuels, renewable energy (wind and solar have been in the raise), fuel cells and rechargeable batteries. Lithium-ion batteries have become one of the most extensively used energy storage devices due to the unparalleled combination of high energy and power densities, making it the ideal technology of choice for portable devices, power tools and hybrid electric vehicles [1–3]. Further, the high energy efficiency may allow Li-ion batteries to find use grid applications, including storing energy harvested from wind, solar and other renewable sources for later use [4]. Therefore, an optimal design for these broad applications is paramount. One of the tools to optimize battery performance is modelling.

The battery models are critical for a better understanding of the effect of design variables, operating conditions on the performance of battery performance with regards to efficiency, degradation and safety. Modelling is an also cost-effective way for the determination of an optimised design thus can lessen the necessity for experimental trial and error [5]. Additionally, most variables that underline the battery operation cannot be measured directly, whereas these variables can be predicted via a validated model.

The common electrochemical models include single-particle models, porous-electrode models and pseudo-two-dimensional models [6]. The main difference between these models is the level of complexity and the computational time required. A given efficient model can be used to address real challenges such as transport and kinetic properties identification, improving capacity fade and lifetime as well as the power/energy density. For example, the energy/power density can be improved by manipulating either the design parameters or operating protocols [7]. Modelling work to improve the performance of batteries has been reported. The important parameters that can be varied in the design to achieve the optimal battery performance are electrode thickness, porosity, particle size, electrode surface area, geometry and the dimensions of current collectors.

Newman and co-workers developed an analytical model of a Li-ion battery to optimise porosity and thickness of the positive electrode for maximum specific energy while holding other parameters constant [8,9].

In this work, we formulate experimental work is validated with a mathematical model suitable for approaching the design, optimization and control of Li-ion batteries. The formulation and experimental work

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have been published. Here, we focus on mathematical modelling using commercial software that is based on the model presented by Doyle and Newman [10]. Since the electrochemical model contains temperature-dependent variables, coupling it with a thermal model gives more accurate predictions.

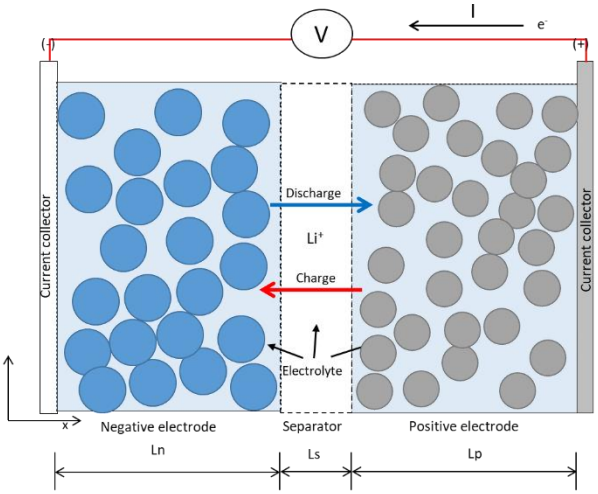

Fig 1: A schematic of the battery model

1.1 Model description

Fig 1 shows an electrochemical model for the Li-ion battery. A sandwich structure of two current collectors, the positive and negative electrodes and a separator were set. It is considered that electricity is generated by the simultaneous insertion/deinsertion of lithium ion in the cathode and anode respectively. In the deinsertion process, electrons released go into the electric circuit and are accepted on the other side to cause Li-ion insertion. Inside the battery, i.e., between the electrodes, positively charged lithium ions move from the anode to the cathode closing the electric loop. The difference phase potential between the current collector and the active material is described by Ohm's law. The electrodes are considered as porous consisting of uniformly-sized spherical active particles. An electrochemical model describing the Li-ion battery cell was set up and solved in COMSOL Multiphysics. Table 1 present the electrochemical model parameters.

1.2 Material and methods

Lithium cobalt oxide (LCO) particles investigated were prepared by Freeport Cobalt, and were synthesized using the same Co_3O_4 - precursor. LCO was synthesized using the Li/Co ratio of 1.005. Galvanostatic measurement was used to electrochemically characterize materials of Li-ion batteries. A current pulse was applied on the cell and the potential was measured as a function of time until a cut-off potential was attained. Full description of the materials and procedure applied can be obtained in already published [11].

1.3 Results and Discussion

The results got from simulations were compared to experimental data [11]. The agreement between the simulated and experimental data is presented in Fig. 2. The results show good agreement and are considered a base case for which modified design parameters i.e. electrode thickness and the porosity of electrode would be compared to. Although the measurements were carried out at room temperature, neither the room

Name of equation	Expression of equation	Nomenclature
Ohm's law	$-\sigma_s^{eff}\frac{\partial \varphi_s}{\partial x} = i_s$	φ- electrical potential, σ- conductivity, s- solid, e- electrolyte, i- electrode current density
Charge conservation, electrode	$-\frac{\partial i_s}{\partial x} = \sigma_s^{eff}\frac{\partial^2 \varphi_s}{\partial x^2} = aFj$	F – Faraday constant, j – pore wall flux of Li-ions, a- specific surface area
Charge conservation, electrolyte	$\frac{\partial}{\partial x}\left(\sigma_e^{eff}\frac{\partial \varphi_e}{\partial x}\right) = -aFj + \frac{2RT(1-t_+^0)}{F}\frac{\partial}{\partial x}\left(\sigma_e^{eff}\frac{\partial lnc_e}{\partial x}\right)$	c- concentration of binary electrolyte, t_+- transference number
Concentration conservation, electrode	$\frac{\partial c_s}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(D_s r^2 \frac{\partial c_s}{\partial r}\right)$	D_s - Diffusivity of Li-ions, r- particle radius,
Concentration conservation, electrolyte	$\varepsilon_e\frac{\partial c_e}{\partial t} = \frac{\partial}{\partial x}\left(D_e^{eff}\frac{\partial c_e}{\partial x}\right) + (1-t_+^0)aj$	ε-porosity
Butler-Volmer equation	$j = i_0 \cdot \left[\exp\left(\frac{\alpha_n F}{RT}\eta_s\right) - exp\left(-\frac{\alpha_n F}{RT}\eta_p\right)\right]$	
Exchange current density	$i_0 = k \cdot (c_e)^{\alpha_n}\left(c_{s,max} - c_{s,e}\right)^{\alpha_n}\left(c_{s,e}\right)^{\alpha_p}$	k- reaction rate constant,
State of charge in the particle	$y = \frac{3}{R_s^3}\int_0^{R_s} r^2 \frac{c_s}{c_{s,max}} dr$	
Reaction overpotential	$\eta_s = \varphi_s + \varphi_e - U - j \cdot R_{SEI}$	U- open circuit potential

Table 1: electrochemical model equations

temperature nor the internal heat generation in the cell was constant. This can be attributed to the variation between the measured data and the simulation results. It is worth pointing out that additional studies need to be done to ascertain the inference.

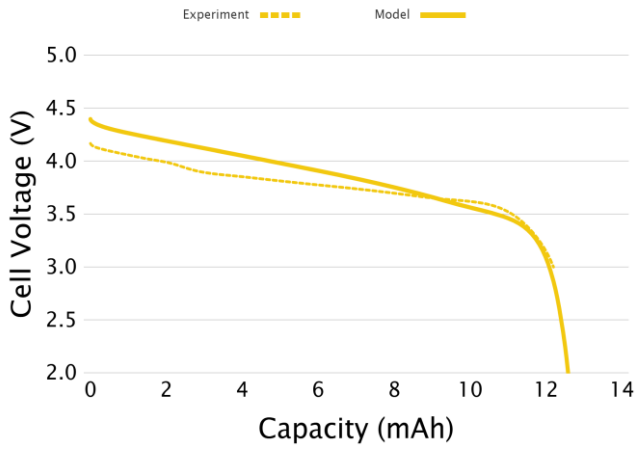

Fig 2: Comparison between simulation (continuous line) and experimental data (dashed line)

The performance of the battery is studied by varying the electrode width and positive electrode porosity design parameters.

The electrodes thickness determines the amount of active material and the resistance to transport in the battery operation. As seen in Fig 3, when the thickness of the electrodes was increased, the battery capacity also increased. This increase in battery performance can be directly attributed to an increase in the quantity of active material available for reaction. Although a subject under investigation, to what extent can the thickness be increased to have a mass transport resistance influencing the performance.

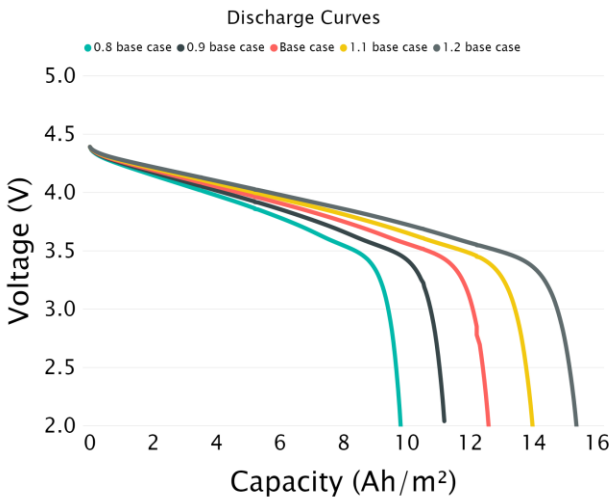

Fig 3: Discharge rate variation from the validated model when the electrode thickness is altered

The porosity of the electrodes affects the effective diffusivity of the electrolyte in the pores as well as mass transference resistance. A reduction of electrode porosity as shown in Fig 4 results in reduced battery capacity and vice versa. It is interesting to point out that a non-proportionate change in battery capacity was observed as the porosity was decreased and increased. Lowering the porosity implies an increase in active material content, however, the diffusion path, (tortuosity) becomes long and possible of non-connectivity of the pores may arise. It was observed that by making the electrode more porous, the capacity increased in a non-linear manner, thus an opportunity to optimize the cell.

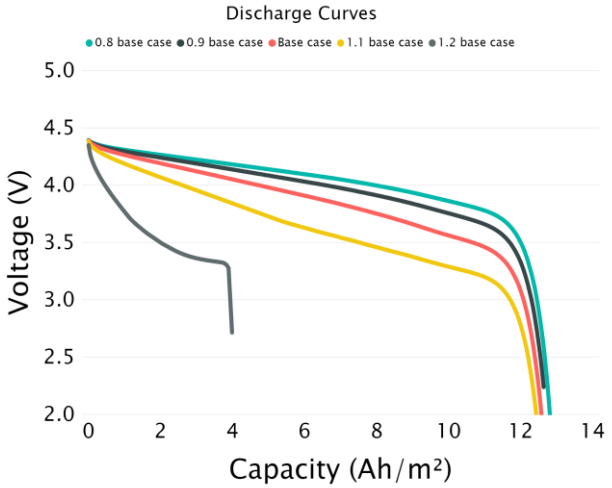

Fig 4: Discharge rate variation from the validated model as the porosity of the electrode is altered

1.4 Conclusions

The growth and demand for renewable energy sources and the need to shift to environmental-friendly powered modes of transportation such as the electric/hybrid vehicles demand safe, effective, reliable and better storage facilities. Li-ion batteries may provide part of solution due to it high power density. In this work, the model was validated using experimental data and used to predict what-if design parameters were shift. It was found that simulation can be an effective tool to optimize performance for different battery applications. Future studies include comparing experiment studies and simulation at elevated temperature to understand deeply the kinetics and validate models for battery suitable harsh environment.

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