



# Ion cell performance using single particle representation of battery electrode



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## ABSTRACT

The aim of study is to predict the performance of lithium-ion cells using the single particle representation of battery electrode model. The model is developed starting from the concentration solution theory and porous-electrode formulation, with Fick's law governing the diffusion of ions in the solid electrode. Since the solution of the governing equations is difficult due to their non-linear nature, simplifying assumptions are made that considerably reduce the computational time needed to predict cell performance. The model is then used to determine the concentration of lithium in solid phase and the electrode potential, assuming that the lithium concentration remains fixed in electrolyte. Further this model is compared with the pseudo two-dimensional model to simulate cyclic performance of lithium-ion cells under various operating conditions.

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## 1. Introduction

The lithium-ion rechargeable battery is a relatively new type of battery. With their high voltage and high energy density, these batteries are widely used for consumer electronics applications, such as mobile phones and laptop computers. Due to enhanced consumer concerns for the environment and fuel savings, the automobile industry has also been developing these batteries for hybrid vehicle (HV) and electric vehicle (EV) applications, which should lead to enhanced output, efficiency and performance.

Lithium-ion (Li-ion) batteries are becoming popular for energy storage in portable electronic devices. Compared to alternative battery technologies, Li-ion batteries provide one of the best energy-to-weight ratios, exhibit no memory effect, and experience low self-discharge when not in use. These beneficial properties, as well as decreasing costs, have established Li-ion batteries as a leading candidate for the next generation of automotive and aerospace applications. Li-ion batteries are also suitable for green technology. As the higher dimension models to analyze performance of Li-ion batteries are computationally expensive.

Miranda et al. [1] reviewed the recent developments and present status of the theoretical models for the simulation of the performance of lithium ion batteries. Preceded by a description of the main materials used for each of the components of a battery anode, cathode and separator and how material characteristics affect battery performance, a description of the main theoretical models describing the operation and

performance of a battery were presented. The influence of the most relevant parameters of the models, such as boundary conditions, geometry and material characteristics were discussed. Baddour et al. [2] investigated the electrochemical lithium insertion reaction into the vanadium pentoxide xerogel  $V_2O_5 \cdot 1.6 H_2O$  (noted VXG) in propylene carbonate solution by structural, thermodynamic and kinetic studies. This material, obtained via a sol-gel process, is a lamellar compound whose high anisotropic structure is characterized by the stacking of ribbons in the c direction. Srinivasan et al. [3] reviewed and presented the current status and expected progress status of the fuel cell research and development programs in the U.S.A., electrochemical problem areas, techno-economic assessments of fuel cells for electric and/or gas utilities and for transportation and other candidate fuel cells and their applications.

Tanim et al. [4] presented a seventh-order, electrolyte enhanced single particle model with electrolyte diffusion and temperature dependent parameters. The impedance transfer function coefficients are explicit in terms of the model parameters, simplifying the implementation of temperature dependence. The present study develops a numerical framework using the simplified single-particle representation of battery electrodes without any temperature dependence.

White et al. [5] cycled Lithium-ion pouch cells at five different temperatures 5, 15, 25, 35, and 45 °C, and performed rate capability studies after every hundred cycles. The data were used with a simple physics-based model to estimate parameters that capture the capacity fade in the cell, with cycling. The weight of active material within each electrode was estimated as a function of time, using rate capability data at the C/33 rate. The C-rate for these cells is 1.656 A. The capacity fade due to the loss of active material and that due to the loss of cyclable lithium were quantified. In the present investigation capacity fade

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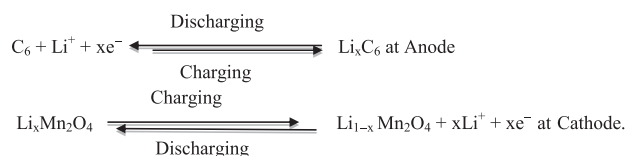
### Nomenclature

$A$	cell area ( $\text{m}^2$ )
$A_j$	surface area of electrode ( $\text{m}^2$ )
$a_n$	specific interfacial is of negative electrode ( $\text{m}^2/\text{m}^3$ )
$a_p$	specific interfacial is of positive electrode ( $\text{m}^2/\text{m}^3$ )
$C_e$	concentration of electrolyte ( $\text{mol}/\text{m}^3$ )
$C_j$	concentration of lithium in solid phase of electrode 'j' ( $\text{mol}/\text{m}^3$ )
$C_{aj}$	average concentration of lithium in solid phase of electrode 'j' ( $\text{mol}/\text{m}^3$ )
$C_{sj}$	solid phase concentration of lithium at the surface of electrode 'j' ( $\text{mol}/\text{m}^3$ )
$D_j$	diffusion coefficient of lithium in the solid phase of electrode 'j' ( $\text{m}^2/\text{s}$ )
$F$	Faraday's constant (96,487 C/mol)
$I$	discharge rate ( $\text{A}/\text{m}^2$ )
$J_j$	current for intercalation reaction of electrode 'j' (A)
$j_j$	current density of electrode 'j' ( $\text{A}/\text{m}^2$ )
$k_j$	rate constant of lithium intercalation/deintercalation. ( $\text{A}\text{m}^{2.5}/(\text{C}\text{mol}^{2.5})$ )
$L_j$	length of electrode 'j' (m)
$M$	molecular weight (kg/mol)
$r$	radial coordinate (m)
$R_j$	radius of particle (m)
$R$	universal gas constant (8.314 J/(mol K))
$T$	temperature (K)
$t$	time (s)
$U_j$	open circuit potential of electrode 'j' (V)
$V_j$	volume of electrode 'j'
$\alpha_a/\alpha_c$	anodic/cathodic transfer coefficient of electrochemical reaction.
$\epsilon_j$	porosity of electrode 'j'.
$\phi_j$	local potential of electrode 'j' (V)
$\phi$	cell potential (V)
$\eta_j$	over potential of electrode 'j' (V).

fast response and accurate control of Li ion batteries. The model developed in this work can be readily used to simulate the cyclic condition of cell.

## 2. Methodology

Fig. 1 shows the schematic of single particle lithium-ion cell. The system consists of two electrodes: positive and negative. The presence of the separator is neglected in the development of the single particle model. Positive electrode is made of lithium manganese oxide and negative electrode is made of carbon. During charging, lithium ions deintercalate from positive electrode and intercalate in negative electrode. While discharging, lithium ions deintercalate from negative electrode and intercalate into positive electrode. The charging and discharging reactions are shown below:



### 2.1. Discharging

In the non-aqueous lithium cells during discharge, lithium ions are inserted into the vacant sites while the  $\text{Mn}_{4+}$  ions are replaced by  $\text{Mn}_{3+}$  ions, which explains the electrochemical behavior of  $\gamma\text{-MnO}_2$  associated with the discharge of Li-MnO<sub>2</sub> batteries [6].

In single particle model each electrode is represented by a single spherical particle whose area is equivalent to that of the active area of the solid phase in porous electrode. A schematic of single particle is shown in Fig. 1. This model assumes that the limitation posed by the solution phase is not considered while developing the model equations. This model is further simplified when the concentration within the sphere is approximated by a parabolic profile. The solid phase concentration is represented by a second order polynomial whose coefficient are expressed in term of average concentration  $C_{a,j}$  and the concentration at the surface  $C_{s,j}$  [7]. This reduce the Fick's law and associated boundary condition to a first order ODE and an algebraic equation.

with cycling was not considered. A new MATLAB code was developed and solved by using forward time marching discretization method. The single-particle model was developed for obtaining

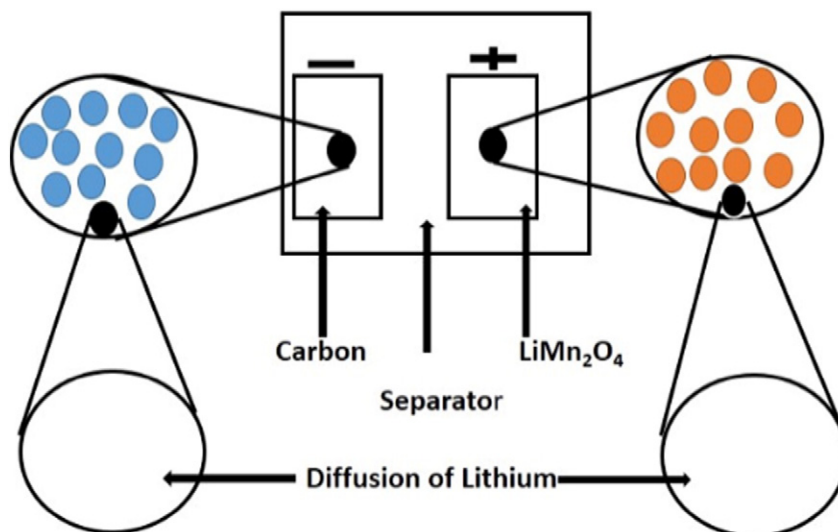


Fig. 1. Schematic representation of the single particle model.

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