

# An Algorithm for Optimal Charging of Li<sup>+</sup> Ion Batteries Using a Single Particle Model\*

Y. Tsai and R. B. Gopaluni

Abstract—Li+-ion batteries are widely used in a variety of products ranging from consumer gadgets such as cell phones and laptops to electric vehicles. Their popularity can be attributed to high energy density and minimal maintenance. Charging these batteries can take anywhere from a few hours for low powered gadgets to many hours for high powered automobiles. Although theoretically possible, fast charging is not preferred because it can lead to unsafe operating temperatures and side reactions that degrade the life of a battery. An optimal algorithm to charge these batteries must therefore account for these constraints in addition to the complex battery dynamics. The battery dynamics are often defined by a large interconnected set of partial differential equations. However, this model is too complex and often takes many hours to solve for relevant battery variables. Single Particle Model is an approximation of this set of partial differential equations. In this article, we develop a constrained moving horizon algorithm to generate an optimal charging profile. The algorithm is based on minimizing the total charge time while meeting the operating safety constraints. The algorithm is illustrated through simulations. Simulations show that the Moving Horizon approach significantly reduces the total charging time by more than 20 percent, compared to a static optimization problem which produces a constant current over the entire charging period.

# I. INTRODUCTION

Lithium ion (Li<sup>+</sup>) batteries are a relatively new type of energy storage technology, developed to replace the older and less efficient lead-acid and transition-metal hydride batteries. Compared to other types of batteries, Li<sup>+</sup> batteries possess certain important advantages: superior energy-to-weight ratios and low levels of idle self-discharge. Consequently, Li<sup>+</sup> batteries are now used in most everyday hand-held appliances such as laptops and cellphones, and are seeing an increased use in hybrid-electric vehicles (HEVs).

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The general operational goal behind Li<sup>+</sup> batteries is to have them deliver specified amounts of power safely and reliably. One interesting problem at hand concerns the optimal charging method of the battery. The widely used charging methods are extremely conservative and are designed to mainly meet the safety constraints. In fact, these charging strategies often take many hours to fully charge a battery. The trade-off between overcharging and undercharging can be qualitatively described as the following: If the charge (coulomb) rate is too high, these batteries can become explosive due to undesired, runaway exothermic reactions that occur at unsafe high temperatures. At low charge rates, the battery is simply charging too slowly, and more current can be utilized to bring the battery to full charge more quickly. In this article, we define the optimal charging profile as a vector of current values that minimizes the total charging time of the battery or maximizes the State of Charge (SOC) of the battery.

The charging of a battery is a batch process and its optimal profile can be theoretically obtained if a battery model is available. Such a battery model must characterize the dynamics of the electrochemical and transport properties. The important properties in a battery are the concentration of Li<sup>+</sup> ions in the electrolyte and in the solid particles (C), temperature (T), current (I), voltage (V), and SOC of the battery. A variety of dynamics models starting from simple electrical circuit equivalent models to complex molecular dynamics models have been developed over many years to describe the behaviour of Li<sup>+</sup> batteries. The electrical circuit models are too simplistic and are not accurate enough, however, molecular dynamics models are more accurate but too complex for use in any optimization algorithm (Ramadesigan, Northrop, De, Santhanagopalan, Braatz & Subramanian 2012). Doyle, Fuller & Newman (1993) have constructed a complete physical model of a typical Li<sup>+</sup> battery, consisting of coupled nonlinear partial and ordinary differential equations (PDEs and ODEs), which allow the previously stated variables to be determined at any time t.

This is known as the "Pseudo Two-Dimensional" (P2D) model. Numerous other models have also been used for state estimation (Plett 2004, Santhanagopalan & White 2006, Gopaluni & Braatz 2012). From a control perspective, however, the P2D approximation is too complex to be simulated. Instead, Chaturvedi, Klein, Christensen, Ahmed & Kojic (2010) have simplified the battery physical model from a solid-electrolyte, dualphase system, into a "Single-Particle Model" (SPM) model. By doing so, the coupled partial differential equations are now approximated as a system of recursive algebraic equations. This approximation is accurate for low coulomb rates. In this article, we use this model to design an optimal charging profile.

The first step is to define an optimization objective to determine the optimal charging profile. Klein, Chaturvedi, Christensen, Ahmed, Findeisen & Kojic (2011) have proposed a Nonlinear Model Predictive Control (NMPC) scheme for fast battery charging, utilizing the a simplified version of the full, complex physical model provided by Doyle et al. (1993). The constrained variables for the optimization are T, SOC, and overpotential  $(\eta)$  of the battery, according to data given by the battery manufacturer. In this paper, we use the approximate, single-particle model given by Chaturvedi et al. (2010) and develop a different methodology based on a moving horizon optimization. In this method, we select an appropriate time period or window (that is a fraction of the total charging time) and find a current profile that maximizes the SOC of the battery, such that all the physical constraints are met. In section II, the SP model and the approximate, algebraic state equations will be discussed in full. We will detail the Moving Horizon Optimization approach in section III and present an optimal charging profile in Section IV, given a set of typical material properties for a Li<sup>+</sup> battery. Finally, Section V will conclude this study and identify areas necessary for future improvements.

## II. LI+ BATTERY FULL PHYSICAL MODEL

Within the core anatomy of a typical Li<sup>+</sup> battery, three distinct domains are identified: the negative electrode, separator, and the positive electrode. Doyle et al. (1993) have proposed a full, 1-dimensional physical model interrelating the state variables of (V, I, C)between the Solid (s) and Electrolyte (e) phases of the battery. The 1-dimensional (in terms of horizontal coordinate x) approximation is based on the assumption that the width and height of the battery (y and z,respectively) are more than 100 times greater in magnitude compared to the length (in the x-direction) of the electrode domain. In this study, we make a further assumption that the state variables (V, I, C) do not vary with x. In other words, we are visualizing each electrode as a giant particle with the same diameter as the length of that electrode. As a result, each state variable (V, I, C) is only a function of particle radius (r) and time (t). This simplification eliminates most of the coupled PDEs in the P2D model and leaves us with the Fickian diffusion of Li<sup>+</sup>:

$$\frac{\partial c_s(x,r,t)}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} (D_s r^2 \frac{\partial c_s(x,r,t)}{\partial r}) \tag{1}$$

With the boundary conditions:

$$\frac{\partial c_s}{\partial r}|_{r=0} = 0 \tag{2}$$

$$\frac{\partial c_s}{\partial r}|_{r=0} = 0$$

$$\frac{\partial c_s}{\partial r}|_{r=R_p} = -\frac{j_n}{D_s}$$
(3)

$$c_s(x, r, 0) = c_s^0 \tag{4}$$

The variable  $c_s(x, r, t)$  represents Li<sup>+</sup> concentration, rthe radius of the hypothetical particle, D the diffusion coefficient, and x the horizontal coordinate. The superscript 0 indicates the quantity at initial time (i.e. t = 0), s the solid particle phase, and n a molar quantity. The molar fluxes of Li<sup>+</sup> for the positive and negative electrodes are calculated using the formulas provided by Chaturvedi et al. (2010):

$$j_n^p = -\frac{I}{Fa^p L^p} \tag{5}$$

$$j_n^n = -\frac{I}{Fa^n L^n} \tag{6}$$

The superscripts p and n indicate the positive and negative electrodes, respectively. Treating  $D_s$  as a constant, this PDE and its corresponding Boundary Conditions (BCs) can be solved using a simple finite-difference method to determine  $c_p$  and  $c_n$  at any time t. However, the computational power required can become increasingly intense as the specified grid size shrinks. Instead, we use the algebraic formulas provided by Northrop, Ramadesignan, De & Subramanian (2011) to calculate the average and particle surface values of  $c_p$  and  $c_n$  in succession:

$$\frac{\partial}{\partial t}c_{avg}^{i} = -3\frac{j_{n}^{i}}{R^{i}} \tag{7}$$

The superscript i can be either p or n. From (5) and (6) we see that applying a constant current I to the battery from t = 0 to t = t\* results in a constant molar Li<sup>+</sup> flux in that period. Therefore, (7) becomes algebraic in the sense that dt becomes a constant, and each  $c_{avq}$  at  $t = t_i + 1$  can be recursively calculated from  $c_{avq}$  at  $t_i$ . To accomplish this, the time domain is divided into a grid space of  $t_n$  equally-spaced nodes  $[t_1, t_2, t_{t_n}]$ . Then, after determining values of  $c_{avg}$ , we calculate  $c_{surf}$  using a similar recursive method. After obtaining the values of  $c_{surf}$  and  $c_{avg}$ , we transform them into dimensionless concentrations by dividing over the maximum solid-phase concentrations in each electrode:

$$\theta_{surf} = \frac{c_{surf}}{c_{max}}$$

$$\theta_{avg} = \frac{c_{avg}}{c_{max}}$$
(9)

$$\theta_{avg} = \frac{c_{avg}}{c_{max}} \tag{9}$$

Next, the Open-Circuit Potentials (OCP, denoted by U) for the positive and negative electrodes can be calculated separately using the following formulas provided by Northrop et al. (2011) (note that either  $\theta_{surf}$  or  $\theta_{avg}$ can be substituted in to find the surface and average OCPs, respectively):

$$U^p = \frac{U_{num}^p}{U_{denom}^p} \tag{10}$$

$$U_{num}^p = -4.656 + 88.669(\theta^p)^2 - 401.119(\theta^p)^4$$

$$+342.909(\theta^p)^6 - 462.471(\theta^p)^8 + 433.434(\theta^p)^{10}$$
(11)

$$U_{denom}^p = -1.0 + 18.993(\theta^p)^2 - 79.532(\theta^p)^4$$

$$+37.311(\theta^p)^6 - 73.083(\theta^p)^8 + 95.960(\theta^p)^{10}$$
 (12)

$$U^{n} = 0.7222 + 0.1387(\theta^{n}) + 0.029(\theta^{n})^{0.5} - \frac{0.0172}{\theta^{n}} + \frac{0.0019}{(\theta^{n})^{1.5}} + 0.2808exp(0.90 - 15\theta^{n}) - 0.7984exp(0.4465\theta^{n} - 0.4108)$$
(13)

The positive and negative electrode potentials  $(\phi)$  are calculated using the OCPs as such:

$$\phi^{i} = U_{surf}^{i} + \frac{2RT}{F}$$

$$sinh^{-1}\left(\frac{I}{2a^{i}L^{i}r_{eff}\sqrt{c_{\epsilon}^{0}c_{surf}^{i}(t)(c_{max}^{i} - c_{surf}^{i}(t))}}\right)$$

Again, the superscript i indicates that one may use the formula for either the positive or negative electrode. Finally, using these potentials, the overall battery voltage is determined as the difference between these potentials:

$$V = \phi^p - \phi^n \tag{14}$$

Besides the existing state variables (V, I, C), another state variable, namely temperature (T), must also be monitored as a function of time for each electrode. This is because temperature is one of the constrained variables in optimizing the charging profile. Klein et al. (2011) have proposed a set of equations relating the temperature change in the cell to the heat of reaction generated by charging, ohmic heat generation, and heat loss to the surroundings. Again, using the model simplification that T does not change with respect to x, the set of PDEs reduce to a single ODE to be solved. Assuming that the OCP of each cell does not vary with T, the single ODE of T with respect to t (and subject to material properties of the battery) is:

$$\frac{dT}{dt}|^{i} = \frac{1}{\rho C_{p}} (h_{cell}(T_{amb} - T^{i}) + \frac{I^{2}}{\theta^{i}} + \frac{3\epsilon^{i}}{0.5L^{i}Fj_{n}^{i}U_{avg}^{i}})$$
(15)

This ODE can simply be solved by a  $4^{th}$ -order Runge Kutta (RK4) routine to find  $T_p$  or  $T_n$  at any time t. Due to the simplicity of Matlab simulations, we select it as the program of choice in this study. The relevant state variables of the battery (V, C, T) are calculated as a function of a single input, which is the current density (I) to the battery. Although Iwould normally be considered as varying with time and spatial domain x, the single-particle and time-invariant assumptions eliminate these complexities. Here, I is treated as a constant current density. The outputs are the positive and negative electrode concentrations (C)and temperatures (T), as well as the final SOC of the negative electrode, since during charging the negative electrode is filled up from zero charge. C and T are outputted and stored as global variables. The reason behind this is as follows: we wish to calculate C and T from t = 0 to  $t = t_1$ , then use these values to determine the optimal charging profile from t = 0 to  $t=t_1$ . Then we repeat the process from  $t=t_1$  to  $t = t_2$ , and so on. The details of this optimization are covered in the following section.

### III. ALGORITHM FOR OPTIMAL CHARGING

## A. Methodology

Suppose that the dead battery (at zero SOC) starts charging with a chosen current density, I, from a certain initial temperature T and concentration C (Note: Tand C contain both values of positive and negative electrodes, and are treated as column vectors, i.e.  $T_0 =$  $[T_{0p},T_{0n}]^T$  and  $C_0=[C_{0p},C_{0n}]^T$ . Next, the material constraints on this charging process are identified. They are the maximum allowable temperature  $T_{max}$  of the battery, the maximum SOC  $SOC_{max}$  of the battery (i.e. the fully charged SOC value), as well as the governing physical model equations discussed in section II. The Moving Horizon Optimization approach is as follows. First, we break down the total charging time required to bring the battery to full charge,  $t_{charge}$ , into fractional periods called windows. The period of each window is denoted by W. Within each window, we break down the time domain further into N sub-windows dW = W/N. The charging profile is then defined as  $I = [I_1, I_2, \dots, I_N]^T$ , with each element corresponding to the current density applied to the battery at t = $[0, dW, \dots, NdW]^T$ . Each element  $I_i$  is determined by applying the previous charge  $I_{i-1}$  to the battery from  $t_i - 1$  to  $t_i$  for dW seconds, and calculating  $T_{i-1}$  and  $C_{i-1}$  of the battery at the end of the dW seconds.  $T_{i-1}$ and  $C_{i-1}$  are then used as initial conditions, with the present current  $I_i$  being applied to the battery from  $t_i$ to  $t_{i+1}$ . This process is repeated until  $I_N$  is determined. The objective is to maximize  $SOC_n$  at the end of the charging period (i.e. at t = W). This problem can be written mathematically as the following non-linear optimization program:

> maximize  $SOC_n(x)$ subject to  $1.T(I) \leq T_{max}$ ,  $2.SOCn(I) \leq SOCn_{max}$ ,  $3.I \leq I_{max}$ ,  $4.I \geq I_{min}$ , 5.Physical Model Equations.

Starting at t=0, solving the non-linear optimization problem yields the optimal charging profile from t=0 to  $t=W,\ I_{0,opt}=[I_{0,opt1},\ldots,I_{0,optN}].$  Here, we take only the first element of  $I_{0,opt}$  and apply it to the actual battery for dW seconds. In other words, we solve the algebraic model equations and single ODE to find the actual  $T_1$  and  $C_1$  of the battery at t=dW,

given initial conditions  $T_0$ ,  $C_0$  and applying the current density  $I_{ont1}$  from t = 0 to t = dW. We then repeat the whole process, shifting the window from t = dW to t = W + dW.  $T_1$  and  $C_1$  are used as initial conditions to find the second optimal current profile  $I_{1,opt}$ , using the same non-linear optimization problem. The first element of  $I_{1,opt}$  is then applied to the actual battery from t = dW to t = 2dW, and so on until the battery reaches its fully-charged SOC. The following is one way to interpret the Moving Horizon approach physically. The temperature of the battery at a time Wseconds from present is predicted. The present current is only applied to the cell for dW seconds, while all the remaining currents between  $t = t_{present}$  and  $t = t_{present} + W$  are adjusted such that the battery is charging as fast as it can while simultaneously staying within its physical bounds. In the worst case scenario, one can simply charge the battery at any desired current density, risking overheating and/or overcharging. The first improvement is the static non-linear optimization problem which generates one constant current value from t = 0 to  $t = t_{charged}$  that guarantees satisfaction of all physical constraints. We will show in Section IV that the optimal charging profile determined by using the Moving Horizon results in a shorter charging time, compared to the two scenarios previously described.

#### B. Implementation

The built-in Matlab function fmincon is used to find the optimal current profiles  $I_{opt} = [I_{opt1}, \dots, I_{optN}]$ with respect to the non-linear optimization. The objective function calculates SOCn at the end of the charging period given  $I_{opt}$ . The first constraint of the non-linear optimization requires T to be calculated as a column vector with N elements  $(T = [T_1, T_2, \dots, T_N])$ along with I. This is simply accomplished by writing a program which outputs a temperature profile given I, using the physical model equations as a basis. The second constraint is simply dealt with using a WHILE loop. The third and fourth constraints are stated as upper and lower bounds on I. Finally, the fifth constraint merely points to the validity of the modelling equations in the program, and does not need to be formulated as a real constraint.

# IV. RESULTS AND ANALYSIS

In this study, the charging of a 5V Li<sup>+</sup> battery (possessing material properties in the paper by Klein et al. (2011) is simulated using Matlab. During charging, Li<sup>+</sup> ions move from the positive to the negative electrode.

Therefore, the limits of zero charge and full charge are defined as the SOC of the negative electrode, which are SOCn=0 and SOCn=0.5, respectively. Suppose the operational limits of this Li<sup>+</sup> battery are as follows: charging current density constraint of  $0 < I_{applied} < 20A/m^2$ , and temperature constraint of  $T_{cell} < 313K(40^{\circ}C)$ . In Case 1, we aggressively charge the battery at  $I_{applied,max}=20A/m^2$ , paying no attention to any constraints. The battery will reach full charge after 3,000 seconds, but the cell temperature will reach 325K, grossly violating the temperature constraint. This is illustrated in the following Fig. 1.

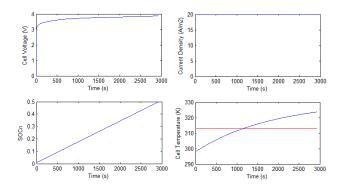


Fig. 1. Simulation results showing battery charging at the upper current density,  $20A/m^2$ . Notice that although the total charging time is only 3,000s, the cell has overheated significantly (the red line indicates the upper temperature constraint).

Risking battery overheating and/or explosion is clearly not acceptable. Case 2 applies the first obvious improvement over Case 1, where we optimize  $I_{applied}$  using a static non-linear program with the constraints stated in Section IIIA over the entire charging period (Fig. 2). This provides the optimal  $I_{applied} = 9.7 A/m^2$ , which brings the battery to full charge in 6,000s while just reaching the temperature constraint by the end of the charging period.

Notice that none of the constraints stated in Section IIIA are violated. However, Iapplied does not need to be constant. Intuitively, we can charge at the maximum  $I_{applied} = 20 A/m^2$  at the beginning of the charging period, where the temperature is still low. Then, we predict ahead of time whether the temperature constraint will be violated, and decrease the current accordingly. This is exactly the essence of the Moving Horizon approach, and we take full advantage of it in Case 3. In Fig. 3, we use a window size W=100s, and a fractional window period of dW=W/N=10s with (N=10). The optimal charging profile is no longer a constant  $I_{applied}$ , but a vector containing many optimal current densities over the entire charging period. Using

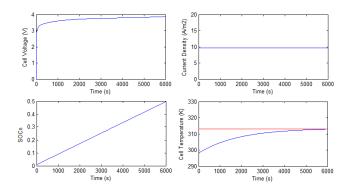


Fig. 2. Simulation results showing battery charging at  $I_{applied} = 9.7 A/m^2$ , determined by a static, non-linear optimization problem. The temperature constraint (red line) is just reached at end of the charging period, indicating that  $9.7 A/m^2$  is indeed the maximum constant current which would charge the battery most quickly.

this method, the battery reaches full charge after 5,000 seconds without violating any material constraint, presenting a clear improvement over the static, non-linear optimization. A further interesting result is obtained when the window size and fractional window sizes are reduced to W = 20s and dW = 2s, respectively. By doing so, we obtain another significant reduction in the total charging time, from 5,000s down to 3,600s. This is due to the Matlab optimizer fmincon giving more aggressive currents in the beginning of the charging period. The increased aggressiveness is a result of the reduction of window size. Previously, the optimizer was generating current values based on what the cell temperature would be 100s from present. Now, the optimizer is only looking 20s from the present into the future. This phenomenon can easily be explained by the analogy of driving a car towards a wall. If the wall exists 100m from the car, a Moving Horizon optimizer with W = 100m will see the wall and slow the car speed accordingly, such that the car stops safely just as it reaches the wall. However, a Moving Horizon optimizer with W = 20m will not see a wall at the end of its window, and hence will tell the car to continue with full speed.

A note of caution is in order. Even though reducing the window size W will decrease the total charging time further, which is parallel to our goal, it may provide infeasible charging profiles if W is made too small. Again we use the car analogy to illustrate this concept. If we use an optimizer with W=1m with a wall 100m away from the cars present position, the car will drive at full speed towards the wall until it has travelled 99m (i.e. is only 1m away from the wall). The optimizer will then tell the car to slow down abruptly,

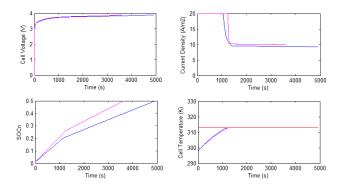


Fig. 3. Blue curves indicate Moving Horizon simulation results, with W=100s and dW=10s. The optimal current profile is  $I_{applied}=20A/m^2$  for the first 1,000s, then dropping down to  $9.3A/m^2$  for the remaining 4,000s. Magenta curves represent results with W=20s and dW=2s. The optimal current profile is  $I_{applied}=20A/m^2$  for the first 1,250s, then decreasing down to  $9.5A/m^2$  for the remaining 2,650s. The total charging time is reduced from 5,000s to 3,600s by using the smaller window.

but the brakes of the car may not be able to achieve this physically. In this study we do not address the issue of finding the feasible bounds of the Moving Horizon optimizer. Here we simply suggest the use of a reasonably large window size W and prove that it is indeed superior over the static optimizer approach.

## V. CONCLUSIONS

The Moving Horizon approach is used to determine the optimal charging profile for a Li<sup>+</sup> battery. This charging profile is one out of many feasible ones (i.e. those that do not violate the material constraints of the battery, namely the State of Charge (SOC), Current Density (I), and Temperature (T)) that brings the battery to full charge within the shortest period of time. The new algorithm for optimal charging results in a superior (decreased) total charging time over the static, constant-current non-linear optimization. This is because the algorithm varies the current over time based on the gap between the state variables and their constraints. When applied on a typical 5V Li<sup>+</sup> battery, the static non-linear optimization charges the Li<sup>+</sup> battery from 0 to 0.5 SOC in 6,000 seconds. On the other hand, the Moving Horizon algorithm can reduce this charging period down to 5,000 and 3,600 seconds, depending on the window size used. When using the Moving Horizon approach, a reasonable prediction window size (W) must be used. If W is too large (i.e. if its magnitude is significant compared to the total charging time), the optimization result would resemble that of the static non-linear program. On the other hand, if W is too small, the optimization may produce an infeasible result. In other words, the optimizer may react too slowly to decrease the current, such that the state variables end up exceeding the material constraints. This study does not explore the optimal range of W, but it is an important concept to consider in a follow-up study.

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