Real-Time State-of-Charge Simulation and Dynamic Optimization of Lithium-Ion Batteries

by Vijayasekaran Boovaragavan

The current and future energy demands for industrial and other applications are now more dependent on electrochemical power sources due to their clean, safe, and reliable energy. Ultimately, modeling of these power sources, which include batteries, fuel cells, and/or super-capacitors has gained momentum and advances have been made detailed enough to model process (voltage, power, energy, etc.,) and intrinsic (solid-phase concentration, electrolyte potential, local current density, etc.,) variables of power sources. Real-time simulation and dynamic optimization of battery models is motivated by this current requirement and is the next step towards realizing energy needs.

Battery models are derived based on concentrated solution theory, porous electrode theory, modified Ohm's law, and other transport and kinetic phenomena.[1] It consists of three regions as shown in Fig. 1 and has ten partial differential equations or 4800 differential algebraic equations (DAEs) in discretized form to solve for intrinsic variables. This rigorous model takes 1-3 minutes to run and is not ideal for hybrid systems modeling and on-line control. In this work, the existing model has been reformulated based on various mathematical methods guided by experimental/theoretical observations.[2] The reformulated model obtained work as well as rigorous model predictions without loss of accuracy and the reformulated model also includes all physical, chemical, and electrochemical phenomena and predicts the exact behavior with a reduced computation time of 75-125 milliseconds. Figure 2 shows good agreement among model predictions for discharge at different rates.

With the current state-of-the-art technology, one cannot estimate the parameters like solid-state diffusion coefficient and/or exchange current densities in milliseconds to predict the state-of-charge or state-of-health of the batteries. But, with this novel reformulated model one can simulate the battery models in milliseconds to estimate the parameters in real-time. This facilitates the capabilities to exactly predict the state-of-charge of the batteries in real-time and to help in optimizing the operating conditions, state-of-health and to minimize capacity fade of the lithium-ion batteries for emerging applications. This approach is useful to analyze batteries in stack and hybrid environments with on-line control and monitoring capabilities.

Having successfully developed the battery models and simulation techniques, the next step in any given application optimization of operating conditions. Here, type of dynamic optimization methodology by the author for the electro-organic has been effectively applied to improve electrochemical performances of a planar used in the batteries and fuel cells. The model consists of a nonlinear diffusion that governs the mass transport limitation planar electrode. The discretized differential-model is solved using piecewise constant vector iteration method with an formulation of a dynamic optimization statement.[4] The results obtained using the control profile is compared with the current discharge and also with another error approach that uses linear current is found that the optimal control method 20% more state of discharge against constant current discharge method with better energy efficiency and battery use (Fig. 3). The results are encouraging and the approach will be extended to porous

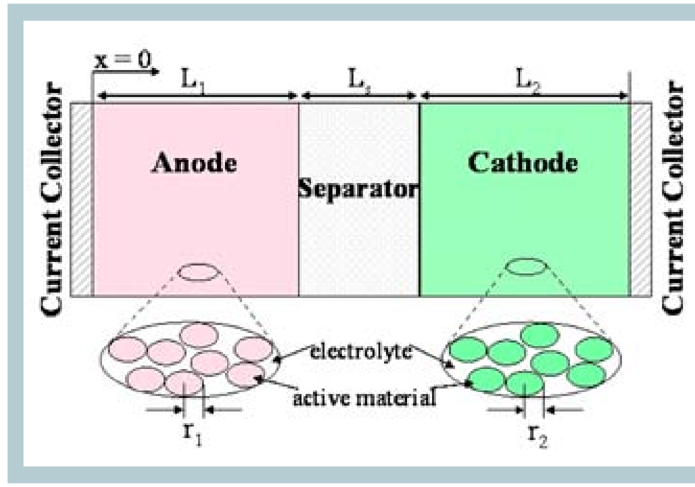

Fig. 1. *Schematic of a lithium-ion cell sandwich.*

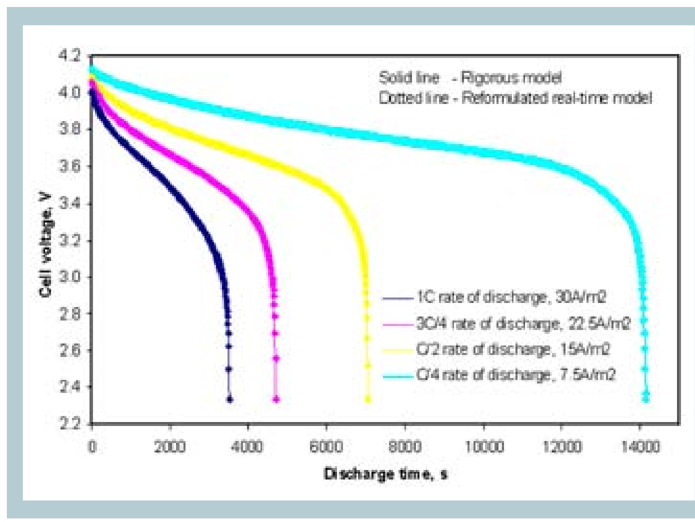

Fig. 2. *Discharge curve at different rates in comparison with the rigorous numerical model of a lithium-ion cell sandwich.*

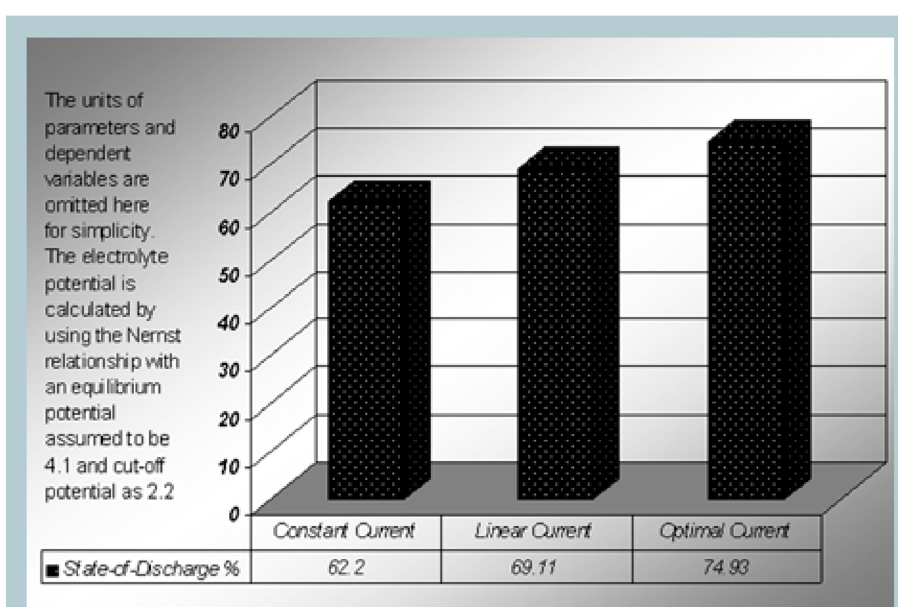

Fig. 3. *Improved electrochemical performances of a planar electrode using optimal operating conditions.*

electrodes governed by a rigorous electrochemical model. The proposed approach can also be extended to optimizing complex situations such as operating an electrochemical energy source in hybrid environments that require proper control over nonlinear energy distribution among the hybrid components.

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