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Optimal Control and State Estimation of Lithium-ion Batteries Using Reformulated Models

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Abstract—**First-principles models that incorporate all of the key physics that affect the internal states of a lithium-ion battery are in the form of coupled nonlinear PDEs. While these models are very accurate in terms of prediction capability, the models cannot be employed for on-line control and monitoring purposes due to the huge computational cost. A reformulated model [1] is capable of predicting the internal states of battery with a full simulation running in milliseconds without compromising on accuracy. This paper demonstrates the feasibility of using this reformulated model for control-relevant real-time applications. The reformulated model is used to compute optimal protocols for battery operations to demonstrate that the computational cost of each optimal control calculation is low enough to be completed within the sampling interval in model predictive control (MPC). Observability studies are then presented to confirm that this model can be used for state-estimation-based MPC. A moving horizon estimator (MHE) technique was implemented due to its ability to explicitly address constraints and nonlinear dynamics. The MHE uses the reformulated model to be computationally feasible in real time. The feature of reformulated model to be solved in real time opens up the possibility of incorporating detailed physics-based model in battery management systems (BMS) to design and implement better monitoring and control strategies.**

I. Introduction

Lithium-ion chemistries are more attractive for many applications due to high cell voltage, high volumetric and gravimetric energy density (100 Wh/kg), high power density (300 W/kg), good temperature range, low memory effect, and relatively long battery life [2-4]. Capacity fade, underutilization, and thermal runaway are the main issues that need to be addressed in order to use a lithium-ion battery efficiently and safely for a long life. Detailed models that incorporate electrochemical, transport, and thermodynamic processes along with geometry of the underlying system can be used to monitor and control internal states of a battery [5-9]. These electrochemical models tend to be computationally very expensive, which has prohibited their use in the control and monitoring of internal states in real time. The observability of these electrochemical models has remained a challenging issue since the dynamics of some internal states are excited only at higher charging rates and the contribution from some states are significant only during either charging or discharging. Depending on the above factors, the observability of internal states can vary significantly and hence various approximations have been made in order to make the model locally strongly observable [10-13].

The use of detailed electrochemical models in control has been limited due to computational cost and issues related to observability. Several simplified/reduced electrochemical models have been proposed and control-relevant studies performed to try to address these issues [10-16]. Efforts in optimal control and nonlinear model predictive control incorporating a Single Particle Model (SPM) and other reduced order models have been published [17, 18].

A mathematical reformulation method [1, 19-21] gives rise to a computationally efficient model that can be solved in milliseconds without compromising on accuracy. A reformulated model with <35 states can be valid for a wide range of battery operations, and includes more meaningful physical states (e.g., volume-averaged flux). These qualities make the reformulated model a suitable candidate for embedded applications and in BMS. The model consists of two collocation points (after taking care of the boundary conditions) in each region (anode, cathode, and separator) to produce a system of Differential Algebraic Equations (DAEs).

This paper evaluates the feasibility of the reformulated model for real-time implementation in receding-horizon approaches to control and estimation (aka model predictive control and moving-horizon estimation). Section II discusses BMS and the application of electrochemical models for advanced BMS. Section III illustrates the use of the reformulated model in computing optimal protocols for battery operations along with a feasibility study on state estimation using the moving horizon technique. Section IV presents results and discussion, which are followed by conclusions and future direction.

II. Battery Management Systems

A BMS is needed to employ batteries aggressively at high efficiency and utilization in electric and hybrid vehicles in a reliable way. A BMS monitors and controls the flow of energy in such a way as to optimally use the energy in the battery, prevent damage to the battery, and ensure safety [4].

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A basic BMS provides overvoltage protection, undervoltage protection, short-circuit protection, thermal protection, and cell balancing or cell equalization [3]. To function efficiently, a BMS needs knowledge of the internal states of the battery, which can be described by the State-of-Charge (SoC), the State-of-Health (SoH), and the remaining runtime (t_r). The accurate determination of these variables is key to the optimal battery use. State inaccuracies can cause severe loss in performance and damage, which creates a need for models that can accurately predict the state of the battery.

Accurate battery models are required not only for design purposes but also on the systems side to maximize the operating performance of lithium-ion batteries. Batteries are overdesigned because full utilization during each cycle very quickly degrades battery lifetime if the charging protocol does not take into account capacity fade of these systems in a reliable manner. The best performance of batteries under different conditions can only be ensured if the model predictions are accurate. For the model to be usable for on-line estimation and control, the model must be efficient.

Models are available for lithium-ion batteries ranging from atomistic to continuum scale [22]. Empirical models are based on experimentally fitted relations in which the parameters have no physical insight. These models are very easy to develop but are not accurate outside of very limited conditions, and prediction confidence decreases significantly as the battery grows older or temperature changes occur. Equivalent circuit models [23-25] describe the input-output behavior by employing capacitors, resistors, voltage sources, and lookup tables. Capacity fade is often represented as a linearly decreasing capacity of a capacitor. Temperature dependence is modeled by a resistor-capacitor combination. A lookup table is often used for nonlinear voltage-current coupling. These models are efficient but lack the intimate coupling to the physics required to accurately predict battery degradation as a function of operating parameters.

Electrochemical models based on porous electrode theory and macro-homogeneous approximation have been validated for many chemistries and designs. The accuracy of these models have attracted the designers and manufacturers of batteries. Despite being accurate in describing the characteristics of battery, these models have found limited use in industrial control applications [26]. The dynamic optimization can take large number of simulation iterations for estimating the optimum value of a objective function, so a computationally expensive model would result in a very long CPU time to obtain optimization results. The computation of the objective function for a single charging profile using a first-principles porous electrode-based electrochemical engineering model could take up to minutes or hours [17] depending on the solver, operating system, and computer. Due to the computational constraints, dynamic optimization of batteries in real-time or online using first-principles-based models has not been attempted or reported in the literature to our knowledge. This situation is not ideal for emerging applications in hybrid power systems or for on-line control, optimization, and monitoring of batteries and other electrochemical power sources.

Recent work on model reduction and reformulation provides a new direction in incorporating simplified and reduced order or reformulated models in BMS design. This paper demonstrates use of a reformulated physics model for prediction and control of internal states in real time. Chaturvedi et al. [27] present a general architecture of an advanced BMS that advocates use of simplified/reduced-order physics-based model at the core of the advanced BMS. Similarly, the following BMS architecture is proposed with emphasis on use of an experimentally validated reformulated model for computational efficiency that is optimized for locally strong observability (Figure 1). The key difference in this paper is the use of a reformulation method that is optimized for best performance for parameter estimation, state estimation and optimization strategies for BMS and performance in a microprocessor environment.

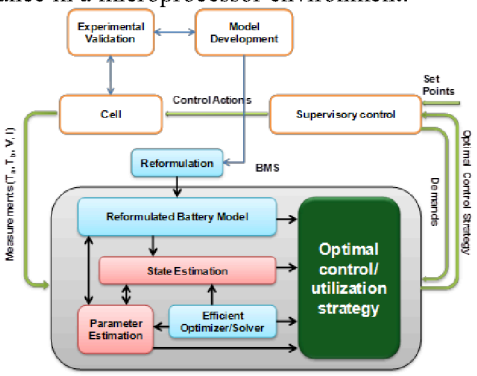

Figure 1. Architecture of an advanced BMS.

I. Optimal Control and State Estimation

A. Optimal Control

To demonstrate the applicability of a reformulated model for deriving control action in real time, the maximization of charge transferred (Q) in a limited time with voltage and temperature constraints is considered. For this optimization study, a variant of the reformulated pseudo-2D thermal model is used with convective boundary conditions.

Numerous methods are available for solving constrained dynamic optimization problems, including (*i*) variational calculus, (*ii*) Pontryagin's maximum principle, (*iii*) control vector iteration, (*iv*) control vector parameterization, and (*v*) simultaneous nonlinear programming [29-31]. Control vector parameterization (CVP) and simultaneous nonlinear programming are commonly used strategies that employ nonlinear programming (NLP) solvers [30]. This paper uses simultaneous nonlinear programming.

The optimal control problem under consideration is:

$$\max_{i_{applied}(k)} Q = \sum_{k=1}^{N} i_{applied}(k); \quad \text{such that:}$$

$$F_k(z(k+1), z(k), y(k), i_{applied}(k)) = 0$$

$$G_k(z(k), y(k), i_{applied}(k)) = 0 \qquad (1)$$

initial conditions $z(k=1) = z_0$ bounds:

$$i_{\min} \le i_{applied}(k) \le i_{\max}, y_{\min} \le y(k) \le y_{\max}, z_{\min} \le z(k) \le z_{\max}$$

with F_k differential equations constraints, G_k algebraic equations constraints, N time discretizations, z differential states, y algebraic states, and an applied current of $i_{applied}$. The differential state constraints include physically meaningful bounds on the solid-phase lithium concentration in the anode and cathode regions, bounds on electrolyte concentration and temperature in the three regions (300 to 320 K in anode, separator, and cathode). Meaningful bounds were provided for algebraic states (e.g., voltage across the cell should be less than 4.2 V).

In simultaneous nonlinear programming [29-31], both the control variables and state variables are discretized, which results into a large set of nonlinear equations to be solved simultaneously for obtaining the optimum charging profile.

B. State Estimation

In order for any model to be useful for closed-loop control, the internal states of the model should be observable from the experimental data. Physics-based models for lithium-ion batteries are very accurate for the prediction of the internal states but their complexity makes it very difficult to use for observer design. Many studies have published observer designs for simplified models [10-13, 15, 32, 33]. Since only the voltage difference is experimentally observable, the observability of open-circuit voltages of the individual electrodes is not guaranteed [11]. Also some states of the model can be weakly observable based on charging rate, SoC, etc. For example, some battery dynamics may not be excited for small rates of charging, in which case it is better to have a suitable assumption or reduction to derive a locally strong observable model. Observability in case of linear systems is easily defined; any linear system will either have one optimal estimate or it will be unobservable. But in the case of nonlinear systems, multiple estimates can exist that are locally optimal estimates that can reconstruct the data arbitrarily closely [34, 35]. Battery models, being highly nonlinear and poorly conditioned, require state estimation techniques that can incorporate bounds on the states in an efficient manner. Moving horizon estimation is one of the state estimation techniques that, although computationally expensive compared to other techniques, can give better estimates due to its ability to explicitly incorporate nonlinear models and bounds on states and parameters.

Moving Horizon Estimation (MHE):

MHE is an optimization-based strategy for state estimation and process monitoring that is especially useful for nonlinear systems with constraints [36]. To limit the online computational cost, a fixed-size moving window of model predictions and process measurements is chosen. As soon as a new measurement arrives, the oldest measurement is discarded and the model states are updated based on the new information.

The optimization solved at each time step in moving horizon estimation is to minimize the difference between the available process measurements and model predictions for a fixed-size moving window to estimate the states and/or parameters at the current time [37]:

$$\min_{\hat{x}(t_k)} \sum_{i=k-N_{est}}^{k} \left\| V(k) - V(k)^{meas} \right\|^2 \tag{2}$$

subject to

$$F_k(z(k+1), z(k), y(k), i_{applied}(k)\ ) = 0 \tag{3}$$

$$G_k(z(k), y(k), i_{applied}(k)) = 0 \tag{4}$$

$$y_{\min} \le y(k) \le y_{\max}, \quad z_{\min} \le z(k) \le z_{\max}, \tag{5}$$

with model voltage $V(k)$ (an algebraic state), voltage output $V(k)^{meas}$, N_{est} past samples used in the estimation window, algebraic states y, differential states z, and applied current $i_{applied}$. MHE is usually desirable when constraints are present or when measurements are available infrequently and at various sampling periods, as these features can be easily incorporated in the MHE formulation.

Two sets of operations of practical importance in evaluating state estimation performance are (*i*) a randomly perturbed discharge profile and (*ii*) an optimal charging profile calculated by open-loop optimal control for a given cost function.

Since the optimal charging profile calculation for maximizing charge storage in a given time will require knowledge of the initial states to perform optimization, it is of practical importance to study the observability for a randomly perturbed discharge profile that mimics an urban driving cycle [38]. The aim is to determine whether the estimated states at the beginning of charging are within a given specified limit from the true states. Once the optimal profile is calculated based on the initial states, it is important to determine whether, for a given optimal charging profile, the states are still observable within a satisfactory tolerance given that the optimal charging profile might not be able to excite all the dynamics. This will enable the implementation of an updated optimal profile as charging progresses that will form a base for model predictive control. Due to space limitations, the estimation performance for only the first set of operating conditions is presented here.

A simulation of the reformulated model is performed using the current values specified in Figure 2. Based on the current values, the model was solved for the state variables, with a current value of 30 A/m^2 corresponding to a 1C rate of charge.

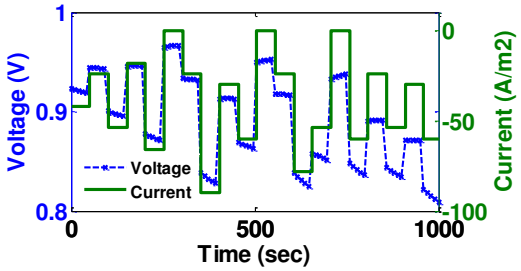

Figure 2. Current and voltage profiles.

II. Results and Discussion

A. Optimal Control

The optimal control problem is to maximize the charge stored in a specified amount of time subject to model equations and bounds on the state variables (temperature and voltage) as well as control variable (current). An upper bound of 320 K was placed on temperature and 4.15 V was placed on the voltage across the battery. Figures 3 and 4 show the optimal current profile and corresponding voltage and temperature profiles. The optimization was solved for 1 h of operation. In Figure 3 the current is shown in C rate of charging. The maximum current in this case was restricted to a 2C rate to minimize capacity fade in the battery.

The voltage and current profile qualitatively follow a constant-current charge followed by a constant-potential charge, but deviate significantly from the conventional method of charging batteries currently used in industry.

Battery lifetime modeling can be incorporated into this model to pose constraints on the overpotential of side reactions to avoid capacity fade during continuous operation [17] rather than only on the voltage difference, which would more aggressively utilize the battery.

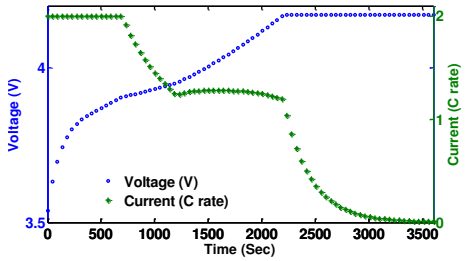

Figure 3. Optimal charging profiles (Voltage and current).

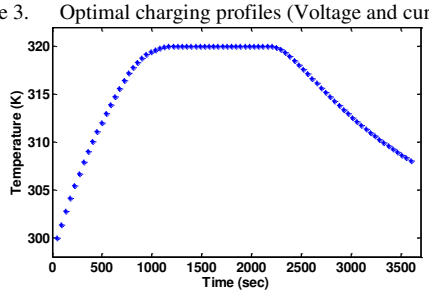

Figure 4. Temperature profile associated with the optimal current profile

B. State Estimation:

In this study, reformulated isothermal pseudo 2D model is used that is composed of a system of 25 equations having 10 differential states and 15 algebraic states. Reformulation is performed in such a way that the reduced number of resultant states also represents the true value of the original states at the collocation points. The differential states corresponds to concentration in three regions: electrolyte concentration in anode (2 states), lithium concentration in anode (2 states), electrolyte concentration in separator (2 states), electrolyte concentration in cathode (2 states), and solid-phase concentration in cathode (2 states). 100 data points were taken to simulate 1000 seconds of battery operation.

For moving horizon estimation, a window of 100 data points was used. The model was discretized for 100 points, resulting in 2500 equations. The 25 equations at the first data point require an estimate of the states at the 0^{th} data point, which adds 10 degrees of freedom. Values of current $i_{applied}$ were directly assigned in the equations. IPOPT [39] was used to solve this simultaneous nonlinear program to obtain the optimized profile that minimizes the difference between experimentally measured voltage (synthetically generated voltage) and predicted values at the 100 data points.

Since the robustness of NLP is dependent on the initial guess, a consistent set of states was obtained by simulating discharge of the same battery from an equilibrated condition (where internal states of the battery are known with good confidence) with the first value of the current profile until the battery reaches the first value of the voltage profile (3.9 V in this case). The obtained states were used as initial values and the model was solved with the given current profile to obtain the initial guesses for all the discretized states. The initial guess obtained in this manner will be consistent with the nonlinear model of the battery.

The estimation problem was solved for three different cases with different level of noises. Random noise was applied with normal distribution with 0 mean and 1 mV, 10 mV, and 50 mV standard deviation to simulated voltage data to predict the experimental data. Figures 5 to 9 show the comparison of three different cases with noise level 1 mV (dashed blue line), 10 mV (dotted red line), and 50 mV (black circle) with true states (green curve). During discharging, the electrolyte concentration in all three cases converges to the true states very rapidly in anode and cathode (Figures 5 and 8). The solid-phase concentration in the anode and cathode are weakly observable and converges to true states rather slowly (Figures 6 and 9). Similar observations were found for the electrolyte concentration in separator region (Figure 7).

Although some state estimates converge rather quickly to the true states, other state estimates converge much more slowly (compare the state profiles in Figure 7). We are currently investigating the use of regularization and Bayesian estimation to improve the accuracy of the estimates of more weakly observable states, and in computing more formal observability metrics. These techniques will be especially useful for state estimation during constant-current or optimal charging, when some of the states may be less excited.

While designing the moving horizon estimator, several factors are important. The size of the moving window is very critical for the performance of estimation. Better estimations are generally achieved when using a larger window size. Conversely, increasing the window size increases the online computational load, which might not be desirable for the best real-time performance. Moreover, reliable and increased precision in voltage and current can significantly affect the performance of the estimator. If the window size is small or the initial guesses in the nonlinear program are poor, then some of the state estimates can poorly converge while producing an estimated voltage output that is close to the true voltage output. Understanding the physics behind

battery operation can affect the performance in a significant way. Physically meaningful bounds on the state variables can be used to ensure that the estimated states converge in to the correct neighborhood values. Including the skin temperature in the model and experiments can provide better estimation results, however, this would require a detailed 2D model that would have to be reformulated for efficient simulation.

III. Conclusion and Future Directions`

As a first step towards model predictive control using physics-based reformulated models for lithium-ion batteries, open-loop optimal control was performed with a computation time of less than a minute. Further, state estimation using a moving horizon technique was performed and the preliminary results showed that performing MPC and closed-loop control using this model is feasible.

The low observability of some of the states in lithium-ion batteries motivates the inclusion of additional measurements into the state estimation. Most sensors that could be inserted into a battery result in operational problems; however, the temperatures at external surfaces of the battery are measurable quantities that could be employed in estimation. Including these temperatures in the model, however, would require a reformulated detailed 2D model to be implemented that is fast enough for real-time implementation.

The MHE results presented here were based on a 2-point collocation. In our experience, a larger number of collocation points (at least 3) are needed for accurate prediction at higher rates. While these points may increase the CPU time somewhat, they may give better observability and robustness in estimation. In addition, employing collocation or higher-order discretization schemes in time will yield faster CPU times.

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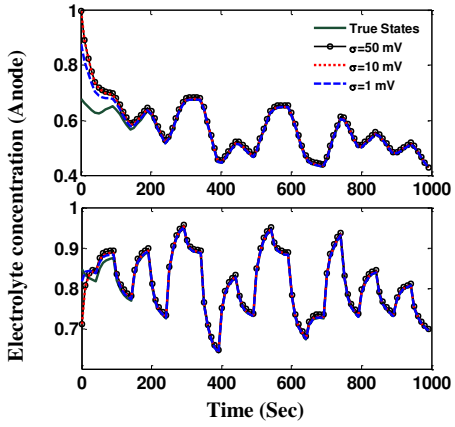

Figure 5. True states and estimated states with different noise.

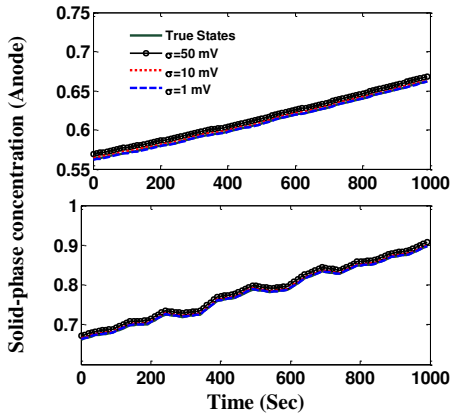

Figure 6. True states and estimated states with different noise.

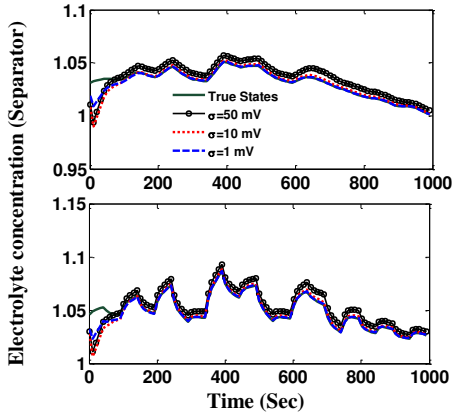

Figure 7. True states and estimated states with different noises.

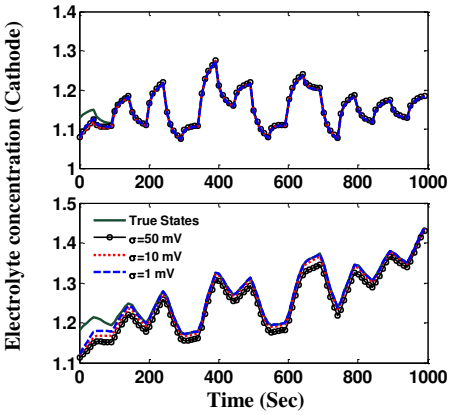

Figure 8. True states and estimated states with different noise.

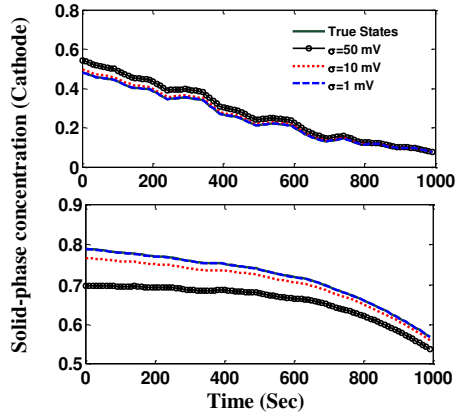

Figure 9. True states and estimated states with different noise.

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