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Reduction of high fidelity lithium-ion battery model via data-driven system identification

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Abstract

The battery management system of a hybrid electric vehicle requires a computationally simple yet accurate model of the battery. In this paper a reduced order battery model is developed using a stochastic top-down approach. Firstly a pseudo-2D, multi-particle electrochemical model, considered as a surrogate for the real system, is used to obtain the observational data. Then the model structure is inferred directly from the data. The dependencies between the states and the model parameters are analysed, which results in a 5^{th} order piecewise state dependent parameter model which can describe the non-linear relationship between the current, the voltage and the state of charge of the battery.

1 Introduction

The recent drive in advancement of hybrid electric vehicles (HEVs) and battery electric vehicles (BEVs) as alternative modes of transport to traditional internal combustion engine (ICE) vehicles has further accelerated the need for improving battery technology. Current Li-ion batteries offer potential benefits as alternative energy storage devices. They are sensitive to extreme temperatures and excessive transient loads. If not controlled, these can lead to thermal runaway (resulting in instability in the internal chemistry) and accelerated aging. Battery packs therefore need a battery management system (BMS) which monitors the state of the battery taking into account temperature, terminal voltage and load current to apply specific charging or discharging strategies for optimised operation. For efficient management, the BMS requires an accurate battery model to estimate internal states of the battery which are not measurable but essential to control degradation mechanisms. These are state of charge (SOC), which indicates the available energy, state of power (SOP), which specifies maximum available charge/discharge rate and state of health (SOH), which gives information on power and capacity fade. Most BMS designs thus far have been based on equivalent circuit models (ECM), which offer simplicity in structure and short computation times due to their relatively high energy density and good cyclability [1, 2, 3, 4]. While they tend to agree well with test data under near-equilibrium conditions, for sustained high-power conditions as is often the case in HEV application, battery dynamics drift far from equilibrium, rendering the ECM model insufficient for prediction of battery performance. To account for the non-linear dynamics observed in battery operation, an extension to a simple ECM structure has been developed [5], where hysteresis is modelled as a complex function to account for the relaxation effect between charge and discharge cycles. In addition a filter was added to incorporate unaccounted dynamics for minimal mismatch to the real system. Whilst gaining in accuracy, the extended ECM model also gained in complexity. In contrast to simple ECMs which lack the predictive qualities of Li-ion electrochemical diffusion dynamics, fundamental electrochemical models, as presented in [6, 7], mathematically describe the internal electrochemical process. These models are accurately able to describe battery dynamics over a wide range of operating conditions and can be used as surrogates to the real system. However, based on coupled partial differential equations, these models tend to be computationally intensive and are thus inappropriate for on board BMS implementation. The requirement for model based state algorithms to take diffusion dynamics into account has led to the development of several reduced order models based on the fundamental electrochemical model [8]. For computational efficiency, these models are derived under various assumptions of quasi-linear behaviour to decouple the partial differential equations. Di Domenico et al. proposed the electrode averaged model (EAM) [9] where the solid concentration distribution along the electrode is neglected and electrolyte concentration is considered to be constant. The model was found to accurately predict output voltage when compared to experimental data. However, due to non-linearity in parameter dependence, difficulty in online parameter estimation led to greater prediction error. In comparison, Smith et al. derived an impedance model [10] under assumptions of linear model behaviour and decoupling reaction current from electrolyte concentration. This impedance model is further reduced to low order single-input-multiple-output (SIMO) state variable models (SVM). The SVM presented poor SOC estimation but accurately predicted output voltage. Errors in both models are clearly attributed to the loss in dynamics due to assumptions

for linearisation. From the models discussed it can be seen that the reduced order models have been derived based on a bottom-up approach where the models are described by deterministic mathematical equations based on well known scientific laws.

As an alternative, in this paper a reduced order battery model is presented as a stochastic, dynamic model using a top-down approach. The methodology termed data-based mechanistic modelling [11] follows an inductive approach, whereby the model structure is not pre-specified but rather inferred directly from the observational data. Once matching accuracy is achieved, the model is interpreted from a physical perspective [11]. A pseudo-2D, multi-particle electrochemical model, considered as a surrogate for the real system, is used to obtain the observational data. Using system identification techniques, a state dependent reduced order model is obtained. The following sections describe the electrochemical model as well as the procedure for obtaining a reduced order model. At this stage in the study, the reduced order battery model only defines the current-voltage relationship having the ability to estimate SOC. The methodology described herein serves as a framework for further work to include higher fidelity for accurate prediction of the essential states for a wide operation range, as well as the ability to predict aging and degradation.

2 Pseudo 2-D electrochemical lithium-ion cell model

The HFM is a pseudo 2-D coupled thermal electrochemical model, where the fundamental governing equations are based on the work of Smith and Wang [12]. The performance of the cell under load is characterised by the solution of four partial differential equations describing the time evolution of the lithium concentration profile in the electrode and electrolyte phases, due to diffusion and charge transfer reactions, under the constraint of charge conservation. The reaction current density is described via the Butler-Volmer equation.

A lumped unsteady state heat transfer model is coupled to this electrochemical description [13]. The three sources of heat considered are: electronic ohmic heat from internal contact resistances, heat from the reaction current and overpotentials, and ionic ohmic heat from the motion of lithium/lithium-ions through the solid and electrolyte phase. As heat generation due to entropy changes in the structure of the electrodes during intercalation/deintercalation was shown to be significant particularly at low discharge rates, its contribution at the high loads typical in automotive applications was neglected [12]. There is heat transfer with an ambient sink through convection. The lumped value of the cell temperature affects, in turn, a number of parameters in the electrochemical model, according to the Arrhenius law dependence.

This model inherently accounts for the dependence of the internal impedance of the cell on temperature, instantanoeus load current, and load history, making it ideal for the task at hand. However, it does rely on detailed knowledge of the cell chemistry and inner structure. Parameter values for the coupled thermal and electrochemical models are chosen for a graphite anode/LiCoO2 cathode as in [12], Geometrical parameters and open circuit voltage curves were chosen to describe a 4.8Ah Kokam pouch cell. The system of equations is solved iteratively by a Finite Difference Method, programmed in MATLAB and embedded into MATLABs Simulink SimPower Systems toolbox.

3 Identification process

This paper focuses of the impact of the SOC and the sign of the current on the dynamics of the cell. As a result a piecewise state-dependent parameter (SDP) single-input-two-output model is devised, whose input is the current $I(t)$ drawn from or supplied to the cell, whilst the cell voltage $V(t)$ and the SOC are outputs of the model.

The first step in the identification process is to develop a set of linear single input single output (SISO) models, each of which can describe either the current to the SOC or the current to the voltage relationship. Each model from the bank should refer to a different value of the SOC. Furthermore, different sets of models are developed for the charge mode (positive current) and the discharge mode (negative current). In order to obtain such a bank of linear models, the HFM has been used to generate the voltage $V(t)$ and the SOC responses to a given current input signal $I(t)$. The input $I(t)$ used for the identification process is a staircase signal with the maximal magnitude of 4.5 A. A staircase signal has been selected due to its broad frequency spectrum which allows one for an accurate data-based identification. Due to the fact that the internal temperature of the battery changes as the current is drawn from or supplied to a battery, the duration time of a single experiment is limited. (If a single experiment was carried out for relatively long time, the internal temperature of the cell would change significantly throughout the experiment causing the HFM to move to different operating range.) During each experiment the input signal consists of three steps each of duration between 15 to 35 seconds. The experiment has been conducted for different values of the initial values of the SOC. This set of experiments has been repeated twice: firstly for the positive current (charging), then for a negative current (discharging). The simplified refined instrumental variable method for continuous time system identification (SRIVC), see [14], has been used to derive the bank of linear SISO models which describe relationships either between $I(t)$ and $V(t)$ or between $I(t)$ and the SOC. Subsequently, the relationships between the parameters of the obtained models, the SOC, and the sign of the current input have been examined. This lead to the overall piecewise SDP model described in Subsection 3.3. The process of developing the current to the SOC and the current to the voltage models is described in Subsections 3.1 and 3.2, respectively.

3.1 Current to SOC model

It has been observed that a type one third order linear model with two zeros

$$G_{soc}(s) = \frac{b_{11}s^2 + b_{21}s + b_{31}}{s^3 + a_{11}s^2 + a_{21}s} \tag{1}$$

provides a sufficient trade-off between the model accuracy and its complexity for all data sets. The term s denotes the Laplace variable, whilst a_{11}, a_{21}, b_{11}, b_21, and b_31 are model parameters. Subsequently, model parameters obtained for different data sets using SRIVC have been analysed; however, no visible relationship between the SOC, the sign of $I(t)$ and the parameters has been observed. Thus, it is concluded that the relationship between the current $I(t)$ and the SOC can be modelled by a linear model given by Equation (1). The parameters of the transfer function (1) differ for different data sets, due to the unmodelled nonlinearities and noise resulting from the use of the HFM solver. The average values of the identified parameters do not provide an optimal solution. Therefore, the Nedler-Mead simplex method (implemented in the built-in Matlab *fminsearch* routine) has been used to find an optimal set of parameters for Equation (1) which are given by

$$\begin{aligned} a_{11} &= 1.28 \cdot 10^{-1} & a_{21} &= 4.62 \cdot 10^{-3} \\ b_{11} &= 4.84 \cdot 10^{-5} & b_{21} &= 4.31 \cdot 10^{-6} \\ b_{31} &= 3.46 \cdot 10^{-7} \end{aligned} \tag{2}$$

Note that the SOC calculated using Equations (1) and (2) is expressed as a number between 0 (0% charge) and one (fully charged cell).

3.2 Current to voltage model

A similar approach has been used to identify the relationship between the current and the voltage, which has been modelled by a type one second order model with a feedthrough term. Unlike the current to the SOC relationship, the parameters of the current to the voltage dependency exhibit a strong correlation to the SOC and the sign of the current. Thus, the current to the voltage relationship is modelled by the following transfer function

$$Z(s) = \frac{b_{02}(soc,m)s^2 + b_{12}(soc,m)s + b_{22}(soc,m)}{s^2 + a_{12}(soc,m)s} \tag{3}$$

where

$$m = \text{sign}\,(I(t)) \tag{4}$$

and a_{12}, b_{12}, and b_{22} are model parameters. The relationship between the SOC and each parameter is modelled using a third order polynomial. Thus, it can be defined by a matrix Γ such that

$$\begin{bmatrix} a_{12} \\ b_{02} \\ b_{12} \\ b_{22} \end{bmatrix} = \Gamma \begin{bmatrix} 1 \\ soc \\ soc^2 \\ soc^3 \end{bmatrix} \tag{5}$$

where the term soc is the SOC expressed as number between 0 and 1 and

$$\Gamma = \begin{cases} \Gamma_c & \text{if } I(t) \geq 0 \\ \Gamma_d & \text{if } I(t) < 0 \end{cases} \tag{6}$$

The optimal values of matrices Γ_c and Γ_d have been found using the Nedler-Mead simplex method and are given by:

$$\Gamma_c = \begin{bmatrix} 0.179 & 1.108 & -1.090 & -0.009 \\ 0.256 & -0.348 & 0.049 & 0.398 \\ 0.271 & 0.369 & -0.315 & -0.063 \\ 0.004 & -0.001 & -0.004 & 0.007 \end{bmatrix} \tag{7a}$$

$$\Gamma_d = \begin{bmatrix} 0.305 & 0.931 & -1.210 & 0.168 \\ -0.095 & 2.022 & -4.188 & 2.673 \\ 0.383 & 0.071 & -0.302 & 0.123 \\ 0.009 & -0.023 & 0.027 & -0.009 \end{bmatrix} \tag{7b}$$

3.3 Overall piecewise SDP model

By combining the two models described in Subsections 3.1 and 3.2, the following two-input-single-output state-space piecewise SDP model is obtained

$$\dot{x}(t) = Ax(t) + BI(t) \tag{8a}$$

$$y(t) = Cx(t) + DI(t) \tag{8b}$$

where the output of the system is

$$y(t) = \begin{bmatrix} soc(t) & V(t) \end{bmatrix}^T \tag{8c}$$

The voltage $V(t)$ is expressed in V·10^{-2} in order to improve the numerical stability of the model. Matrices A, B, C, and D are given by

$$A = \begin{bmatrix} -a_{11} & 1 & 0 & 0 & 0 \\ -a_{21} & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -a_{21}(soc,m) & 1 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \tag{8d}$$

$$B = \begin{bmatrix} b_{11} \\ b_{21} \\ b_{31} \\ b_{12}(soc,m) - b_{02}(soc,m)a_{12}(soc,m) \\ b_{22}(soc,m) - b_{02}(soc,m)a_{22}(soc,m) \end{bmatrix} \tag{8e}$$

$$C = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix} \quad D = \begin{bmatrix} 0 \\ b_{02}(soc,m) \end{bmatrix} \tag{8f}$$

and the parameters in the matrices A, B, C, and D are given by Equations (2), (5), and (7).

The Nyquist plots of the current to the voltage transfer functions (cell impedances) for different values of the SOC are presented in Figure 1. Due to the fact that the LOM is piecewise, i.e. its parameters and the steady state gain differ for different sign of $I(t)$, the LOM can replicate the voltage hysteresis, see Figure 2. A sample behaviour of the LOM is presented in Figures 3 and 4, displaying a good fit to the HFM.

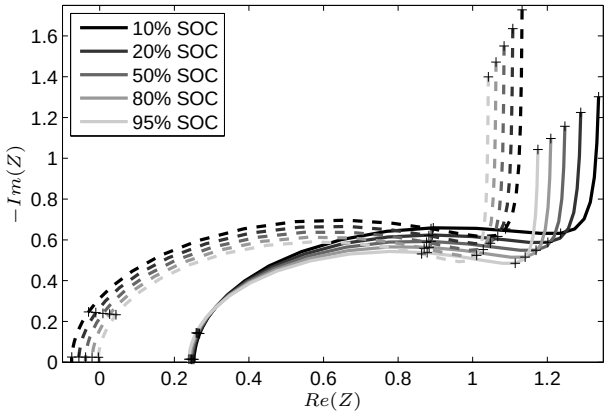

Figure 1: Nyquist plot of current to voltage transfer functions for different operating regions. Solid line represents the charging model, whilst dashed line refers to discharging mode. Markers are placed at 0.1 Hz, 0.67 Hz, 1 Hz, 10 Hz, and 100 Hz.

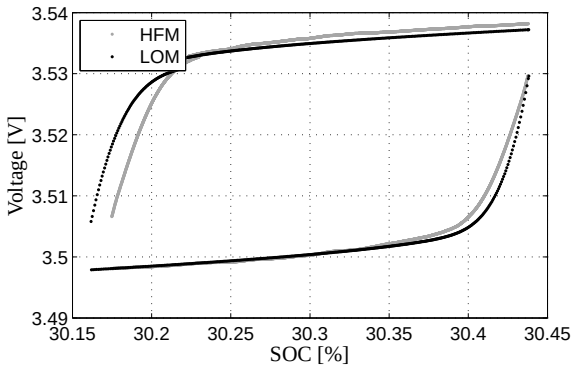

Figure 2: Voltage hysteresis modelled by LOM

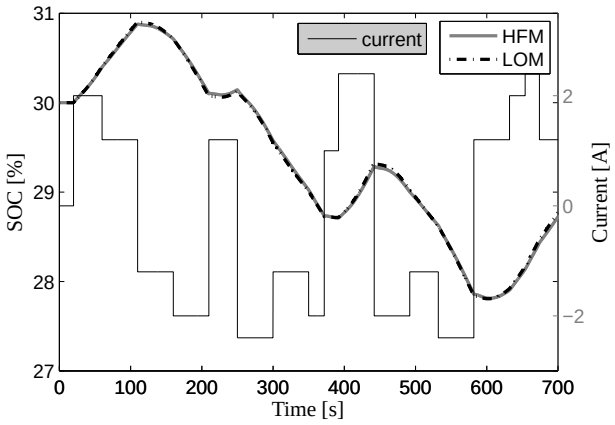

Figure 3: Sample of SOC response to a current input

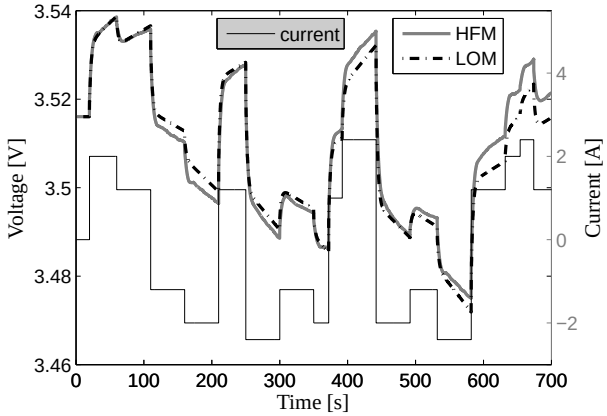

Figure 4: Sample of voltage response to a current input

4 Conclusions and future work

In this paper a framework for devising a reduced order model of a lithium-ion cell is developed. Unlike the methodology commonly found in the literature, this approach utilises data collected from the HFM in order to identify a piecewise SDP model describing the relationship between the current drawn from or supplied to the cell, its SOC and the terminal voltage. The model developed using this framework is computationally simple, which makes it applicable for control, yet sufficiently accurate to describe the nonlinear behaviour of the system including the voltage hysteresis. The difference between the voltage simulation by LOM and HFM could possibly result from the noise in the training data. The current to the voltage relationship contains an integrator, thus the LOM virtually describes the dependency between the current and the derivative of the voltage. It has been observed that the derivative of the voltage acquired from the HFM contains noise which may be a result of a solver. This which obstructs the identification process and leads to modelling errors. Other possible reason for this discrepancy could be the fact the the LOM does not have a built-in memory/history effect. However, the limited information on this effect can be present in the LOM to the extent it has been 'taught' it by the training data.

The future work aims to introduce temperature effects of cell performance as part of the LOM model. Furthermore, the reduced order model developed in this paper may not be sufficiently accurate for high values of current. It has been observed that the Li-ion cell dynamic behaviour change as the value of current significantly increases (above 8 A). This could be modelled by, for example, piecewise bilinear model. Other effects which the authors plan to include into the model are SOH and aging.

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