



Parameter identification of a lithium-ion cell single-particle model through non-invasive testing[☆]



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ABSTRACT

Physics-based models of electrochemical cells are of great interest for the future battery management systems (BMSs), due to their accuracy and capability to predict cell physical states. One of their main disadvantages, when compared to equivalent circuit models, is the fact that they rely on numerous parameters. The identification of these parameters is difficult and usually needs the tear-down of the cell and detailed electrochemical analyses. In this work, we address this issue by developing a novel non-invasive procedure for the parameter identification of a single-particle model (SPM) of a Li-ion cell. The main contributions are: (i) the reformulation of the SPM in order to achieve a minimum number of grouped parameters to be identified; (ii) the formulation of a series of experimental tests capable to identify individually and non-invasively given subsets of these parameters. Notably, we craft specific tests to identify separately the parameters related to equilibrium, intercalation and diffusive phenomena that occur within the cell; (iii) the validation of the reformulated SPM and the associated parameter identification procedure through comparison of simulation results with both synthetic and experimental data. The former are obtained from a detailed pseudo-2-dimensional (P2D) model of a MCMB-LiCoO₂ cell. The latter are obtained through experimental tests performed on a Lithium-titanate cell. Both are cycled with current profiles representative of power-grid and electric-vehicles (EVs) operating conditions. For these profiles, the model identified versus synthetic data achieves a root-mean-square error lower than 0.3% on the cell states and lower than 0.75% on the cell voltage. The model identified versus experimental data achieves a root-mean-square error on cell voltage lower than 1%.

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1. Introduction

In order to achieve cost-efficient and reliable operation of Li-ion cell based battery energy storage systems (BESSs), new advanced BMSs are needed [1]. BMSs need to be able to estimate the state of charge (SOC) and state of health (SOH) of the cells as well as their instantaneous power limits. Ideally, a BMS should also be able to estimate the internal states of the electrochemical cells. The knowledge of ion concentration and internal potential levels is, in fact, useful to detect, and eventually avoid, the degradation of these devices and the occurrence of faults and detrimental usage condition [1–3].

A common technique for SOC and SOH estimation of Li-ion cells in nowadays BMSs is through model-based estimation [4–7]. The cell models most frequently used are the so-called equivalent circuit models (ECMs) [8–10]. ECMs model the voltage output of the cells as a function of current and SOC through simplified electrical circuits. These models, while simple and easy to implement, cannot estimate the physical states of the cells (e.g. concentrations and potentials in the various parts of the cell). Physics-based models (PBMs), on the contrary, are able to represent the physical phenomena occurring in the cells and are, therefore, more suited for these tasks. A BMS based on a PBM may provide more accurate and detailed cell state estimation and enable the perspective of control policies that explicitly minimize specific cell degradation mechanisms.

Most Li-ion cell PBMs rely on the porous electrode theory [11], and the most common models are the pseudo-2-dimensional (P2D) [12] model and the single-particle model (SPM) [13]. The P2D model describes the reaction kinetics, diffusive and conductive phenomena within the two electrodes and within the electrolyte of a Li-ion cell. The SPM simplifies the P2D model by

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neglecting the diffusive phenomena in the electrolyte [13]. This simplification is valid at low applied current densities and in the case of thin and highly conductive electrodes. In several power-systems BESS applications [14], current rates often do not exceed 1 C and these assumptions can be considered valid. The SPM is therefore a valid candidate to serve as PBM in BMSs for such BESSs [15].

Drawbacks of PBMs are (i) their computational complexity (tackled by techniques of model order reduction [16–18]) and (ii) the high number of parameters on which these models rely and that need therefore to be identified. In the present work, we propose a method to tackle this second issue. Depending on the assumptions made, PBMs presented in the literature have several tens of parameters. This makes the model identification procedure very difficult without a cell teardown and complex electrochemical analyses, which is something often not desirable. For this reason and contrarily to ECMs, for which many works exist concerning both offline [8,19,20] and online [6,21,22] model identification, the literature about parameter identification of PBM of Li-ion cells is scarcer and – to date – focused solely on offline methods. Refs. [13,23] identify a subset of parameters for Li-ion PBMs, while relying on literature values for the remaining ones. Ref. [24] identifies a set of 88 parameters of a P2D model through a genetic algorithm approach. While succeeding in its goal, the proposed model relies on a complex procedure and on the usage of a computational cluster for several weeks. Ref. [25] identifies the parameters of a lumped model derived from an SPM through non-linear least-squares fitting of voltage profiles from a set of cycling experiments. Finally, Ref. [26] proposes a method to assess 24 parameters of a reformulated PBM through a series of tests crafted to identify specific subset of parameters and validates the approach by identifying the parameters of a simulated cell.

As in the latter reference, in this work we propose a series of tests specifically built to completely identify the parameters of a PBM. Specifically, and differently from [26], we rely only on data from time domain analysis (i.e. on cell cycling) and based on the considerations above, we seek the identification of the parameters of an SPM rather than of other kinds of PBM. Finally, we validate the method through comparison of simulated experimental profiles from an actual Li-ion cell. The original contributions of this paper are:

- 1 The definition of a new set of parameters for the SPM, by grouping and normalizing the original ones. The newly defined set of parameters is smaller but does not compromise the generality of the model. The reformulated SPM has therefore the same accuracy as the original one while relying on less parameters. This allows for an easier characterization through experimental tests.
- 2 The design of an experimental procedure capable to effectively identify the newly defined parameters. This procedure differentiates and isolates three subsets of parameters. Three experiments are then performed, each one related to a specific subset. In the present work we use a low-current-rate test to identify the electrode equilibrium properties, a series of pulse tests to identify the parameters causing instantaneous voltage drops and a series of galvanostatic intermittent titration technique (GITT) cycles to identify the diffusive parameters. The proposed procedure differentiates itself from the one in [26] in two important aspects: (i) it is based on an SPM (ii) it relies only on cycling experiments, rather than both cycling and electrochemical impedance spectroscopy (EIS) experiments. In this sense, the required experimental setup is lighter.
- 3 The proposed procedure is first applied in a controlled experiment to the P2D model of a 30 Ah MCMC-LiCoO₂ cell whose parameters are known and internal states accessible. This allows to verify the correct identification of the parameters and

the ability of the obtained SPM to properly represent the cell states. The same procedure is then applied to a real 30 Ah cell having Lithium-titanate (LTO) as anode active material and Nickel-Cobalt-Aluminium Oxide (NCA) as cathode active material. In this latter case, the validation of the proposed model identification method is performed through comparison of simulated and experimental voltage profiles. The excitation profiles we selected for this validation are: (i) a realistic profile for a grid-level application such the one described in [14] and (ii) a Dynamic Stress Test (DST) profile, i.e. a profile for testing of battery packs in electric vehicles applications.

The paper is structured as follows. Section 2 recalls the theory at the basis of the SPM for Li-ion cells and describes the model reformulation performed in order to reduce the number of parameters to be identified. Section 3 illustrates the parameter identification procedure. Section 4 presents a validation carried out against synthetic data from a reference P2D model. Section 5 presents the results of the proposed procedure to a 30 Ah Li-ion cell and shows the validation of the identified model against data from battery cycling with realistic profiles for both grid and automotive applications. Finally, Section 6 summarizes the results and contributions of the proposed work and presents the directions of future research.

2. Model formulation

2.1. The single-particle model

The model on which this paper is based is described in [13]. The SPM describes the main phenomena taking place in a Li-ion cell: solid state diffusion, intercalation and de-intercalation and conduction. It neglects the diffusion in the electrolyte. This simplification allows for a considerable simplification in the model structure and dimension and is generally considered to be acceptable as long as the current rates are low and electrodes are thin and highly conductive. Following this assumption, diffusion and intercalation phenomena occur uniformly in all the anode and cathode volume and the two electrodes can be therefore modeled by two spherical particles. The model structure and the relevant phenomena occurring within the cell and modeled by an SPM are

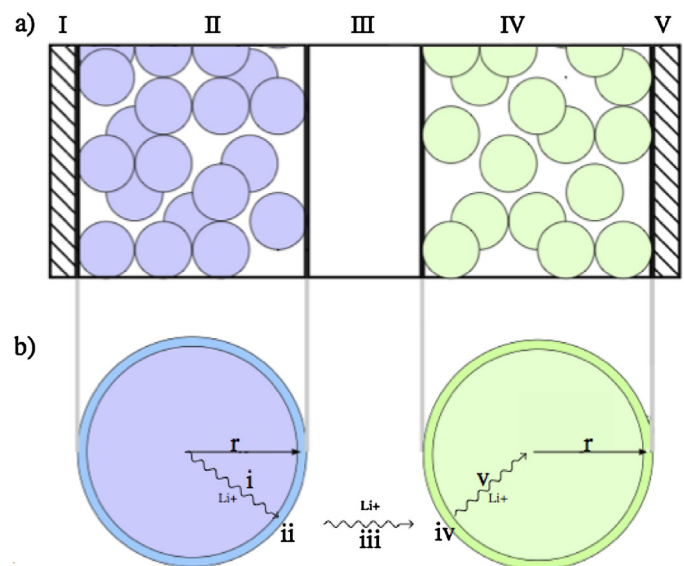


Fig. 1. (a) Structure of a Li-ion cell: (I) negative current collector; (II) anode; (III) separator; (IV) cathode; (V) positive current collector. (b) single-particle model schematic.

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