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Model-based state detection and efficiency testing of advanced electrochemical energy storage devices

Thesis booklet

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1. INTRODUCTION

Lithium-ion (Li-ion) batteries are the primary, popular source of energy storage for electric vehicles and commercially available portable applications such as laptops and mobile phones, thanks to their favourable energy and performance characteristics. Through decades of continuous R&D, many major manufacturers now produce Li-ion batteries with a wide range of electrochemical compositions. These efforts have led to the development of Lithium-Nickel-Manganese-Cobalt Oxide (NMC), Lithium-Nickel-Cobalt-Aluminium Oxide (NCA), Lithium-Titanate Oxide (LTO) and Lithium-Iron-Phosphate (LFP) batteries, which are the most widely used advanced compounds on the market today. Samsung, Panasonic, Sony, Ultrafire, LG, A123 and CATL are major players in the Li-ion battery market, having developed their own component mixes and commercialised batteries in various shapes such as cylindrical, pouch, prismatic or coin-shaped. For the reliable and safe use of batteries of any of the above types, it is important to know the 'State-of-Charge' (SOC) and the output voltage of the battery. For the sake of clarity, the SOC parameter can be considered as a kind of 'fuel level meter' for the battery. Battery voltage can generally be measured without any particular difficulty, but reliable and reliable measurement of SOC requires considerable technical equipment and attention, as it is not a directly measurable parameter. Over the past decades, a number of solutions have been developed for SOC determination, ranging from the simplest and fastest open circuit voltage-based approach, through the well-known Coulomb counting technique, to model and artificial intelligence-based estimators. Model-based and artificial intelligence-based estimation techniques can be used to successfully estimate SOC in demanding applications such as automotive applications, where the battery is mostly in transient mode due to the constantly changing charging and discharging processes and never reaches equilibrium. Under these conditions, the previously mentioned Coulomb counting and voltage-based techniques are highly erroneous and are not recommended.

The key to model-based state estimation of Li-ion batteries is the Doyle-Fuller-Newman (DFN) model, which is the basic electrochemical modelling framework for Li-ion batteries. The model identifies the electrochemical driving processes within the Li-ion battery and describes the dynamic behaviour of the battery in terms of concentrations and potentials [1]. The DFN model is advantageous for SOC determination when the material property functions and parameters such as porosity, diffusion coefficients, conductivity, ageing factors and electrode geometries are known or can be measured, and when the significant computational requirements of calculating model PDEs are not a problem. DFN models are preferred for numerical calculations, such as finite element simulations, where the aim is to analyse the dynamics and thermal response of the battery and to optimise the structure at particle or continuum scales [2-8]. The parameters describing the battery required for the DFN model are usually determined by direct or indirect measurements. Direct measurements require cell disassembly and special cell preparation and involve some form of microscopic or spectroscopic measurement.

In engineering practice, however, the battery must be measured during operation, without dismantling, which is the requirement that drives the need for indirect measurements. Indirect measurements, as the name suggests, are used to extract "implicit" information about the battery condition from voltage and current data. As voltage, current and temperature are all parameters that are generally easy to measure, a commonly used approach to parameterise a DFN model is the indirect measurement method, where information is typically extracted from voltage and current values using an equivalent circuit modelling (ECM) technique. The ECM describes the main behaviour of the battery by means of an appropriately parameterised network of concentrated and/or distributed electrical elements. The concentrated elements are resistors, capacitors and inductors, which are suitable for realising the charge transfer and series resistances as well as the double-layer capacitance of the battery. The ion transport due to diffusion and migration in the electrolyte and electrodes of the battery is modelled by distributed elements such as Warburg and Constant Phase Element (CPE). The number and type of constituent elements in a given ECM depends on the desired level of detail of the battery electrochemistry. Some of the popular ECMs are the Rint, Thevenin/Randles and DP models [10]. The goal of constructing an ECM is to obtain a robust and simple model function that can be fitted to voltage and current data, from which battery material structure parameters can be derived.

The ECM is not only a preferred battery model for material structure parameter estimation, but also for state-of-charge estimation (e.g. SOC), as its rather simple structure and well-known mathematical apparatus can be easily integrated into a model-based estimator. In automotive applications, deterministic systems are required for safety reasons, which is an inherent property of the class of Kalman filter-based predictors. These models are based on the ECM.

Recently, different types of Kalman filters, such as linear Kalman filter (LKF), extended Kalman filter (EKF), "odourless" Kalman filter (UKF) and particle filter (PF) have been developed [11-13], tested and successfully applied in electric vehicles.

Another class of state estimators are non-deterministic models that neglect the physical meaning, treating the battery as a grey or black box. These methods are based on Soft Computing, such as artificial neural networks, genetic algorithms or fuzzy networks [14,15]. Artificial Intelligence (AI) has the advantage of superior performance in processing and evaluating huge amounts of data quickly, and the ability to detect more patterns and trends at once and over a longer time horizon than model-based methods. The performance of AI-based models can be improved by increasing the diversity of the datasets used in the learning process that are specific to the downstream application domain.

1.1. Need for SOC estimation supported by finite element simulation

As mentioned earlier, the parameterisation of battery models is based on measurement data, Due to the many variables involved, to obtain this parameter set, batteries are measured under laboratory conditions, following multi-step protocols. This requires that batteries are charged and discharged at different temperatures, with different currents and from different initial SOC levels, which in itself is a

very time and resource consuming task. In addition, if the cyclic lifetime of a battery is to be known, these steps need to be repeated hundreds of times to finally produce ageing data. The total duration of the process can reach several months by the end of the operation. Obviously, the whole process is very time-consuming, not cost-effective and requires a large investment in infrastructure and measuring equipment.

To generate such a huge amount of measurement data, simulations are a reasonable alternative to extending real measurements. In addition, simulation is a very efficient way to analyse use cases for different use conditions and configurations, such as ageing of 18650 batteries in modules or packs [16-21]. Furthermore, Finite Element Analysis (FEA), a category of numerical solvers used in engineering and mathematical modelling, is also useful for 3D investigations of battery internal temperature and cooling dynamics [22], which are challenging and not cost-effective with real measurements. FEA is also a promising platform for running state-of-the-art driving scenarios, such as the Worldwide Harmonised Light Vehicle Test Procedure (WLTP) or the New European Driving Cycle (NEDC) on 2D or 3D battery packs. [23].

1.2. Problem statement and existing solutions

The Li-ion battery is a complex electrochemical system, so most of the material properties such as diffusion coefficients, ionic conductivities, porosities, activation energies, Bruggemann coefficients are related to the field of electrochemistry. Consequently, the tools used to measure these parameters in electrochemistry were also useful for the study of batteries. Krewer et al [1] and Li et al [24] summarized several existing techniques for collecting electrochemical parameters. These measurements can be classified into two types according to their micro- or macroscopic significance:

- direct measurements, which essentially require disassembly of the cell and special cell preparation, such as scanning electron microscopy (SEM), X-ray diffraction (XRD), transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), nuclear magnetic resonance spectroscopy (NMR) [9], etc.
- indirect measurements include electrochemical impedance spectroscopy (EIS), potentiostatic intermittent titration technique (PITT), galvanostatic intermittent titration technique (GITT), galvanometry, potentiometry, chronoamperometry, etc.

It should be stressed here that the above measurements are complementary. Indirect measurements are based on more precise and inherently more direct information, which can be used to further refine the cell under investigation on the spot. Indirect measurements are in fact the most important when only the voltages, currents and temperatures of the cell can be measured.

One of the main advantages of direct measurements is that they allow the investigation of materials at the granular, molecular level, and are therefore useful for studying, for example, porosity, material composition and the effects of ageing [25-28]. Although direct measurements are the most accurate,

they are expensive and the sample has to be specially prepared. Indirect measurements, on the other hand, require the extraction of the cell's enveloped electrochemical parameters from macroscopic dynamic data such as voltage and current using a suitable mathematical or data-driven model and a model-dependent fitting function.

Specific data of a battery can be measured in situ without disassembling the cell. In-service testing of the cell precludes the use of direct measurement techniques. The measured voltage and current data are subjected to post-processing, where the model parameters are determined by parameter fitting (regression) and the resulting characteristics are finally converted into electrochemical quantities. In the time domain, this is usually achieved by fitting to terminal voltage curves, which are the voltage responses of the charging or discharging currents. [It has been found that in the frequency domain, impedance regression is favourable [34,35]. The impedance response of the porous electrode model was studied by Meyers et al [36]. Regression algorithms can be of several types, often using genetic algorithm (GA), Kalman filter and nonlinear least squares using different solvers such as Levenberg-Marquardt, Newton-Raphson, quasi-Newton and Gaussian methods. [37]. Several sources have reported Randles circuit parameters such as charge transfer resistance R_{ct} , double layer capacitance C_{dl} , series resistance R_s , Warburg coefficient σ and diffusion time constant τ_D [38-40] or electrochemical parameters, for example, D_s is the diffusion coefficient of Li ions in the solid phase, the diffusion coefficient D_l of Li ions in the electrolyte, the concentration of Li c_s in the electrode, the porosity ϵ_{sep} of the separator, the porosity ϵ_s of the electrodes, the reaction rate k_0 and the t_+ transference number [41-46]. The relationship between the geometric structures and cell electrochemical parameters such as solid phase diffusion coefficients has been investigated by Cooper et al [47], Sapoval et al [48] and Zou et al [49] in different fractal pore shapes. They pointed out that the pore shape affects the EIS impedance spectrum. However, conventional DFN models rely on simple spherical particles, so the specific shapes of pores and particles are not considered in these models. In addition, Song et al [50] showed that particle geometries and pore shapes have negligible effects on the EIS impedance characteristics in the high-frequency range of the diffusion impedance. Levi et al [51] evaluated and compared several promising equivalent circuit models suitable for fitting EIS impedance spectra, especially in the low frequency range where diffusion dominates. Their comprehensive comparison draws attention to the variations in EIS spectra due to the effects of different particle sizes, ionic and electric conductivities, solid-phase diffusion coefficients and electrode thicknesses. Bisquert and colleagues investigate the effects of these inhomogeneities using a constant phase element diffusion modelling technique. Baker et al [52] studied solid-phase diffusion in multiphase electrode materials and found a strong nonlinear dependence between the solid-phase diffusion coefficient and the SOC during phase transitions. Guo et al [53] published a very promising method for estimating the solid phase diffusion coefficient from the AC excitation signal and showed the dependence of the solid phase diffusion coefficient on the application of different electrochemical parameters. Cabanero et al [54] estimated the solid phase diffusion coefficient of several commercially available Li-ion batteries using GITT. Dong et al [55] presented a

method for parameter estimation using CPE to model diffusion and the double layer effect. They proposed different configurations of ECMs suitable for extracting the values of resistive, capacitive, inductive and distributed elements based on EIS impedance measurements. Useful applications of CPE for diffusion modeling have been reported by Huang et al [56], Guha et al [57] and Zhuang et al [58]. Scipioni et al [59] used a generalized transmission line model for estimating equivalent circuit parameters, where instead of using a single CPE, multiple *RC* branches were implemented to model diffusion. The electrochemical parameters of batteries can be estimated by fitting a physicochemical model to dynamic discharge curves according to Park et al [60].

In these scientific reports, the estimated electrochemical parameters are associated with different types and configurations of cells, and there is a lack of a complete, consistent list of material data required for the DFN model in FEA. Furthermore, no significant techniques have been reported on how to obtain the characteristic cell dimensions to be implemented in the DFN model to make the model valid by indirect measurements. The two characteristics of the characteristic size are the cross-sectional area of the electrode plate A_{cell} and the thickness of the modeled cell "sandwich" (unit cell thickness) L_{cell}.

1.3. Research topic and objectives

To overcome the problems mentioned above, I developed a technique to derive the missing geometric data from the diffusion impedance. Classical estimation techniques, as indicated in the previous paragraph, derive the diffusion-related parameters from the solid-phase diffusion impedance using a surrogate electrical model with a Warburg element and CPE. However, data collection and parameter fitting in the low frequency range where solid phase diffusion dominates transport processes - approximately the frequency interval 0.1-10 mHz - is very time consuming and challenging in function fitting. In terms of fitting, the main problem in this range is the highly non-linear complex impedance characteristic with multiple "curvatures", to which a model function must be fitted in such a way that it retains its physical meaning with the best possible accuracy and results in a convergent system of equations for the fitting algorithm.

In addition, solid phase diffusion is obviously related to the diffusion of particles within the solid electrode matrix, which can be succinctly called the microlevel. Here, the typical dimensions of the particles that make up the electrode material are on the order of a few micrometers and do not carry useful information about macroscale dimensions, such as the cross-sectional areas of the cell. Consequently, my attention has been focused on extracting data from the early part of the diffusion impedance reduced to the frequency interval 100 mHz - 10 mHz - the so-called "tail part" of the diffusion impedance - instead of solid phase diffusion. The merit of using this method was motivated by the previous work of Huang et al [58].

Based on this, my main hypothesis is that there is sufficient time in the tail frequency region for ion transport to develop in the electrolyte within the full cross section of the cell, but not sufficient time for the majority of ions to intercalate into the electrode matrix. In other words, for a given active particle i,

the frequency-dependent diffusion length $l_{d,i} = \sqrt{D_i/j\omega}$ is short in this frequency range, and therefore the effect of solid-phase diffusion can be considered negligible when examining the tail particle. Under these conditions, the diffusion-related parameters of ions in the electrolyte can indeed characterize the macroscale structure of the cell and can be used to determine battery-specific macroscale electrochemical parameters.

To prove this hypothesis, I first performed EIS measurements to obtain impedance data from the cell. Subsequently, I fitted the impedance characteristics using the Randles equivalent circuit model with a generalized Warburg element extension to model non-ideal - so-called non-Fickian - fluid phase diffusion in the tail section. An additional advantage of extracting the data from the tail section, as opposed to examining the full diffusion impedance spectrum, is the possibility of accelerated data acquisition and more robust impedance fitting. Based on the results of the fitting, I determined the fundamental parameters $D_{l,0}$, A_{sep}, L_{cell} and D_s as well as the characteristic parameter vector for a given 18650 Li-ion cell. Time domain dynamic measurements were also performed to evaluate the internal resistance of the battery in the time domain. In order to reduce measurement errors, the internal resistance of the cell was measured both in frequency and time domain.

1.4. Research methods

To achieve the objectives, I modelled, measured and simulated. In the modelling phase, I built a DFN model in a finite element analysis environment to faithfully implement the behaviour of a Samsung ICR18650 26F cell. The parameters required for the DFN model were determined by indirect measurements. In frequency domain EIS, in time domain GITT and resistance measurements were performed. The EIS measurement yields an impedance data set from which the electrochemical characteristics that can be incorporated into the DFN model are decoded in an intermediate step. In this I first created a matching function based on a Randles model, whose resulting impedance characteristics match the EIS measured data series as closely as possible. Then, from the Randles parameters determined as a result of the fitting, such as resistance and capacitance values, I deconvolved the material properties that can now be incorporated into the DFN model by constructing a so-called characteristic cell. The key to the function fitting is the use of a suitable electrical surrogate model, where the use of distributed elements such as Warburg elements and CPE is a key element. This process requires careful attention to ensure that the fitting function is convergent and is derived from a physically meaningful surrogate model. The EIS measurements were performed with Schlumberger and Solartron instruments, and the function fitting was performed in ZView. The GITT and resistivity measurements provided an alternative way to verify the EIS measurements and geometric layout and gave information about the available capacity of the cell. Data acquisition software for these time domain measurements was created in LabVIEW on National Instruments PXI target hardware. The geometric layout of the cell under test was verified using a Nikon XT H 225 ST CT. With the DFN model parameterized in this way, I generated simulation data series on Comsol finite element platform, where I reproduced the cell voltage

and SOC variation under different loading scenarios. The results were compared with real measurements covering both tempered (ESPEC LU-113 climate chamber) and non-tempered (natural cooling) measurement environments.

2. NOVEL SCIENTIFIC RESULTS

1. Thesis group

Description: Electrochemical Impedance Spectroscopy I have demonstrated that Samsung 18650 Li-ion cells exhibit non-Fickian lithium ion diffusion in the impedance spectrum from 100 mHz to 10 mHz due to their high porosity. This is indicated by a phase difference of more than 45° between excitation current and voltage response in the Nyquist diagram of the battery impedance.

1.1. **sub-thesis:** The results show that the Randles model based on the standard Warburg element is not suitable for modelling non-ideal diffusion.

1.2. **sub-thesis:** I have shown that, among several electrical surrogate models used in the literature, the so-called extended Randles model with generalized Warburg element and CPE fits the measured impedance curve best. The former is the element suitable for describing non-ideal diffusion, the latter the non-ideal double layer effect.

Publication(s) supporting the thesis group:

Csomós, B. and Fodor, D. "Identification of the material properties of an 18650 Li-ion battery for improving the electrochemical model used in cell testing", Hungarian Journal of Industry and Chemistry, vol. 48, no.1, pp. 33–41., (2020), https://doi.org/10.33927/hjic-2020-06

2. Thesis group

Description: Based on literature sources and the results of my measurements, I proved my hypothesis that the highly non-linear characteristics of Samsung 18650 Li-ion cells in the impedance spectrum from 100 mHz to 1 mHz indicate diffusion in two different phases.

2.1. **sub-thesis:** I proved my hypothesis that they can be separated into Li-ion diffusion in liquid and solid phases, and a transient region between the two.

2.2. **sub-thesis:** I have proved my hypothesis that both the liquid phase diffusion diffusion coefficients D_l and the solid phase diffusion coefficients D_s are diffusion coefficients of the liquid and solid phase diffusion, respectively, obtained from impedance data in these two ranges and from the full impedance spectrum modelling, as well as the cross-sectional area of the A_{sep} cell separator, the thickness of the L_{cell} cell, the overall cell exchange current density i_0 and the reaction rate coefficient k_0 can be estimated, provided that the main geometric parameters of the cell, the porosity and the composition of the electrodes are known.

Publication(s) supporting the thesis group:

Csomós, B., Fodor, D. és Vajda I., „Estimation of Battery Separator Area, Cell Thickness and Diffusion Coeffcient Based on Non-Ideal Liquid-Phase Di_usion Modeling", Energies, vol. 13., pp. 6238., (2020), doi:10.3390/en13236238

3. Thesis group

Description: I have demonstrated by measurements and simulation results that the pseudo-2D electrochemical battery model, built as described in Chapter 4, is capable of generating standard charge-discharge and dynamic load profiles consistent with reality, and can be used to generate voltage and current data series suitable for accelerated training of machine learning algorithms using a direct prediction strategy to estimate battery charge and/or operating time. Based on a comparison with reference measurements, it is demonstrated that the model is suitable for simulating standard vehicle driving test cycles (e.g. WLTP), allowing accelerated battery testing under realistic load scenarios.

Publication(s) supporting the thesis group:

Adrienn Dineva, Bence Csomós, Szabolcs Kocsis Sz. and István Vajda, „Investigation of the performance of direct forecasting strategy using machine learning in State-of-Charge prediction of Li-ion batteries exposed to dynamic loads" Journal of Energy Storage, (2021), 36, 102351, doi:10.1016/j.est.2021.102351

3. PUBLICATION LIST

2021

1. Dineva, Adrienn ; Csomós, Bence ; Kocsis Sz., Szabolcs ; Vajda, István
Investigation of the performance of direct forecasting strategy using machine learning in State-of-Charge prediction of Li-ion batteries exposed to dynamic loads
JOURNAL OF ENERGY STORAGE 36 Paper: 102351 (2021)
DOI WoS Scopus Egyéb URL
Közlemény:31869406 Nyilvános Forrás Folyóiratcikk (Szakcikk) Tudományos
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2020

2. Csomós, Bence ; Fodor, Dénes ; Vajda, István
Estimation of Battery Separator Area, Cell Thickness and Diffusion Coefficient Based on Non-Ideal Liquid-Phase Diffusion Modeling
ENERGIES 13 : 23 Paper: 6238 (2020)
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Q2
DOI: 10.3390/en13236238

3. Csomós, Bence ; Fodor, Dénes
Identification of the material properties of an 18650 Li-ion battery for improving the electrochemical model used in cell testing
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IV. Agrártudományok Osztálya IVAO A
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ACTA IMEKO 7 : 1 pp. 20-26. , 7 p. (2018)
DOI Scopus
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Nyilvános idéző összesen: 4 | Független: 3 | Függő: 1 | Nem jelölt: 0 | WoS jelölt: 1 | Scopus jelölt: 1 | WoS/Scopus jelölt: 2 |
DOI jelölt: 1
Q3
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