35th International Electric Vehicle Symposium and Exhibition (EVS35)
Oslo, Norway, June 11-15, 2022

Synthetic Modeling of Batteries – a Case Study

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Summary

To analyze the behavior of cells with future battery materials, before a prototype cell is even built, a Synthetic Battery Modeling Toolchain is developed at the authors' institute. With this toolchain, major parameters regarding the electrical behavior of battery cells can be calculated. To demonstrate the functionality of the toolchain, a case study with two battery cells, of which one is well known at the institute, is performed, and the validation results are presented in this work.

Keywords: Battery, Battery Model, Case-Study, Materials, Simulation

1 Introduction

Upcoming battery materials are frequently published in the scientific literature as cathode [1] or anode [2] active materials. How these materials influence cell performance cannot be easily estimated from the material properties as long as no prototype cell is built with these new materials. Due to a prototype cell's time- and money-intensive construction process, it is advantageous to make an initial approximation on a simulative basis. The development of the "Synthetic Battery Modeling Toolchain" aims to make assumptions about the battery's electrical behavior in the application based on parameters at the material level.

2 Toolchain

As shown in Fig. 1, the structure of the toolchain consists of four individual components, a database with material to cell parameters, a physico-chemical battery model, an impedance-based battery model, and a framework in which batteries can be simulated in various applications. In the database, material parameters from literature and lab measurements are collected. With those parameters, batteries are virtually assembled, and the properties on the cell level are calculated. A sophisticated physico-chemical battery model (PCM) is parameterized and simulated in different operating points to estimate the battery's electrical behavior with the calculated parameters.

The resulting voltage output of pulse and EIS simulations is used to parameterize an impedance-based equivalent circuit model (ECM), which, e.g., allows accelerated system scale simulations and diagnostics in the battery management system [3]. The entire toolchain is widely automated, enabling the investigation of parameter variations on a large scale.

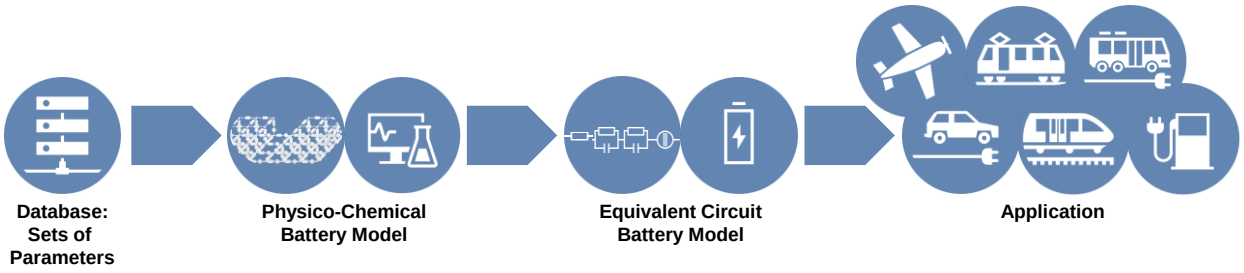

Figure 2.1: General structure of the Synthetic Battery Modeling Toolchain

2.1 Structure

The database structure is inspired by the real-world production process of battery cells. Starting from elements of the periodic table, all intermediate products of the production process are created, and the corresponding parameters are calculated. This structure offers the advantage that subsequent parameter variations can be applied at any stage of the production process, and corresponding parameters are automatically recalculated at all subsequent stages. The result of the first tool of the toolchain is a parameter set with static parameters such as dimensions, weight, capacity, voltage curve over SOC and energy. These parameters are extracted in an interface and serve as input for the subsequent physico-chemical battery simulation. This second tool additionally requires current profiles as input. These are based on the routines established at the institute for the electrical characterization of a battery cell. Therefore, the physico-chemical battery simulation includes a quasi-OCV measurement per temperature, where charging and discharging is performed with a shallow current of C/50. Here, the hysteresis effects of the active materials are taken into account.

Subsequently, a sequence of relaxation, EIS and pulse simulations is performed for each temperature in 5% SOC steps between 95% and 5%. All data is stored in a defined directory where it can be used by the following tool in the toolchain. This tool is an automatized routine to parameterize electrical ECM from measurement data or simulation data. The parameters are identified and quantified locally for each combination of temperature and SOC in a hybrid method from EIS data and pulse data and the qOCV data using a least-square fit algorithm and then optimized for continuity in a post-processing step. The final piece of the toolchain is the ECM simulation tool. With the already published "ISEAFrame" [7], electrical and thermal-electrical simulations with aging linked can be performed. This simulation can be done on the single-cell level and module or pack level.

2.2 Implementation

The implementation of the control functions of the entire toolchain is done in Matlab. The individual tools and their execution, on the other hand, are not carried out exclusively in Matlab. While the cell parameter database and the routine for parameter identification of the electrical equivalent circuit models are implemented as GUIs in Matlab, both the PCM battery simulation and the simulation environment for the ECM are written in C++. These C++ programs are called multiple times from Matlab as part of the toolchain. In order to automatize the workflow as much as possible and be prepared for multiple uses of the toolchain, for example, to compare and analyze the behavior of different cells with different parameter variations, a higher-level folder structure is created. The simulation inputs and outputs are collected in this folder structure to ensure functional access to the data from the various tools.

3 Simulation and Validation

To demonstrate the advantages of the toolchain, we conducted a case study using a battery cell produced by the manufacturer Kokam. It is a commercially available cell in a pouch bag housing and has a capacity of 7.5 Ah. This "KOKAM7.5" cell is well known in the literature [4], [5], [6] as well as in the authors' lab and has nickel-cobalt-oxide (NCO) as the cathode's active material and graphite as the anode's active material. Using different measurements from the chemical lab like laser microscopy, ICP mass spectrometry, Mercury porosimetry, GITT, and more, the database is filled with the parameters of the different cell materials and components. The parameters are systematically calculated from the raw material to the cell level. Then, they are compared and validated with the measured full cell data. The reassembling of the battery cell leads to model parameters for the physico-chemical battery simulation. With the steps of the toolchain, an electrical impedance-based equivalent circuit model was parameterized. The model's accuracy is determined and validated using experimental data from electrical measurements, such as electrochemical impedance spectroscopy and pulse measurements. Finally, a real-world drive cycle, measured at the cell level in the lab, is simulated and compared to the measurement data. In conclusion, the toolchain is validated on the cell parameter level, PCM level, and ECM level. The results are promising and can be applied to other cell formats and material compositions based on literature or measurement data.

KOKAM7.5 Cell

For the simulation and measurements in this work, a high-energy pouch lithium-ion polymer battery from the manufacturer Kokam is used. The cell's nominal voltage is 3.7 V, while the end of discharge voltage is 2.7 V and the end of charge voltage is 4.2 V. Between those two limits, the battery can provide a capacity of 7.5 Ah with a current rate of 1C. Concerning the datasheet, the positive electrode consists of $Li(NiCo)O_2$, the negative electrode consists of graphite, and as the electrolyte, an EC/EMC mixture with LiPF6 is used [4]. In Table 1, the datasheet values are compared to the results of the static parameters from the virtual cell design. As can be seen, the results for nominal voltage and capacity and energy are very close and differ only less than 1%.

In contrast, the weight is calculated a lot too high. With 194.6 g, the calculated cell weighs 39.6 g more than the real cell. The volume calculated to be 91.57 cm^3 is also higher than the real volume of 79.5 cm^3. Both deviations are because some uncertainties in the chemical measurements regarding the inactive parts lead to higher amounts of binders and conductive additives, which are necessary to meet the electrical behavior in the simulation.

Table 1: Comparison of real cell parameters from datasheet and calculated parameters

	Real Cell Data	Calculated Cell Data
Nominal voltage	3.7 V	3.72 V
Capacity	7.5 Ah	7.42 Ah
Weight	155 g	194.6 g
Energy	27.75 Wh	27.62 Wh
Volume	79.5 cm^3	91.57 cm^3

In Figure 3.1, the fundamental values are shown in correlation.

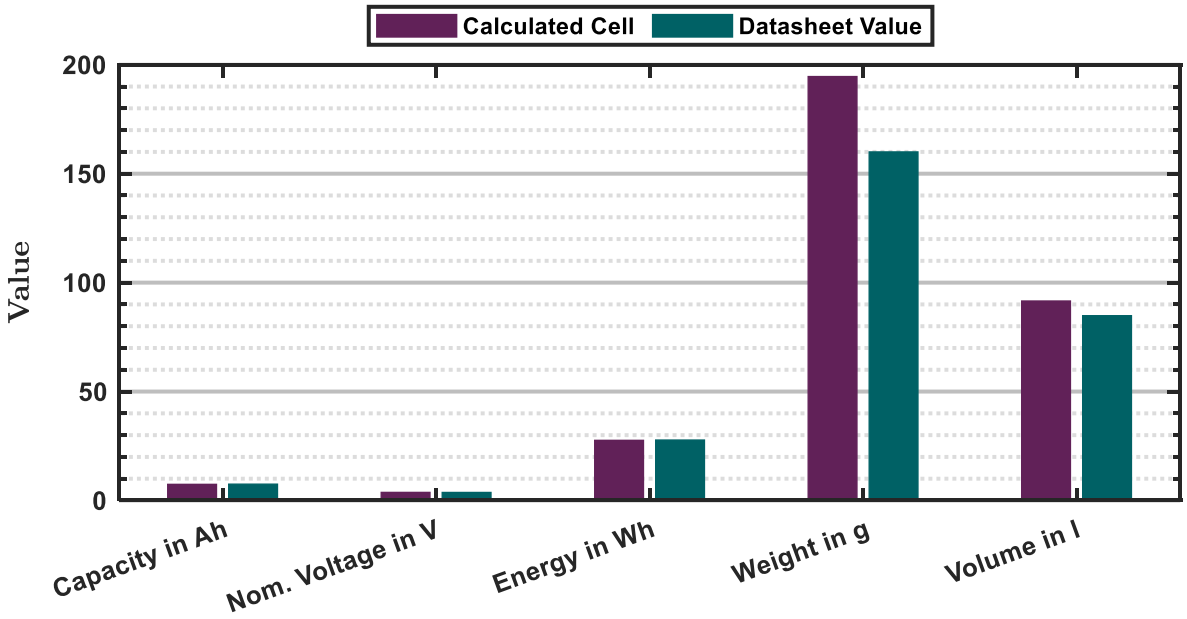

Figure 3.1: Comparison of KOKAM7.5's calculated parameters and the datasheet values

3.1 Frequency Domain

In the frequency domain, we simulate sine wave excitation currents in frequency ranges from 1 mHz to 10 kHz and store the voltage response of the model. The complex impedance can be calculated after analyzing the different voltage courses at different frequencies. The impedance course is shown in Figure 3.2 in a Nyquist-Plot at 25° C and 50 % SOC.

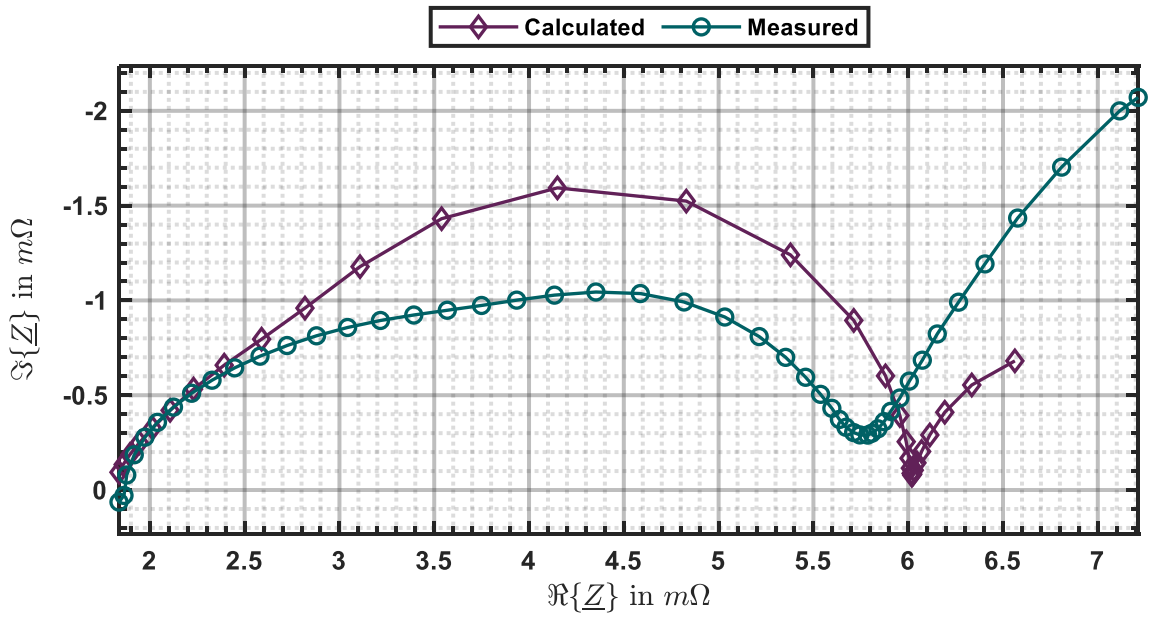

Figure 3.2: Comparison of the complex impedances of the measured and the calculated cell using a Nyquist plot at 25° C and 50% SOC

The Nyquist plot shows the strengths and weaknesses of the present state of the toolchain. The frequencies of the complex impedance increase from left to right. In the high-frequency range, the calculated and measured values almost match. In contrast, deviations can still be seen in the mid-frequency and low-frequency ranges. The medium-frequency semicircle in the Nyquist plot currently still shows a too large time constant. The diffusion processes take place in the low-frequency range. Here in the right part of the figure, there are still notable deviations in the diffusion region. These deviations indicate that the diffusion processes cannot yet be represented precisely in the toolchain.

The complex impedance can be visualized in different ways to be analyzed and compared. In Figure 3.3, the comparison is conducted between the measured and the calculated values. We see minor differences in the explicit comparison of solely the real part (a), as well as comparing the imaginary part (b). The benefits of such visualizations compared to the nyquist plot are comparing the values at specific frequencies. This comparison is also possible in the impedance's magnitude (c) and phase (d).

In (a), it can be seen that the plot of the real part of the complex impedance versus frequency reflects the real behavior of the cell very accurately. There is also a slight deviation in the mid-frequency range analogous to the Nyquist plot. In the imaginary part (b), the deviation is considerably more prominent, especially in the mid-frequency and low-frequency range <100 Hz calculated results and measured data deviate from each other. Analogous to the real part, the magnitude of the complex impedance (c) is also sufficiently well matched. This good match is mainly because the real part is more significant in magnitude than the imaginary part. Therefore deviations in the imaginary part have less influence on the magnitude of the impedance. In the angle of the complex impedance (d), on the contrary, mainly the imaginary part affects the result, whereby the calculated values and the measured values deviate more strongly, similar to the imaginary part consideration.

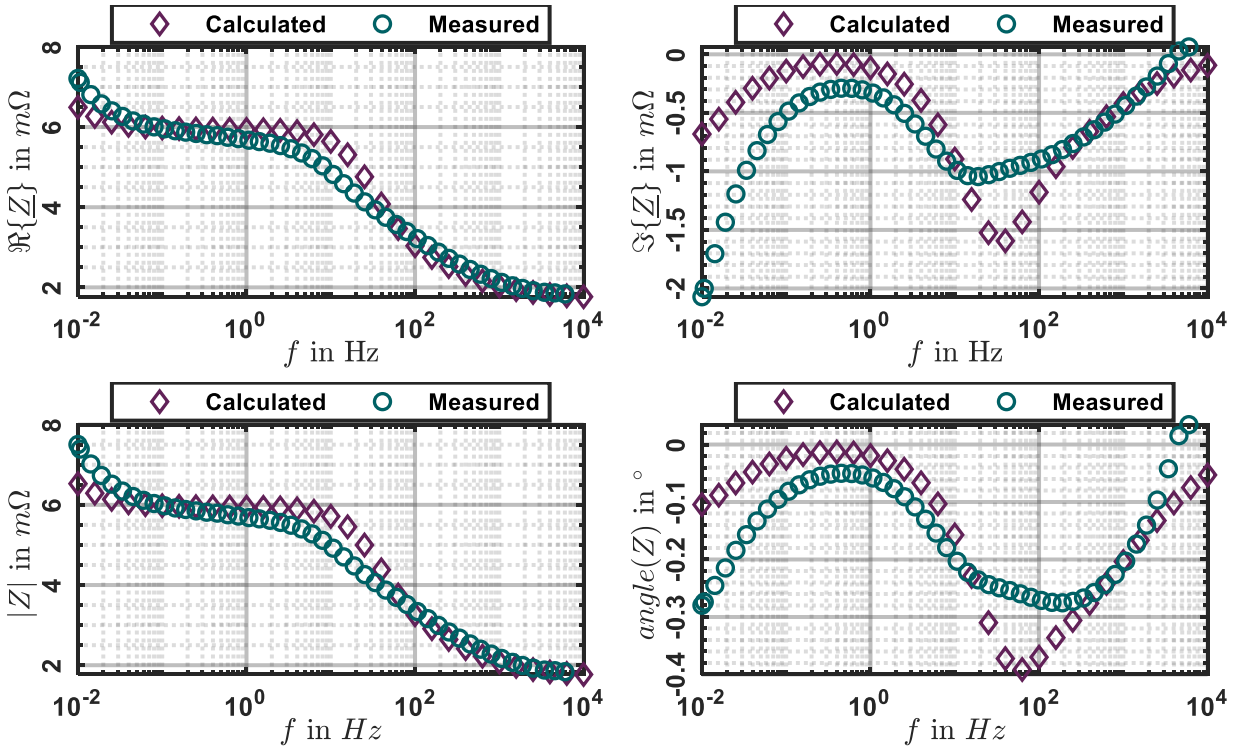

Figure 3.3: Comparison of KOKAM7.5's calculated and measured values (a) real part of the complex impedance Z; (b) imaginary part of Z; (c) magnitude of Z; (d) angle of Z

With a least-square fit algorithm, the model's parameters are estimated to match the Nyquist-Plot for both the calculated virtual cell and the real measured cell. Therefore, the impedance is calculated for every frequency as

a result of the transfer function of the ECM with the fitted parameters. The parameters are optimized to have the least error between ECM-impedance and measured or calculated impedance. The residual for the fit of the virtual cell is 2.45e-5, and for the fit of the measured cell, 1.39e-5. The results are shown in Figure 3.4.

3.2 Time Domain

With the estimated parameters of the frequency domain fit, the model parameters are transformed to the time domain, and the voltage response to the current profile is calculated. The current profile we use for this time domain fitting is several pulses with different current values and short relaxation times of about 15 minutes afterwards. We define specific ECM parameters to be re-fitted in the time domain. The resulting error between both voltage courses has to be minimized by the defined re-fit parameters. The results of the time domain fit are shown in figure 3.4 (c) for the ECM fit with the measured data and (d) with the calculated data.

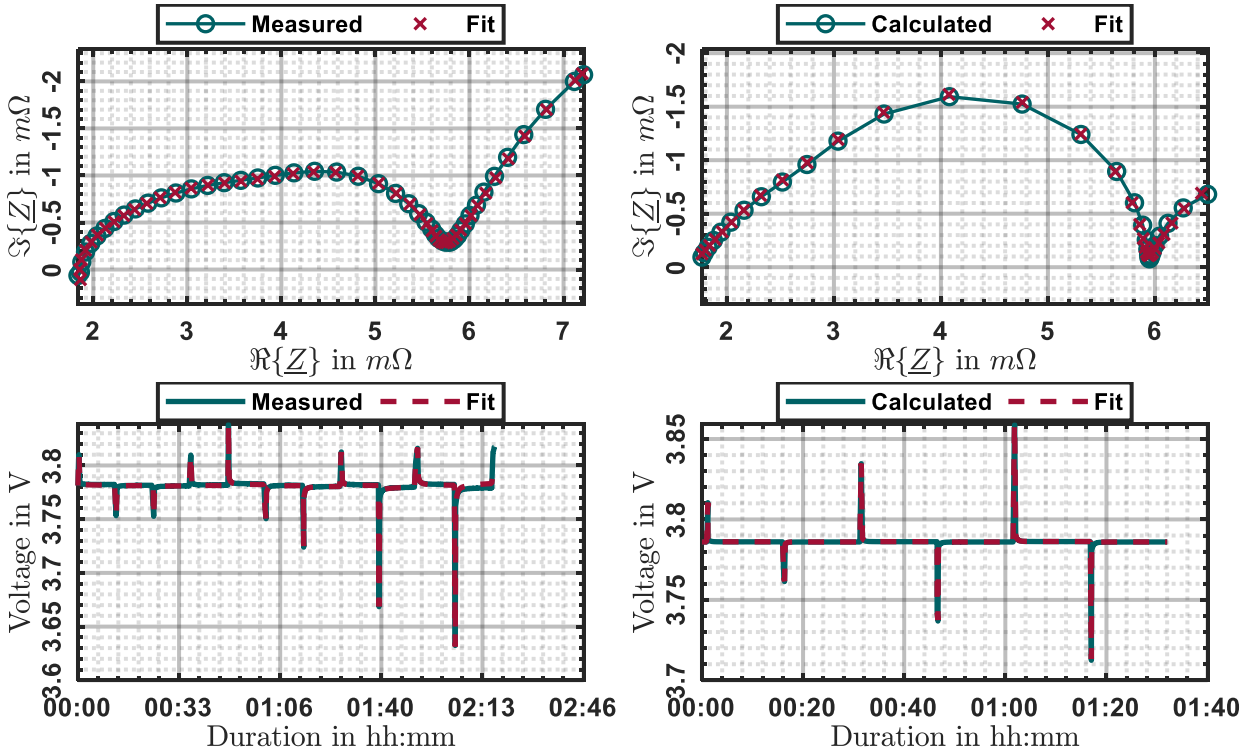

Figure 3.4: Fitting results for (a) the measured impedance in the Nyquist-Plot; (b) the calculated impedance in the Nyquist-Plot; (c) the measured pulse data; (d) the calculated pulse data.

After this hybrid fit and as the last part of the toolchain, a verification simulation is performed for every cell. The pulse profile used for the fit is simulated with the institute's ECM simulation called "ISEAFrame". These simulations are performed at 20% SOC, 50% SOC and 80% SOC at all specified temperatures. The results are shown in Figure 3.4. The simulated voltage course of the measurement data based ECM (M-ECM) (a) and the calculation data based ECM (C-ECM) (b) are compared to their input data. The M-ECM (c) error in the form of pulses is due to an instantaneous current rise in the simulation but a linear ramping current rise in the real measurement. The C-ECM (d) error is small, with only up to 4 mV deviation in the pulse phase.

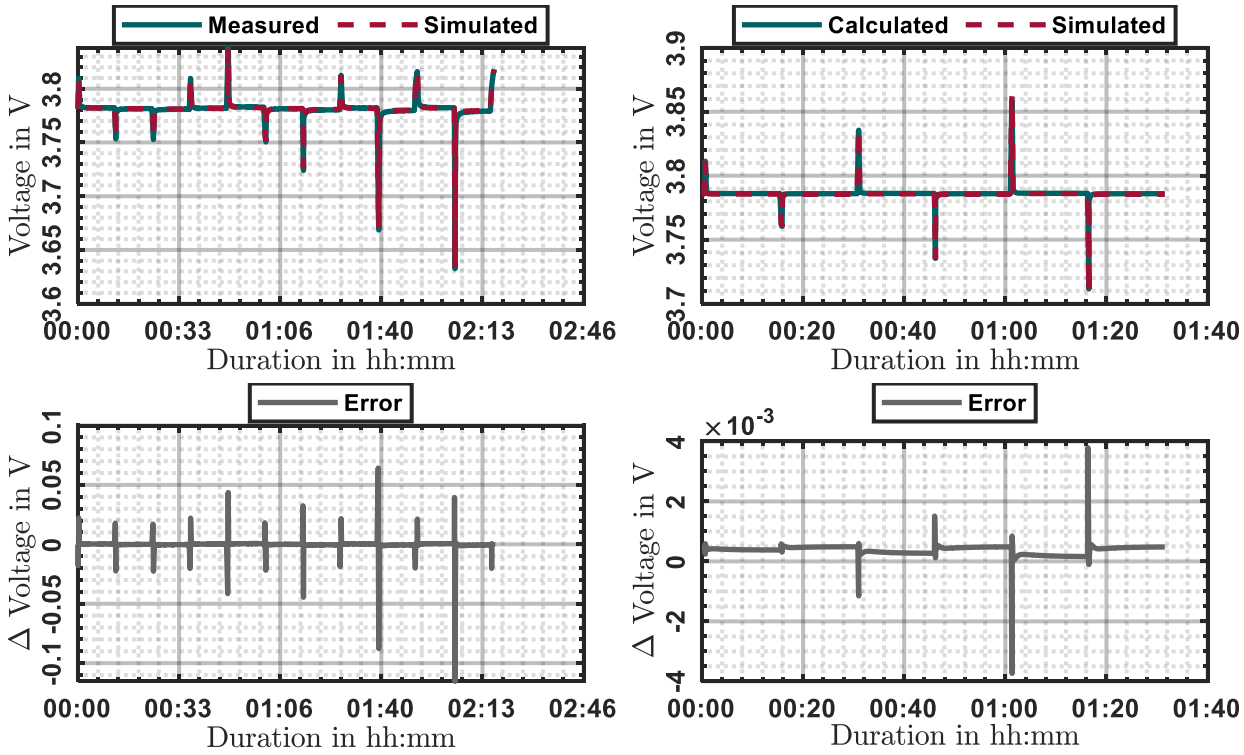

Figure1: Resulting voltage courses of the verification simulation: (a) simulation of the pulses with the model fitted to the measurement data compared to the measured profile; (b) simulation of the pulses with the model fitted to the calculated date compared to the PCM simulation result; (c) error between both voltages in (a); (d) error between both voltages in (b).

3.3 Drive Cycle

To validate the ECMs, we performed measurements on the real cell with two synthetic battery load profiles called SLCA and SLCB designed by colleagues of TU Munich. While the SLCA is only at a more or less constant SOC, the SLCB discharges from 90% SOC to 10% SOC with a highly dynamic current. As a result, the voltage courses are compared. For SLCA, a good simulation result for both ECMs is shown in Figure 3.5. A good result here means a small error in voltage peaks of less than 10 mV and good dynamic behavior of the ECMs.

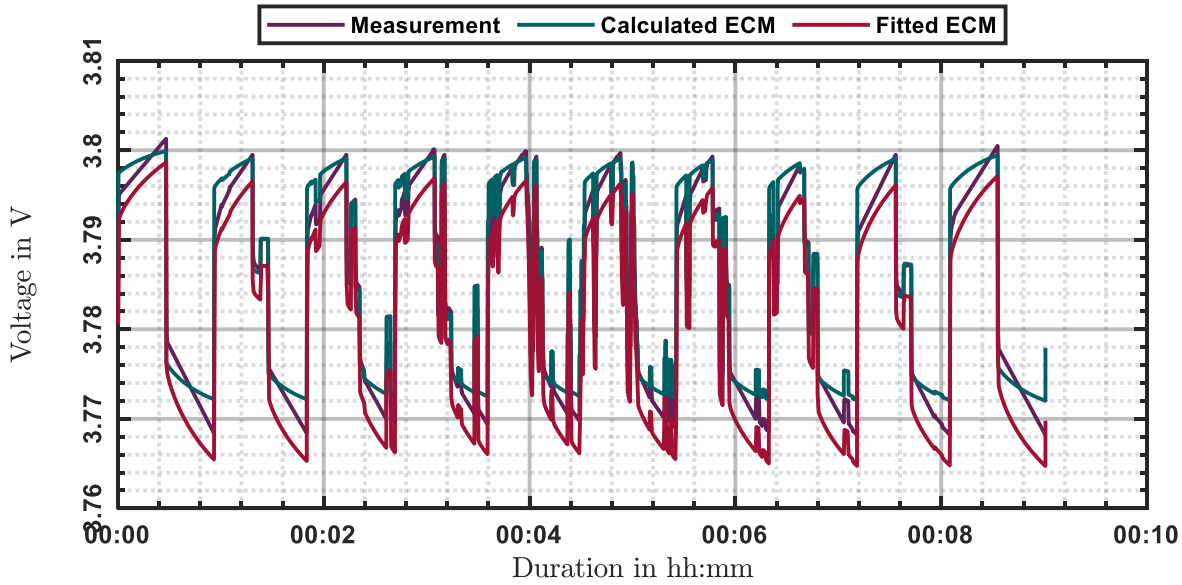

Figure 3.5: Comparison of measurement of the real cell and the ECM simulations of the measurement-data based ECM and the calculation-data based ECM.

The SLCB simulation shows a battery load profile, which is more related to EV applications because we see a significant DOD over the whole time. In Figure 3.6 (a), the voltage result of the M-ECM simulation is compared to the measured voltage. The related error is shown in (c). Additionally, in (b), the voltage result of the C-ECM simulation is compared to the measured voltage. The related error is shown in (d). The results still have some capabilities for improvement but already represent a very appropriate behavior close to that of the real cell. The simulation result of the M-ECM model has maximum error values of up to 25 mV, while the C-ECM model has maximum error values of up to 50 mV. The higher error values of the C-ECM simulation can be seen in the upper and lower SOC range higher than 75% and lower than 25%, while the simulation in between is close to the quality of the M-ECM parameter set.

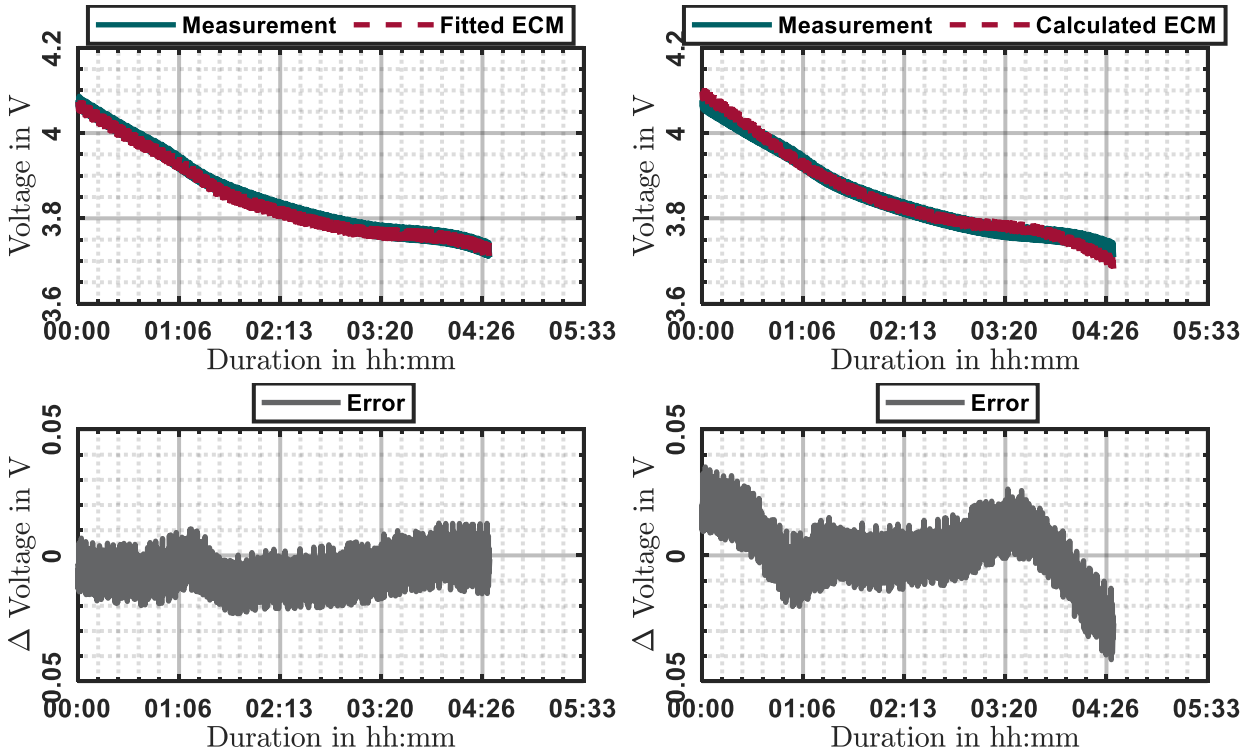

Figure 3.6: Resulting voltage courses of the validation simulation SLCB: (a) comparison of measurement and simulation with the M-ECM; (b) comparison of measurement and simulation with the C-ECM; (c) error between both voltages in (a); (d) error between both voltages in (b).

4 Conclusion

With the Synthetic Battery Modeling Toolchain, we can parameterize electrical impedance-based models from physico-chemical simulations, parameterized by virtually designed battery cells in our database. The resulting models for estimation can accelerate the design process, pre-filter the cell or cell material selection for a specific application, characterize novel materials before prototypes of such cells are available and shorten innovation cycles. In addition, studies that vary individual cell design parameters can be performed for real and virtual designed cell chemistries, thereby identifying optimization potential.

Acknowledgements

This work was financially supported by the German Federal Ministry of Education and Research within the SimBAS project (Grant No. 03XP0338B), managed by Project Management Jülich. The responsibility for this publication rests with the authors.

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