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Parameter Free Model for Diagnosis and Behavior Simulation of Energy Storage Units

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Abstract:
For the characterization, simulation and diagnosis of batteries, different methods can be used. One approach is the separation of static and dynamic behavior, to analyze it separately and to combine them into one model. The dynamic behavior is often characterized by pulse tests and spectroscopic methods. The static behavior is determined by measuring the open circuit potential at different state of charge and temperature. To be useful in an application the measured behavior must be converted into suitable models. The models should be valid over a wide operating range and applicable with only minimal loss of generality. These requirements can be met by nonparametric models. In this work nonparametric modeling of the open circuit potential as well as of the dynamic behavior is presented. Simulations were done and compared to measured results.

Key words: Battery, impedance spectroscopy, distribution of relaxation times, kernel regression, simulation.

Introduction

In applications electric vehicles, hybrids or stationary energy storage batteries as complex electrochemical systems require a powerful battery management system for diagnosis and control. These battery management systems usually contain algorithms for safety, behavior prediction and diagnosis as well as others. These algorithms rely on models of the battery behavior, thus the demand for accurate modeling. The modeling is done by either modeling the open circuit voltage and the dynamic behavior together: the most known are the Shepherd model and others semi empirical, [1][2], or models based on basic electrochemical equations [3]. A second approach would be to split the behavior into a dynamic and a static part. Here the open circuit potential is described using a look-up table [4], imposing strong memory usage, basic relations like the Shepherd, Unnewehr or Nernst model, and a dynamic part usually modeled by a limited number RC-elements [5]. Some of these models link single relaxations to electrochemical processes inside the cell but do not allow deeper insight.

The paper organizes as follows: in the next section it is shown how to calculate parameters for a non-parametric model from lab-measured impedance data, in section three a simplified way to describe the open circuit voltage and in section 4 the combination of both methods to simulate the dynamic behavior. The simulation is then compared with measured data and the differences are discussed.

Impedance Spectroscopy

Impedance spectroscopy is able to measure the linear dynamic behavior of a battery by excitation of single frequency components of the battery current and measurement of the battery voltage. The impedance is then defined as

$$Z(\omega) = {U(\omega)}\big/{I(\omega)} \qquad (1)$$

The resulting impedance spectra contain information on internal electrochemical processes as these processes are sensitive in different frequency ranges, thus allowing investigating different mechanisms with one measurement. For the evaluation of impedance spectra different strategies exist. The first would be direct modeling by complex impedance models including diffusion effects [6][7], modeling of electrode/electrolyte reactions [8] and modeling of porous electrode effects [9][10] beside parasitic effects like inductivities of the measurement setup. Finding a suitable model requires prior knowledge on the investigated system and sometimes overlapping effects make model selection hard. The evaluation using the chosen complex models is an ill-

posed inverse problem which requires the use of advanced fitting algorithms to determine the model parameters [11][12][13] and even then it is not guaranteed that the model will sufficiently describe the measured spectra. If the model is sufficient the determined parameters can be used to track several effects and use them for diagnostics. However, using these models for simulation can be cumbersome as they often include fractional behavior in the frequency domain (s^{α} -terms) leading to non-integer derivatives in the time domain [14].

Another evaluation strategy for impedance spectra is to find another representation of the data in way that it can be used for evaluation of chemical processes as well as for time domain simulations of the battery behavior. One such representation is the distribution of relaxation times [8].

Distribution of Relaxation Times

The distribution of relaxation times (DRT) assumes a density function, $\gamma(\tau)$, over the domain of relaxation times τ. This can be understood as using a measurement model with an infinite number of RC elements each with a fixed τ_i as depicted in fig. 1.

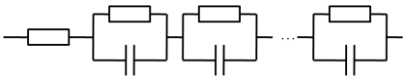

Fig. 1: measurement model used for the DRT aproach

Each RC-element is then weighted by $\gamma(\tau_i)$. The shape and position of components of this density describe different electrochemical processes. Thus it is still possible to identify different electrochemical processes.

DRT Calculation

The reconstruction of the DRT from impedance data is again an ill-posed inverse problem which includes solving a Fredholm integral equation of the first kind:

$$Z''(\omega) = R_{pol} \int_0^{\infty} \frac{\omega\tau}{1+(\omega\tau)^2}\, \gamma(\tau)\, \mathrm{d}\tau \qquad (2)$$

Different solution strategies for the determination of $\gamma(\tau)$ exist: direct fitting of elements of the density function [15], deconvolution approaches [16][17] and regularization techniques [18]. A more general overview is given in [19].

In the paper we will use the regularization approach as it is easily implemented and is handy for the solution of other linear problems.

After discretization eq. 2 becomes a system of linear equations with a coefficient matrix $\mathbf{A}$ with a high condition number and $\tilde{\gamma}(\tau) = R_{pol}\gamma(\tau)$:

$$Z''(\omega) = \mathbf{A}\,\tilde{\gamma}(\tau) \qquad (3)$$

thus calculation of the naive solution

$$\tilde{\gamma}(\tau) = \mathbf{A}^{+^{-1}} Z'' \qquad (4)$$

will lead to a strong amplification of measurement noise. $\mathbf{A}^{+}$ is the pseudo inverse of $\mathbf{A}$ as this matrix is not always square.

To stabilize the solution regularization can be used leading to a modified solution:

$$\tilde{\gamma}(\tau) = (\mathbf{A}^{\mathbf{T}}\mathbf{A} + \lambda^2\mathbf{I})^{-1}\mathbf{A}^{\mathbf{T}}\, Z''(\omega) \qquad (5)$$

enforcing flatness of the solution depending on the regularization parameter λ which is related to the noise in the measurement. This equation can be written in stacked matrix form and solved with standard tools, e.g. MATLAB ®.

The solution now suppresses the amplification of noise but is not necessarily positive as preset by the measurement model which forms the basis of this method. Usually additional non-negativity constraints are employed in eq. 5 leading to sequential algorithms for the solution.

Simulation using the DRT

From fig. 1 the way of simulating the dynamic behavior the linear dynamic response of a battery can be understood as a superposition of the dynamic responses of the single RC-elements. This can be implemented in a numerical efficient way as digital filter. The coefficients can be derived from the DRT: the time constants are given by the support of the DRT in the τ domain and the resistance value is given by the density value $\gamma(\tau_i)$.

Description of the Open Circuit Voltage

Modeling the open circuit voltage (ocv) serves two purposes. First is the simulation of the battery behavior and second it aids in the determination of the state of charge via tracking of the ocv. For the modeling of the ocv of a battery different approaches exist. The simplest way is to store the relation between state of charge, temperature and ocv in a look-up table and use interpolation methods to determine the ocv at different operation points. Another approach would be to use well known models like the Shepherd model [1], or other models that use the diffusion processes inside the bulk material of the electrodes as described in [3].

Another possible way to describe the ocv is to use kernel regression.

Kernel Regression

Kernel regression expands standard linear regression to the nonlinear case by using an implicit mapping of the input data. A linear equation can be rewritten in terms of inner products on the data used for the regression (the training data):

$$y = mx + b = \sum_l w_i \langle x, x_i' \rangle + b \qquad (7)$$

Here $x' \in X$ describes the data used for regression, and w is the weight associated to each input data. By using a nonlinear map $\phi : X \to F$, mapping the input data in some high dimensional feature space, one can expand this method to the nonlinear case:

$$y = \sum_l w_i \langle \phi(x), \phi(x_i') \rangle + b \qquad (8)$$

It can be shown, that the inner product of the input data in F corresponds to calculating some kernel on the input data, [20]:

$$\langle \phi(x), \phi(y) \rangle = k(x, y) \quad x, y \in X \qquad (9)$$

Thus it is possible to calculate the inner product in F without explicit calculation of the mapping $\phi(\cdot)$ as calculation of this mapping can be hard and sometimes impossible. We now have a nonlinear regression that can be easily calculated:

$$y = \sum_l w_i k(x, x_i') + b \qquad (10)$$

Depending on the kernel used, this allows different nonlinear functions to be regressed without having an explicit model. This can be useful if only the behavior should be approximated and no underlying fundamental laws have to be investigated.

The kernel regression can be expanded to select only necessary training data if a small error in the regression is allowed. This expansion leads to the support vector regression. With this method only a small subset of the training data is selected during an optimization process resulting in special support vectors. The determination of the support vectors requires the calculation of a sparse solution; powerful algorithms exist for this problem [20][21].

Experimental

For testing the proposed method a commercial 5 Ah Lithium Polymer cell was used. The cell has an ocv range from 3.3 to 4.2 V. It was modeled with kernel regression as described above using a multi quadric kernel:

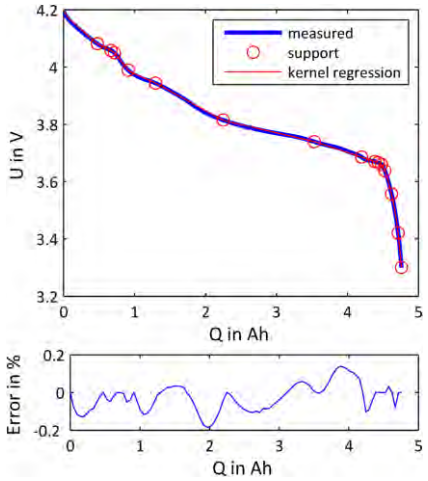

Fig. 2: ocv modeled using kernel regression with multi quadric kernel

Fig. 2 shows the ocv, the training data used for regression and the resulting nonlinear regression with overall only 20 support points used for regression. The second graph shows the relative error which never exceeds 0.2%.

The linear dynamic behavior of the battery was characterized by impedance measurements as shown in fig. 3. From these measurements the DRT, fig. 4, was calculated using regularization method as described above.

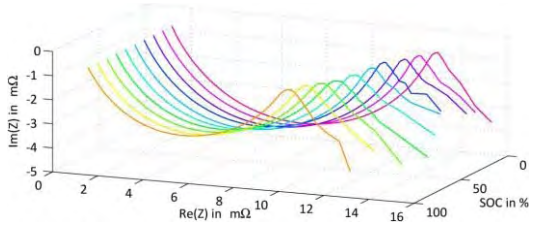

Fig. 3: measured IS spectra

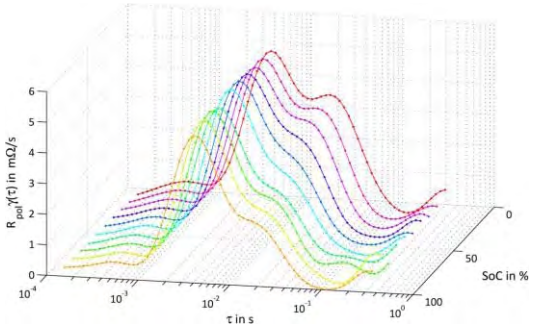

Fig. 4: calculated DRT spectra

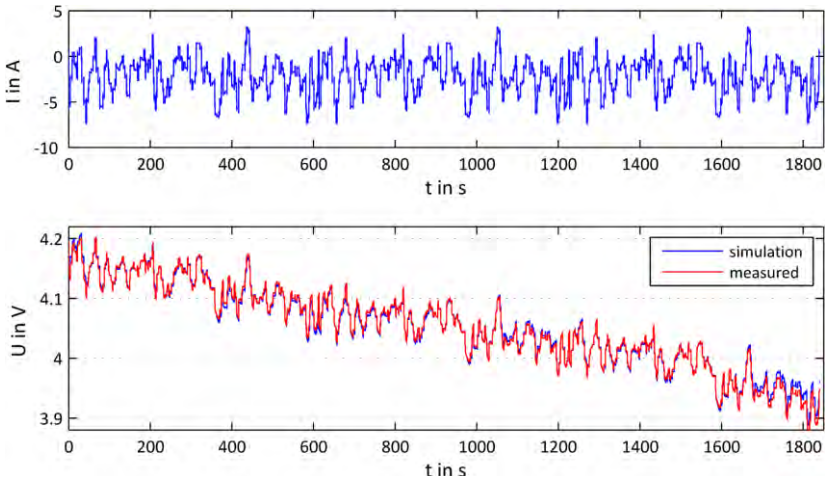

Fig. 5: (top) current used for measurement and simulation, (bottom) measured battery response and simulation results

The data above was used for the simulation of the battery response to random test sequence with an average discharge current of 1 A. Simulation time was 30 min with an overall removed charge of 1.04 Ah starting at 100 % SoC. The simulation was done neglecting temperature and intercalation capacity effects and assuming 98 % discharge and 96 % charge efficiency. The result is shown in fig. 5.

The simulated battery voltage is in good agreement with the measured response. The error is mainly due to inaccuracies in the ocv regression. Fig 6 shows the histogram of the residuals. The resulting overall error has a mean of 0.44 mV and a standard deviation of 5.2 mV which is comparable to the overall error of the ocv regression (μ = 1.1mV, σ = 2.8 mV).

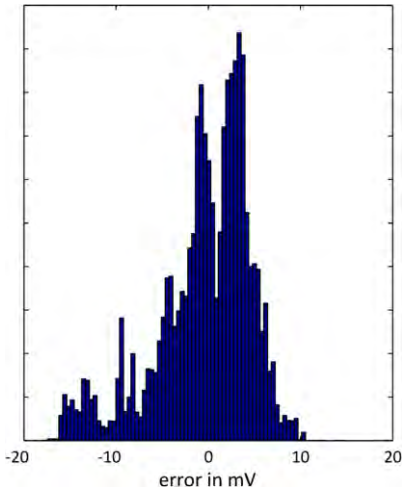

Fig. 6: distribution of the simulation error

Conclusion

A method was shown for the simulation of the dynamic behavior of batteries that uses non-parametric modeling approaches. The description of the dynamic behavior of a battery using the DRT approach serves two purposes: the identification of electrochemical processes and the parameterization of a digital filter for simulation. In combination with the kernel regression a straight forward simulation procedure can be realized. As a benefit the kernel regression needs less memory for the storage of the SoC-ocv relationship (20 coefficients and 20 support points).

The DRT as well as the kernel regression are useful tools for the characterization of batteries and their efficient modeling in various applications.

Further work will focus on the expansion of the DRT method for the use in the nonlinear battery behavior identification. The kernel regression method can aid in the efficient storage of look-up tables or for the development of SoC determination algorithms.

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