A Modelica Based Lithium Ion Battery Model

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Abstract

The initial integration of a large scale battery system in existing end products like cars is usually of experimental nature. So are the simulation models supporting its design process. In the following a comprehensive Modelica model is introduced for the simulative description of the physical behavior of lithium ion battery cells packs for relevant aspects and use cases. It is part of the Modelon Battery Library, a commercial Modelica library to model battery cells and packs of various types, shape and grouping.

Thermal behavior, electrical behavior and the impact of the degradation due to aging are considered as they influence each other.

The model parameters to calculate the electrical behavior are to be derived from measurements; an optimization algorithm to obtain them is integrated in the package using the Optimization Library. Functions to validate the model against these measurements are included as well.

As an application example the simulation of an energetic energy storage system in the model of a battery electrical vehicle is shown.

Keywords: battery model; lithium-ion; behavioral modeling; electrical vehicle

1. Motivation

In Battery Electric Vehicles (BEV) and Hybrid Electric Vehicles (HEV) the majority of car producers focus in lithium ion based battery concepts due to their high performance density in connection with reasonably high lifetime and acceptable thermal behavior. As these vehicles become more accepted on the market, the production numbers are supposed to increase with some positive pricing effect. It is likely that this will also make lithium ion batteries attractive for use in homes and other decentralized energy systems – especially in connection with renewable energy.

Practically all lithium ion based batteries show more or less troublesome aging behavior which reduces the lifetime to inacceptable levels, if no particular provisions are taken to avoid or reduce it. Aging appears as calendric and as cyclic effect according to the number of charging and re-charging events. The main aging effects [1] of current lithium battery systems are:

- Accumulated damages of the solid electrolyte interface (SEI) between anode and electrolyte caused by chemical reactions and physical movement due to temperature changes.
- So-called lithium plating, i.e. the deposition of metallic lithium on the anode.

Aging effects are severely influenced by the thermal load on the battery. Therefore high performance battery systems need to be kept within a certain temperature range by cooling and sometimes heating.

For whatever application, in current battery systems single cells of a certain type are arranged in stacks, modules or packages through serial and parallel alignment of the cell. Cells can have cylindrical, prismatic or so-called coffee bag shape. Apart from the electrical interconnection, the cells are integrated in some thermal design concept to cool them and reduce aging. It should be noticed that car as well as energy system manufacturers design battery systems according to the needs of the general concept of their product. I.e. the design of the battery is not based on a unified single-type approach, but many different concepts are required to cover the large range of system requirements.

Fig. 1, Battery system of the MUTE electrical car project by TU Munich

Therefore, the battery model presented in this paper uses the cell as a base unit to be parameterized with fairly simple data sheet and empiric input. With the help of pre-defined templates, organized as shown in figure 1, the user can easily set-up a battery model as an electrical and thermal system consisting of a single cell.

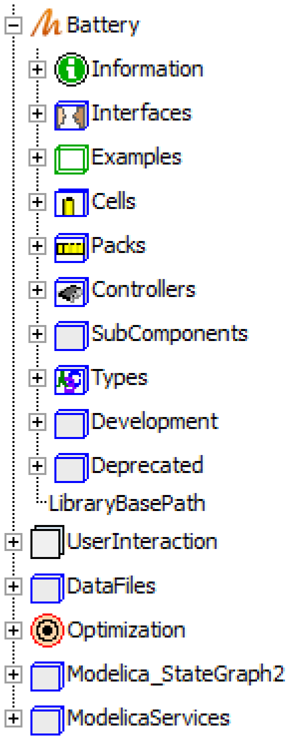

Fig. 2, Content of the Battery Library

Aging information is provided by an integrated aging system or user-defined approach.

While lithium ion battery cells are usually described by RC circuit elements, the electrochemical effects in lead-acid batteries are approximated in a separate model to take account of the specialties of this battery type.

2. Electrical Modelling

The main requirement for cell models used in system simulation is to provide accurate information on the macroscopic characteristics (e.g. voltage, current and state of charge) combined with reasonable computation time. In many applications these requirements are fulfilled by models using an electrical equivalent circuit.

The voltage of a battery U can be described as the difference between the open circuit voltage U_{OCV} and a number of overpotentials η_i caused by different electrochemical effects:

$$U = U_{OCV} - \sum \eta_i$$

These overpotentials can be modelled with electric networks. In figure 2 the voltage characteristic for the step current discharge of a NiMH cell is shown.

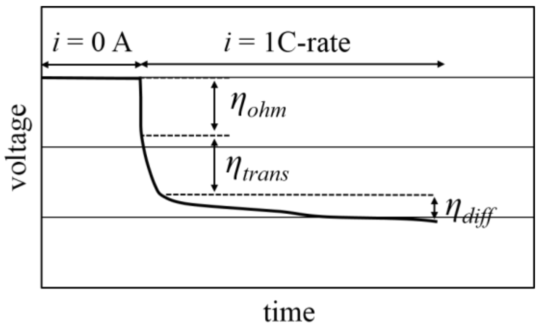

Fig. 3, Voltage characteristic of NiMH cell [1]

The overpotential is divided into an ohmic overpotential η_{ohm}, overpotential caused by charge transfer and the electrical double layer η_{trans} and overpotential due to diffusion η_{diff}. An electrical equivalent circuit capable of reproducing the shown voltage characteristic is shown in figure 3, whereas the dynamic behavior the overpotentials are modelled using RC-circuits.

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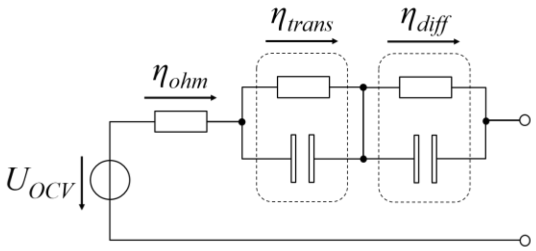

Fig. 3, Equivalent circuit

The performance of a cell is strongly depends the battery current, state of charge, temperature and other factors. To achieve good performance of the model over a wide range of conditions the consideration of these dependencies in the models of the electrical components and their parameterization is crucial.

The presented library offers equation based and table based modeling of the electrical components. As an example of equation based modeling a lithium ion cell model [2] and a lead acid cell model [3] are implemented in the library. The electrical equivalent circuits of the models contain serial resistors, RC-circuits, voltage sources representing the open circuit voltage and current sources describing the leakage current. The functions representing these elements are derived from measurement data and depend on the temperature, state of charge and current.

The table based models perform a table lookup to determine the parameters of the components in the electrical circuit. The library offers pre-defined templates for 2D and 3D interpolation. They enable a variable composition of elements in the equivalent circuit. In the 2d interpolation template the dependency of the lookup tables can easily be configured.

For the simulation of battery packs containing multiple cells, templates using discretized or scaled cell models are implemented. In the discretized pack models every cell is modeled separately. This enables the analysis of the packs' electrical behavior when unconformities of the included cells occur. As the geometric layout usually doesn't correspond to the electrical connections of the cells in the pack, a connection Matrix *M* is defined, that offers the possibility to connect the electric connectors of the cells in a given design.

3. Parameter Estimation

When modeling the electrochemical processes in a battery using a simplified approach like an electrical equivalent circuit, the choice of the circuit's components and the parameterization of these components determine the performance of the model.

A widely used approach to parameterize battery models is the generation of lookup tables from measurement data using numerical optimization algorithms ([6], [7]).

As mentioned before the battery performance is strongly dependent on numerous factors. The number of dependencies that are important for the interaction within the investigated system and the size of the range in which they need to be considered often lead to a complex optimization task.

The developed library provides a Dymola internal approach to execute parameter estimations using the commercial library Optimization developed by the German Aerospace Center (DLR) which includes several numerical optimization algorithms [10]. A template of a parameter estimation for an equivalent circuit containing a serial resistor and two RC-circuits generating 2d lookup tables is implemented. The workflow of the template is illustrated in figure 4.

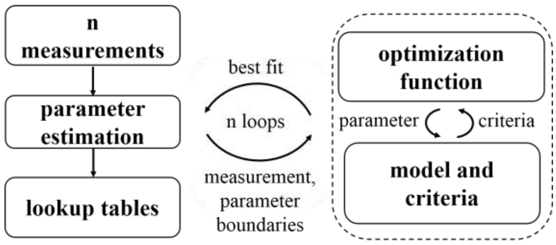

Fig. 4, Parameter estimation workflow

The inputs to the parameter estimation routine are inner resistance measurements from discharging or charging the battery with step currents. For each measurement an optimization function from the Optimization Library is called. The optimization function simulates a model that contains the equivalent circuit and computes the optimization criteria which is returned to the optimization function. The outputs of the parameter estimation are 2D lookup tables for the resistors and the capacitors in the circuit.

When computing the parameters of all components in a single estimation task the generation of plausible lookup tables is a complex challenge [8]. To simplify this challenge and dictate e.g. which RC-circuit represents the fast dynamics and avoid a switch of assignment during the estimation task, the boundary *b* for each parameter can be set by

$$b = k_1 + k_2 \cdot \Delta R^{k_3}$$

ΔR is the increase of the inner resistance during the measurement and k_i are constants defining the boundary. This rather simple method showed acceptable results estimating current and state of charge dependent tables for a NiMH cell.

4. Thermal Model

In order to determine the influence of varying temperatures on electrical and aging behavior a thermal model of the cell and its surrounding environment is required. Heat inside the cell is generated mainly due to Joule effects, the chemical reactions are only weakly exothermic or even endothermic. Thus the generated heat corresponds to the power loss calculated in the resistors of the equivalent electric circuit which are therefore connected to the thermal model.

Cell

The thermal model uses a template/interface structure with a replaceable thermal model such that the discretization level can be adapted by the user. All models are based on a finite volume approach, using heat resistors and thermal capacities. The user can choose between 0D and 1D models, further models can be added easily

Conditional heat ports at the top, side and bottom of the cell reduce the complexity without reducing the flexibility of the thermal management design.

Equations for the calculation of thermal parameters are provided for cylindrical and prismatic forms. Material records for the most common materials are also included.

Packs

In addition to the cell, the thermal model of the pack might consider housing and in case of the discretized pack a filling material in between the cells. Simple heat transfer models for convection and radiation are also included.

For the scaled models, the heat flow of a single instance of the cell is multiplied with total number of cells. Effects such as heat conduction in-between the cells can only be considered in the discretized pack models with several instances of the cell model. Heat transfer via pins can also be modelled; the connections between the pins use the same connection matrix as the electric part.

A two-dimensional heatport simplifies the icon of the housing, Cells, filling, and the exterior heat ports can easily be connected.

The temperature of the pack can be monitored with a provided controller model. Based on given limits. Boolean signals for activation of heating or cooling are emitted.

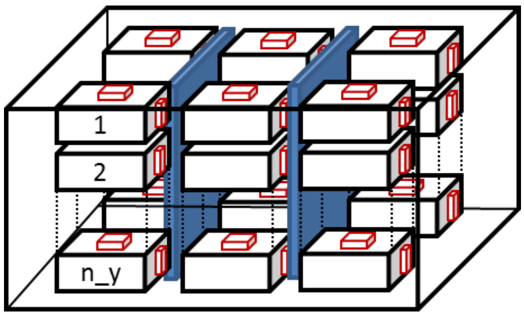

Fig. 6, Structure of thermal model of a discretized battery pack

5. Aging Model

The capacity as well as the behavior of a cell change with age and cycle numbers of the cell. To account for the effects of the most important factors temperature, current rate and SOC, a flexible aging model based on the StateGraph library has been implemented.

The aging factor φ denotes the ratio between the current value and the value at t=0:

$$\varphi_A = \frac{A(t)}{A(t=0)}$$

Using this definition, the actual value can be determined just by multiplying with φ. Resistor and capacitor models have a conditional input for the aging factor that can be activated in the parameter dialog.

The flow chart in figure 6 shows the signal flow structure in the aging model. The cycle detector detects the end of a cycle and triggers the calculation of the aging factors in the cyclic and calendric aging models. Mean values

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for temperature, depth-of-discharge (DOD), voltage and current are calculated for the previous cycle as the aging models are all based on continuous boundary conditions. The aging factors are discrete values, thus they are constant during one cycle until the next calculation is triggered. Therefore, the aging factors represent the age of the cell at the beginning of the next active cycle. Start value for all aging factors is set to 1.

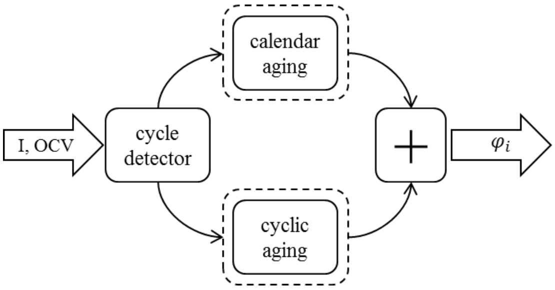

Fig. 7, Flow chart of the aging model mechanism

Both aging models use a semi-empirical approach to determine the aging factor based on recent publications ([4], [5]). The aging models are replaceable and can be switched on/off individually. New aging models can easily be added by using the provided interface.

The aging of cells during storage (calendar aging) is mainly caused by electrolyte decomposition and the growth of the solid electrolyte interface. Ecker et al [5] describe this process with a square root dependency on time. For voltage and temperature, an exponential approach is chosen. The implemented model is based on extensive measurements on 30 NMC cells stored at different SOCs and temperatures. The semi-empiric approach allows the user to adopt the parameters to his data even with a low number of measurements. The calendar model calculates aging factors for the cell capacity, the serial resistance and the parameters of the first RC-circuit. Thus, the degradation of capacity as well as the loss of power and changes in the dynamic behavior due to calendar aging can be shown.

It is supposed that the loss of active lithium due to anode degradation is the cause of capacity loss due to cycling of the cell [5]. Wang et al performed measurements with varying time, temperature, depth of discharge and discharge rate. They developed a generalist model for cyclic aging that can be adapted to different Li-Ion chemistries as long as the aging mechanisms are also based on diffusion processes. By using the energy throughput of the cell as input of the aging factor calculation instead of time, the equation becomes independent of the charge rate. As the experiments showed little influence, the SOC of the cycled cell is neglected.

Figure 7 shows the aging factors for a cell cycled with a constant current rate between 0.5 and 0.55 SOC at 20°C. The aging factors for capacities decrease, those for the resistance increase, both reducing the capacity as well as the power of the cell.

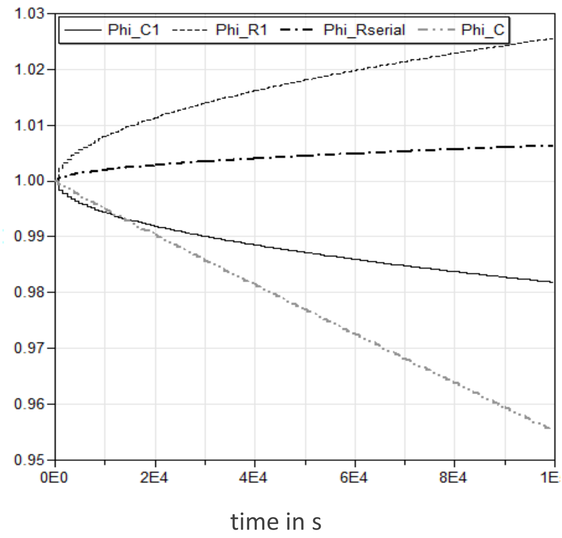

Fig. 8, Aging factors for cycling a cell between 0.5 and 0.55 SOC with 0.5C-Rate at 20°C

6. Application Example

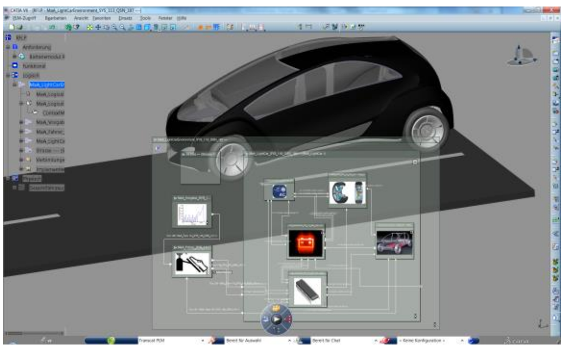

Fig. 9, Battery Lib within a Catia V6 Systems model of an e-car

In order to demonstrate the application of the Battery Library within a vehicle environment, an example project has been created based on the “Light Car” – a battery electric vehicle concept designed by the company EDAG. The development methods applied were chosen to replicate the real-world methods as closely as possible. The partners participating in the project are the companies EDAG (to represent the car development competence), Transcat (to represent Catia V6) and Modelon (to represent system simulation with Modelica). Dimensioning the battery in terms of vehicle autonomy and its aging behavior are also in the scope of the project as well as the first time application of state-of-the-art development tools. In order to realize typical driving scenarios and test cycles like NEDC the system simulation model consists of a longitudinal dynamic vehicle model, the driving resistances and a driver. The focus of the model lies on the battery system, including its electrical, thermal and aging behavior and the battery controller.

In current e-car projects, the battery cells are supplied by cell manufacturers, but combined to a battery system at the OEM car producer. The control of the battery's primary states such as current, cell temperature, state of charge and state of health has to be in line with the entire car concept and is therefore OEM work, too. The key design factors of the battery system are the arrangement of the cells in stacks and packs under maximum utilization of their potential in terms of performance and duration of life. In this context, due to the very high influence of the temperature on the aging, certain limits have to be kept during all conditions of operation. In the presented project, the cooling design is based on air flow. For a maximum precision of the calculations, the 1D system simulation results from the Modelica / Catia V6 Systems environment have been verified using a finite element simulation in the tool Simulia.

A typical simulation result in terms of a cell temperature is shown in Fig. 9.

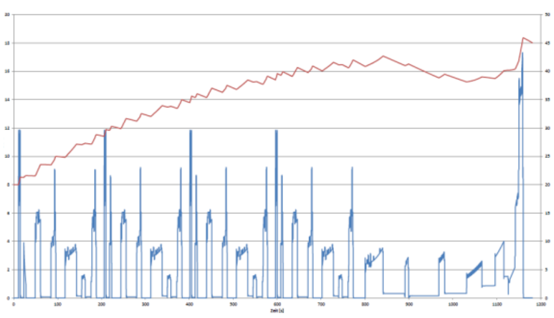

Fig. 10, Temperature (red) and heat performance (blue) of a battery cell within the NEDC drive cycle

7. Summary and Outlook

The battery model of Modelon's Battery Library for Lithium Ion cells has been described in its structure, functionality and employment.

The calculation of the electrical behavior by equivalent circuit models with table based and equation based approaches has been shown as well as its parameterization function based on the Optimization Library. The thermal model has been described for single battery cells and battery packs. The estimation of degradation due to cell aging has been modelled in different ways, calendric aging and cyclical aging. An example for the integration of the battery model in a vehicle simulation of an electrical car has been described in the "Light Car" project.

The Battery Library was designed with the intention to be coupled with other system models in Modelica-based or other simulation frameworks. As the battery model features all necessary interfaces, the code of a battery management system in a signal flow simulation environment can be attached as an FMU. Vice versa, it is possible to use this physical battery model for the prediction of the thermal-electrical behavior as well as aging on a battery management system or for a "model in the loop" approach.

The ongoing development of the Battery Library is heading towards electrochemical modelling of the aging behavior by the implementation of a "Dual-Foil-Model" [9] and the advancement in the thermal modelling of large electrical energy storage systems comprising several battery packs. Introduction of models for capacitors of the "super capacitor" type is also planned.

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