A method of computer modelling the lithium-ion batteries aging process based on the experimental characteristics

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Abstract. The paper presents a method of modelling the processes of aging lithium-ion batteries, its implementation as a computer application and results for battery state estimation. Authors use previously developed behavioural battery model, which was built using battery operating characteristics obtained from the experiment. This model was implemented in the form of a computer program using a database to store battery characteristics. Batteries aging process is a new extended functionality of the model. Algorithm of computer simulation uses a real measurements of battery capacity as a function of the battery charge and discharge cycles number. Simulation allows to take into account the incomplete cycles of charge or discharge battery, which are characteristic for transport powered by electricity. The developed model was used to simulate the battery state estimation for different load profiles, obtained by measuring the movement of the selected means of transport.

1. Introduction
REP SAIL research and development project aims to build an electrically powered yacht. Energy is accumulated in lithium-ion batteries, like in most other electrically powered means of transport. Selection of power source was based on analysis of yacht operating conditions, including predicted energy consumption in various sailing modes, and operation characteristics of the battery obtained with experimental measurements [1, 2].

The REP SAIL model (figure 1) was built using an experimental measurements of battery capacity dependent from currents of charging or discharging. It assumes that the battery is constructed from cells with identical parameters. Operation characteristics for a single battery cell were obtained in the form of discrete functions \{ \( E(I, t) \) \} that represent relationship between collected energy \( E \) and time \( t \) at constant charge/discharge current \( I \), for various currents \( I \in \{ I_1, I_2, \ldots, I_k \} \) in the range between the minimal current \( I_1 \) to the maximum current allowed for specific cell type \( I_k \). Measurement data are stored in the relational database. For other currents than measured, the spline form interpolation of the \( E(I, t) \) is used. The REPSAIL behavioral model consists of measurement data and interpolation method [3, 4, 5]. The algorithm of the computer simulation of the battery exploitation needs an characteristics of charge/discharge battery current in time, and the initial battery charge level. Next the battery state in time \( \hat{E}(I, t) \) is calculated as iterations. The model aims to predict battery condition at any given moment, provided that the load and charging processes over time \( I(t) \) are known.
Proposed model was implemented as a computer program [6] and was subject to validation tests. At the time of writing of this article there was no operational electrical yacht prototype, so the validation process used measurement data obtained with test drives of electrically powered vehicle. We need to notice that versatility is an important feature of the proposed model, which allowed for validation with the use of different input data than initially planned. This model construction method has a drawback of time consuming nature, and advantage of very precise representation of real condition.

Despite the abovementioned advantages, the battery model that authors of the paper proposed does not consider aging processes specific to lithium-ion batteries. Electrically powered vehicles working cycle is usually characterized by frequent changes in battery charge and discharge modes, so the aging process can be a significant factor in predicting the battery charging level and its general state of health.

![Proprietary model of REP SAIL battery.](image)

This paper presents proposition to complement the battery model with aging module, aging module operation algorithm, and computer modelling results of battery behavior at long term operation at a specific profile of cyclic load.

2. **Assumptions in the battery aging model**

Li-Ion batteries are subject to aging process. They gradually lose capacity as the number of the charge and discharge cycles increase. The references describe many models of battery aging. Authors [7, 8] indicate that aging process simulation based on model of electrochemical processes running inside cell requires high computational power and is of little use practically. Empirical models on the other hand require large collection of experimental data, which is money and time consuming. Analytic models of cells offer poor adaptation to various types of batteries. Statistic methods are quite the opposite, they can be easily adjusted to many types of batteries, however effectiveness heavily depends on the size of collected data [9, 10]. Once strong and weak points of specific model types of battery aging have been analysed, we made a decision to construct the REP SAIL aging model based on empirical data. That is due to great scope of experimental data collected during 2 years of the project run. Besides, such approach is compliant with the concept of behavioural model of the battery discussed earlier.
At the foundation of the REP SAIL battery aging model lies an assumption, that the battery aging process is not regular at operation with various currents, which hinders derivation of general approximation formula. Therefore, range of allowed battery operation currents has been divided into intervals. It is assumed that aging process for all currents within one interval range is identical. Interval boundaries are selected based on analysis of the battery cell measurement characteristics. On one hand, it is advantageous to increase number of intervals to eliminate errors that originate from battery behaviour differences for currents near lower and upper limit of an interval. On the other hand, necessity of large number of experimental measurements significantly extends time needed to create the battery model.

A charge/discharge cycle will be defined as such change of the battery cell state, when the total change of energy exceeds maximum capacity of the cell $E_{\text{max}}$. We assume that the energy transferred during the cell charging process (positive value) and the energy consumed during operation (negative value) are counted separately. This allows to count the number of battery cycles in real conditions operation, when the battery cannot be fully discharged or fully charged. At the execution of subsequent cycle $m$ the present maximum cell capacity $E_{\text{max}}$ is reduced by the value $\Delta E(m)$ calculated with the experimental data for the number of cycles $m$.

3. Construction of the battery aging model
Next, we will discuss the aging model construction process for the battery built with Panasonic NCR 18650B cells. The cell type selection was based on the type of batteries in electrically powered vehicle, which was used for experimental measurements of real operating characteristics. This allowed to compare the results of computer modelling with the actual battery wear.

The battery has been built with the cells configured as presented in Table 1 to provide appropriate operating characteristics specific for design of electrically powered vehicle.

| Table 1. Battery configuration. |
|--------------------------------|
| Capacity, [Ah] | Voltage, [V] |
| Single Cell | 3.4 | 3.6 |
| Battery | 408 | 648 |

Next, a computer simulation has been run for the process of battery operation, with real input data acquired with measurements, but aging process was not included. Negative current value $I$ corresponds to battery discharging, positive value corresponds to charging. In the given example, battery charging occurs while driving and braking (partial energy recovery at regenerative braking). Figure 2 presents simulation at a scale of a single battery cell for 200 minutes drive without long stopping periods.

Table 2 presents summary of the modelled section and compares the results of the computer simulation with the real measurements of battery condition changes.

| Table 2. Results of discharge modelling. |
|----------------------------------------|
| Simulation | Real measurement |
| E cell, [Ah] | Cells in battery | E bat, [Ah] | Discharge, % | E bat, [Ah] | Discharge, % |
| Drive start | 1.699 | 120 | 203.88 | 49.97% | 146.79 | 35.98% |
| Drive end | 1.082 | 120 | 129.84 | 31.82% | 88.24 | 21.63% |
| Battery level change, total | 74.04 | 18.15% | 58.55 | 14.35% |
| Battery level change, 1/h | 5.44% | 4.31% |
Figure 2. Battery operation process modelling with the use of real data, without aging.

The data in the Table 2 show that the computer simulation of battery use over 1 hour differs from real measurements by ~1% of maximum capacity, which indicates correct representation of battery operation process in the model.

To include the aging process in the battery model, we carried out experimental measurements that aimed to estimate the battery capacity reduction at repetitive charging and discharging with constant current at selected intervals.

Figure 3. Change of the battery capacity in relation to the number of discharge and charge cycles.

We decide that for each discharging, constant current $I_k \in \{ I \}, k = 0..n$ there will be experimental measurements of relationship $E(I_k, t)$ with the battery fully charged at the beginning, i.e. $E_0(I_k, t = 0) = 100\%$, and fully discharged at the end. The battery is charged with the specified current after each discharge. To obtain characteristics of battery capacity changes as a function of number of cycles $n$, we will do measurements repetitively until the battery capacity is reduced to 50% compared to initial level. Experimental characteristic for battery aging for a specific current $I_k=1C$ is presented on Figure 3. (Note: I=1C denotes charging current, which allows to charge in 1 hour; for battery under tests it is 1.6A.)
By repeating the measurement series for different values of the constant current $I_k$ we can obtain a set of experimental characteristics, as presented in Table 3.

**Table 3. Relationship between battery aging factor and number of cycles.**

| Current interval no. | Maximal charging current in the interval $I_i$ [mA] | Number of cycles $n$ | Battery capacity reduction $E_{\text{max}}$, % |
|----------------------|-----------------------------------------------|----------------------|----------------------------------|
|                      |                                               |                      | Total for $n$ cycles | Averaged for 1 cycle |
| 1                    | 400                                           | 100                  | 2.92%                          | 0.0292%            |
| 2                    | 800                                           | 100                  | 6.08%                          | 0.0608%            |
| 3                    | 1200                                          | 100                  | 14.45%                         | 0.1445%            |
| 4                    | 1600                                          | 100                  | 25.14%                         | 0.2514%            |
| 5                    | 2000                                          | 100                  | 34.07%                         | 0.3407%            |

4. **Consideration of the battery aging process in the computer model**

Studies on how number of battery charging cycles reduces its capacity were carried out for constant currents. In practice, use of a battery in electrically powered transport vehicle means frequent changes of absolute current value and direction of the current. Including this factor in the battery model required to take the following assumptions, which facilitate count of battery work cycles:

1) for any time period $t_i$, where the battery loading current $I(t_i)$ falls into one interval (Table 3) we will assume, that the aging process is in line with characteristics for that specific interval;
2) we will sum up partial changes of energy $\Delta E_i$ within each of the current intervals, positive and negative separately (Figure 4);
3) when total energy flow $\Delta E_i$ in an interval $i$ exceeds maximum running battery capacity $E_{\text{max}}$, counter of total number of cycles will be incremented $n := n + 1$, and the value $\Delta E_i := 0$;
4) after the number of cycles $n$ is increased, the maximum battery capacity $E_{\text{max}}$ is reduced in accordance with the factor defined in Table 3, i.e. $E_{\text{max}} = E_{\text{max}}(100 - W)$, where $W$ is the battery aging coefficient (the last column in Table 3).

![Figure 4. Concept of battery energy changes counting by the current intervals.](image-url)
5. Modelling of the battery aging based on the real drives data
To show the effects in the battery model operation, a computer simulation of electrically powered vehicle drives has been run for a selected route and a long period. Source data contain real electric vehicle drives along the route, obtained by everyday drives over one month. The data has been extrapolated to longer range of time (year) to emphasize effects of the battery aging. Figure 5 shows the simulation result.

![Graph showing battery aging over time and days](image)

Figure 5. The result of the modelling of the battery aging.

The simulation allows for rough estimation of the battery wear at continuous operation over a specified time range. Practical verification of obtained results is complex due to lack of real data over such long time. Therefore, verification of the model is planned only after gathering necessary experimental data, which will allow to evaluate level of the battery aging. Just like for the verification of the battery model without aging, we can expect high consistency between the modelling results and the control measurement at the end of one year operation period.

6. Conclusion
The paper presents enhancement of the computer model of the Li-Ion battery used in electrically powered transport vehicles with the battery aging process caused by repetitive charge and discharge cycles. The battery model has been evaluated by the research team of the Warsaw University of Technology under the REP SAIL project. The model belongs to the class of behavioural models, because it is based on the experimental measurements. Extrapolation of the battery behaviour depending on its load distribution over time is carried out by the computer program, that uses base of measurements that describe relation between battery energy and the standardized currents. Specific character of the proposed model derives from its close relationship with the cell type used in the battery design. Each cell requires separate experimental measurements, and that significantly extends time needed to create the model and requires consideration of its imperfections. Advantages of the model include high level of consistency between modelling results and the actual results obtained with direct measurements. Error of the battery level estimation for 1 hour modelling falls within 2–3% range.

Model extension with the battery aging processes has been proposed. In order to include this feature in the computer model, the battery capacity changes has been studied for specific charging currents, with dependence of number of chargings. Obtained experimental data was the foundation to calculate the battery aging coefficients for specific loading current intervals. Battery work cycle count
format has been proposed, based on integration of function that describes the battery loading power over time, separately for different current intervals.

Modified battery model was demonstrated to assess reduction of the battery capacity in regular operation over one year. Input data included measurement data of electrically powered urban transport vehicle, for which consistency had been experimentally observed between modelling of battery charge level and registered actual state. Verification of the battery aging model is planned once there is available information about actual wear after one year of service.

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