CHARGE AND DISCHARGE BEHAVIOR MODELLING AND SIMULATION OF LI-ION BATTERIES USING QUCS-S SOFTWARE

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Abstract. The paper presents an improved SPICE model of a Li-ion battery cell, simulating its charge and discharge behavior during an accelerated aging procedure. The model is based on our earlier developed model, presented in a research paper. The SPICE model is implemented in the QUCS-S open-source software. In the model, problems related to the convergence of the simulation process have been mostly eliminated. The model is implemented using real measurement data for standard Li-ion batteries with automotive applications. The developed simulation model includes models of the measuring equipment used in the accelerated aging procedure, in addition to the battery model. Results of model verification are presented, including error analysis.

Keywords: circuit simulation; Li-ion battery pack; QUCS-s simulator; SPICE modeling.

1. INTRODUCTION

More and more devices are using rechargeable batteries for power. One of the most widely used rechargeable batteries is the lithium-ion battery [1]. Until recently, this type of battery provided power to portable consumer electronic devices (phones, laptops, watches, headphones, etc.); today, they find much wider application, especially in electric vehicles. In these applications, battery packs with enormous capacity are required, composed of multiple parallel connected groups of lithium-ion cells in series.

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In the development of various electronic systems related to the operation of batteries (chargers, BMS systems), as well as devices powered by these batteries, it is very useful to have a simulation model of a battery cell or pack. It is most convenient for this simulation model to be implemented in the environment that is used in the development of the electronic system. These are most often electronic circuit simulators, of which SPICE-based ones are most often used. [2]

Li-ion battery electric modeling is a widely considered scientific problem [3], [4]. These publications present the widely used first-order equivalent circuit and second-order equivalent circuit.

In our earlier research [2], we presented a model of Li-ion battery cells in the QUCS-S environment, which is suitable for simulating the behavior of the battery in the charging process. The present study aims to develop an advanced model based on the earlier one. The aim is to eliminate its disadvantages, as well as to expand its capabilities, especially in terms of simulation of the discharge process.

The developed model is tailored to the capabilities and specifics of QUCS-S [5] software (used as a graphical environment for development and simulation of the model) and NGSPICE [6] software (used as a SPICE simulation engine). During the development, the concept of using the specific element in the QUCS-S EDD (equation-defined device) has been preserved. This element offers a great deal of flexibility in model development, especially in the modeling of nonlinear dependencies, including those described by different equations for different sections of characteristics. The simulation study of models using reactive elements under nonlinear dependencies, and especially in the case of dynamic model change, presents a challenge mainly in terms of convergence in the application of integration methods for calculating the parameters of the circuit. There is no universal solution to the convergence problem, and specific approaches are applied for each circuit to reduce the risk of the simulation "stuck". The article proposes options in this direction.

The current research is part of the team's research aimed at predicting the functionality of energy converting systems, in particular Li-ion batteries.

Section 2 presents the setup by which the Li-ion battery pack measurement data were obtained. Section 3 presents the stages of the simulation model development. Section 4 presents the results from the verification of the developed model.

2. THE USED BATTERY PACK SCREENING SYSTEM

Data obtained from real measurements of the charge and discharge process of a Li-ion battery were used in the development and verification of the model.

A battery pack screening system was developed to perform these measurements and create a database with the measurement results. The system includes three different modules: a Master Controller board, a Battery Holder board, and an FLIR One

PRO thermographic camera. Figure 1 shows a block diagram of the system. Details about this system are presented in our earlier work [7].

It is used in batches of 6 18650 Li-ion battery cells with a capacity of 2.2 Ah, which are subjected to accelerated aging procedures. The captured data for the battery voltage and current were sampled once every 5 seconds [7]. The data that is recorded is the voltage of each cell and the current through the cells for the charge and discharge processes.

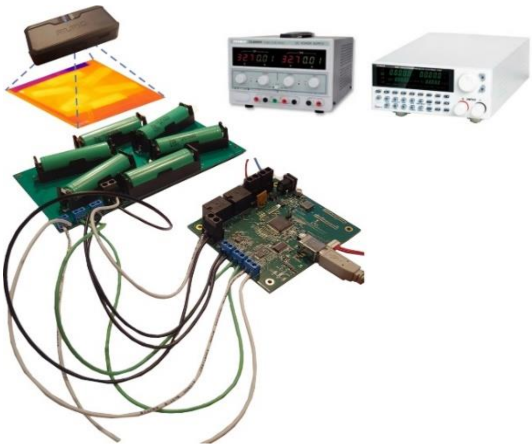


Fig. 1. The hybrid battery-pack screening system [2], [7]

3. STAGES OF THE MODEL DEVELOPMENT

The development of the model involves several stages. The stages do not have a strictly defined sequence, since some of them are performed repeatedly (for example, parameterization). A block diagram presenting the stages is shown in Fig. 2.

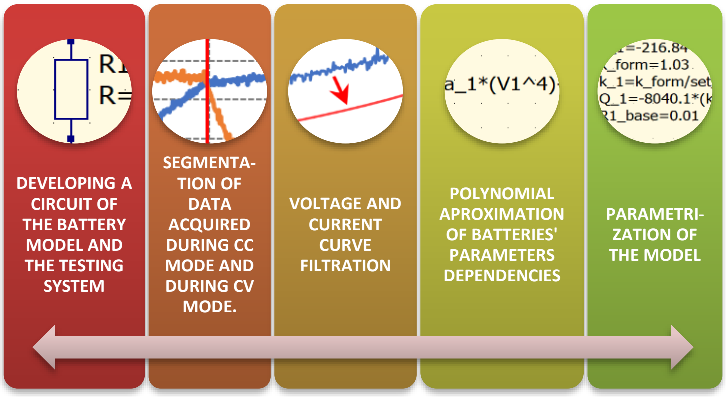


Fig. 2. Stages of the model development [2]

3.1 Developing a circuit of the battery model and the test system

The developed model includes the following modules: the battery, regulated power supply model (for charging behavior simulation), regulated DC electronic load model (for discharging behavior simulation), and switches that switch between charge (SW1) and discharge (SW2) mode.

A block diagram of the model is shown in Fig. 3.

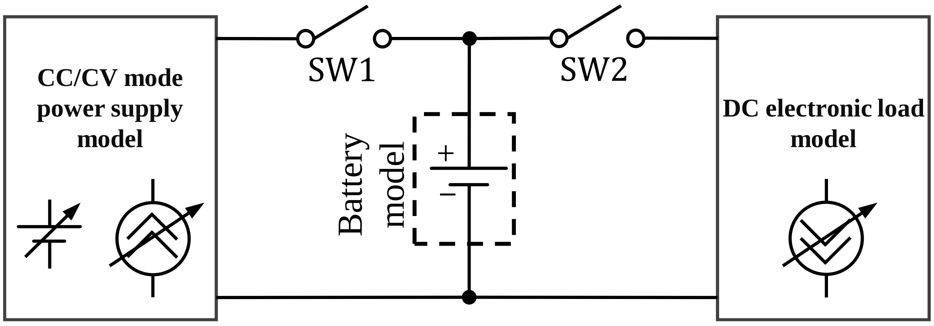


Fig. 3. Block diagram of the model

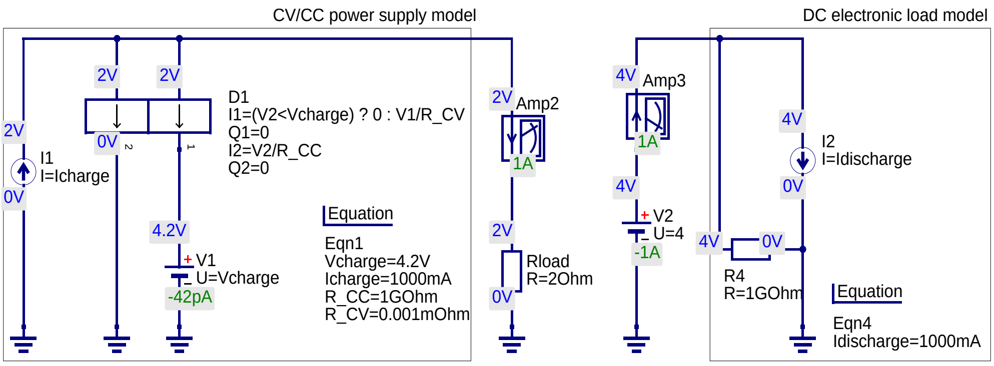


Fig. 4. CV/CC mode power supply and DC electronic load model. View from QUCS-S

The power supply unit can operate in both constant voltage (CV) mode and constant current (CC) mode, switching automatically depending on the output voltage. For its modeling, the element **equation defined device** (EDD), which is available in the QUCS-S component library, was used. The DC electronic load is modeled with a simple current source. The models of the power supply and DC electronic load are presented in Fig. 4. Results from DC operating point simulation at example values for input voltage/current (for CV/CC power supply - 4.2 V, 1 A and load 2 Ω; for DC electronic load - 4 V input voltage and set current 1 A) and load are presented in the figure. There are no changes to the model of the power supply unit compared to the previous model presented in [2]. It has only been confirmed that it works without problems with the current versions of the software products used.

- The battery model is also realized with the element **equation defined device EDD**. There are many changes and improvements to the model compared to the variant presented in [2]. Some of the changes are:
- Branches 4 and 5 have been added, which allow for "memory" of the battery voltage when the charging process is stopped.
- An equation has been added describing the relationship between charge Q_1 and branch 1 voltage V_1 when the battery is discharged.
- For branches 1-3, an automatic change of the analytical model is implemented, depending on whether the battery is being charged or discharged (this is monitored by the voltage direction on the resistor, modeling the serial resistance of the battery R_{ser}).
- Added the ability to automatically turn on a parallel resistor of the capacity of branch 3 at discharge, in order to model the nonlinear nature of the change in battery voltage during discharge.

The battery cell model has the form shown in Fig. 5.

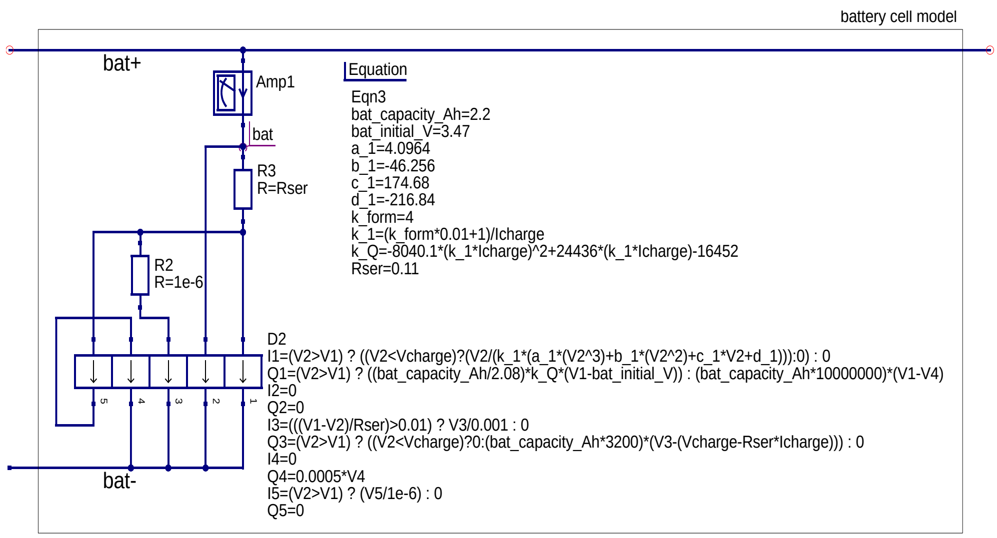


Fig. 5. Battery cell model. View from QUCS-S

As a basis for the development of the model, the data from a real measurement of voltage and current in one of the studied battery cells, during the process of charge and subsequent discharge, will be used. The time diagram is presented in Fig. 6. Due to the nonlinear nature of the change in battery voltage, the parameters charge/discharge in Ah Q_{Ah} and energy stored/given in Wh E_{Wh} carry useful information.

In this particular case, during the charging process, the battery has "received" a charge $Q_{Ah} = +1.599$ Ah (energy $E_{Wh} = +6.205$ Wh). During discharge, the battery has "lost" charge $Q_{Ah} = -0.764$ Ah (energy $E_{Wh} = -2.877$ Wh). These parameters will be used for additional verification of the developed model.

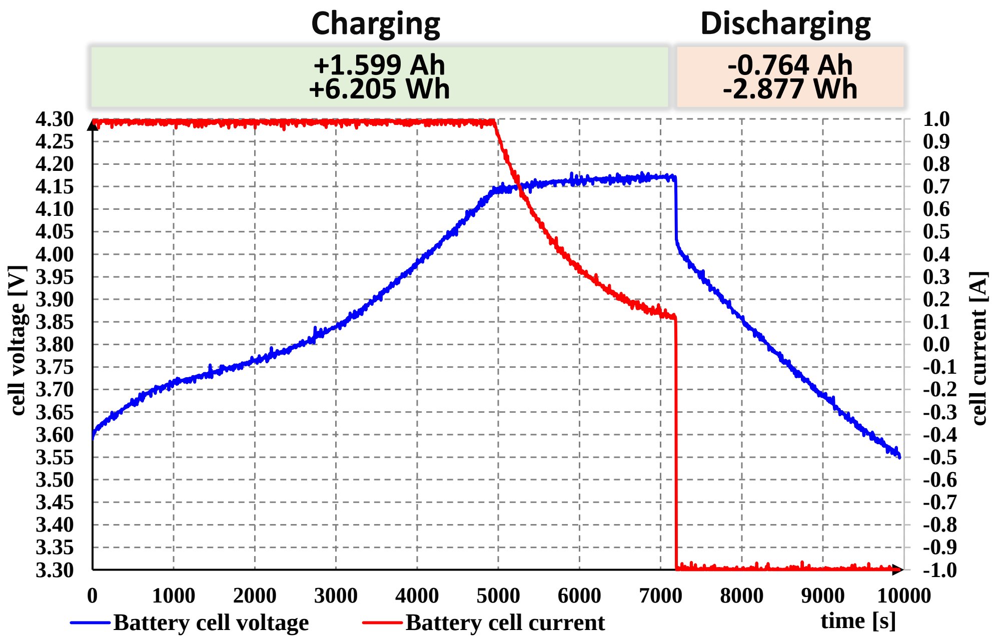


Fig. 6. A time diagram of charge process for one of the investigated cells

3.2 Modeling using a non-linear parallel resistance and linear capacitance

In our previous research, this modeling principle is described in detail as relatively easy to apply in this case. Modeling by nonlinear capacitance is practically impossible for battery voltage values for which experimental data are not available. This is due to the highly nonlinear relationship between the capacitance modeling the energy storage in the battery and the battery voltage [2].

The first step of modeling is to segment the data into three regimes: CC charge mode, CV charge mode, and CC discharge mode. Data filtration and analytical modeling of processes are then performed. At some stages of analytical modeling, parametric analyses are performed for refinement. The steps performed on analytical modeling and optimization cannot be presented here due to the limited volume of the article. Only the final result will be presented.

The equation describing the current through branch 1 of the EDD block D2 is:

$$I_1 = \begin{cases} \text{Charging: } \dfrac{v_{cell}}{k_1(a_1V_2^3 + b_1V_2^2 + c_1V_2 + d_1)} \; when \; v_{cell} < V_{cell_{CV}} \\ 0 \; when \; v_{cell} \geq V_{cell_{CV}} \\ \text{Discharging: } 0 \end{cases}$$

$$k_1 = \frac{k_{form} \times 0.01 + 1}{I_{cell_{CC}}}, a_1 = 4.0964, b_1 = -46.256, c_1 = 174.68, d_1 = -216.84 \quad (1)$$

where $v_{cell}(t)$ is the voltage of the battery at a given moment, $V_{cell_{CV}}$ is the battery cell voltage during the CV phase of charging, $I_{cell_{CC}}$ is the current through the battery during the CC mode phase of charging, k_1 is a coefficient that prescales the polynomial, k_{form} is a coefficient that controls the form of the dependence (values start from 2), V_2 is the voltage of branch 2.

Through coefficient k_{form}, the shape of the charging curve can be changed without affecting the other parameters.

The dependence between the charge and the voltage for branch 1 of the EDD block D2 has been determined by theoretical analysis of the circuit and by parametric analysis, having the following form:

$$Q_1 = \begin{cases} \text{Charging: } \dfrac{C_{batt}}{1.935} k_Q\left(V_1 - V_{batt_{OC}}\right) \\ \text{Discharging: } C_{batt}10^7(V_1 - V_4) \end{cases}$$

$$k_Q = a_2\left(k_1 I_{cell_{CC}}\right)^2 + b_2\left(k_1 I_{cell_{CC}}\right) + c_2, \quad (2)$$

$$a_2 = -8040.1, b_2 = 24436, c_2 = -16452$$

where C_{battt} is the battery capacity in Ah, V_1 is the branch 1 voltage, V_4 is the voltage of branch 4, $V_{batt_{OC}}$ is the battery's open-circuit voltage before the charging process, k_Q is the coefficient that accounts for the dependence of the charge on k_1 and $I_{cell_{CC}}$.

Branch 2 of the EDD block D2 is used to monitor the voltage on the battery. Branch 3 of the EDD block D2 is used to change the parallel capacitance during the CV phase of the charge process. Equations for branch 3 are the following:

$$Q_3 = \begin{cases} \text{Charging: } 3200C_{batt}\left(V_3 - \left(V_{cell_{CV}} - R_{ser}I_{cell_{CC}}\right)\right) \; when \; v_{cell} < V_{cell_{CV}} \\ 0 \; when \; v_{cell} \geq V_{cell_{CV}} \\ \text{Discharging: } 0 \end{cases}, \quad (3)$$

$$I_3 = \begin{cases} \text{Charging: } 0 \\ \text{Discharging: } \frac{V_3}{10^{-3}} \end{cases}. \tag{4}$$

where R_{ser} is the series resistance of the battery in the model, V_3 is the branch 3 voltage.

Branch 4 represents the capacity used to store the voltage value at the time the battery stops charging. Branch 5 acts as a "switch" that switches on and off branch 4 to the battery terminals.

During the development of the model, many problems were encountered related to convergence in the simulation. To avoid these problems, the following options in NGSPICE were used: **`cshunt=1e-12; rshunt=1e11; XMU=0.4.`**

4. VERIFICATION OF THE MODEL

A simulation was performed under the conditions under which the time diagrams in Fig. 6 are obtained. The result is shown in Fig. 7. The value of the cell voltage (the blue curve, left y-axis) and the cell current (the red curve, right y-axis) are presented.

Optimization was performed through parametric analyses, seeking a balance between stored/given charge for the specified time, duration of the CC mode under charge, and voltage form. In terms of stored/given charge, the values differ by several percent. There is no noticeable error during the duration of the CC charge mode. In terms of signal form, the deviations are more significant.

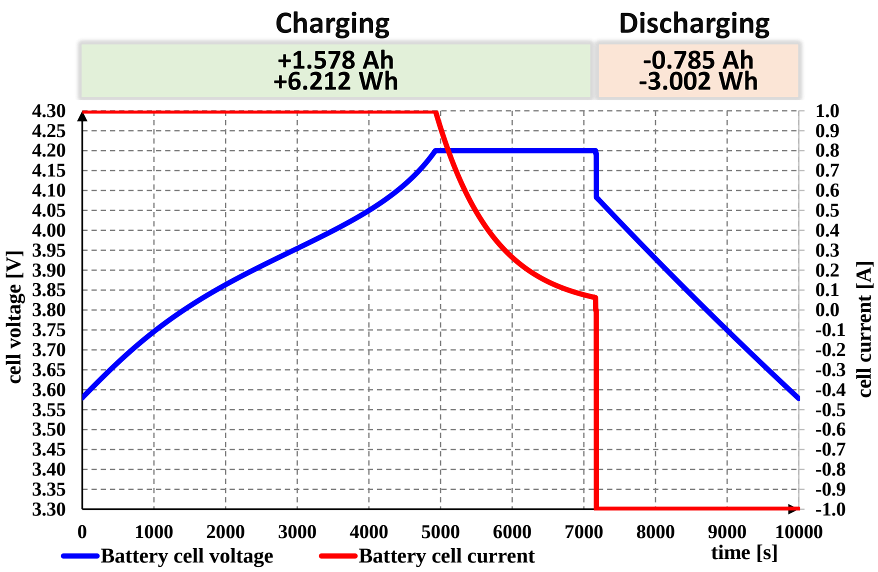


Fig. 7. Results from verification of the battery model – charging curve. View from QUCS-S

The next step of verification is to confirm that the model is correct for any battery capacity and random charging/discharging current. In this way, the correct development of the correction coefficients will be confirmed k_1 и k_Q, which are used precisely to compensate for cross-dependencies between the different parameters of the model.

The simulation study was conducted under the following conditions:

— Initial battery voltage: $V_{batt_{OC}} = 3.47$ V
— Charge voltage: $V_{cell_{CV}} = 4.2$ V
— Charging time (time when open SW1): $t_{charge} = \frac{C_{batt}}{2.2} \times \frac{7200}{I_{cell_{CC}}}$ [s]
— Discharging time (time when open SW2): $t_{discharge} = \frac{C_{batt}}{2.2} \times \frac{10000}{I_{cell_{CC}}}$ [s]
— Discharging current: $I_{dischrage} = I_{cell_{CC}}$
— Curve form control coefficient: $k_{form} = 4$

Under these conditions, it is expected that the charge/energy stored/given by the battery will always be:

— during charge: $Q_{Ah} = +1.578 \frac{C_{batt}}{2.2}$ Ah, $E_{Wh} = +6.212 \frac{C_{batt}}{2.2}$ Wh
— during discharge: $Q_{Ah} = -0.785 \frac{C_{batt}}{2.2}$ Ah, $E_{Wh} = -3.002 \frac{C_{batt}}{2.2}$ Wh

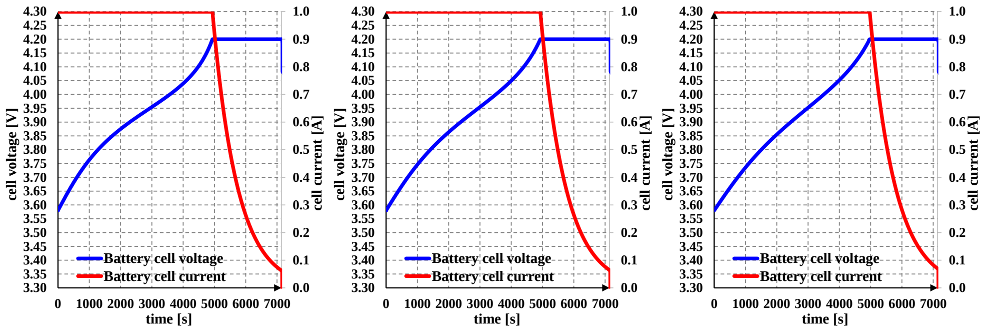
The results are presented in Table 1.

Table 1. Verification of model behavior at different charge/discharge current and capacity

Battery capacity C_{batt} [Ah]	**Charge current $I_{cell_{CC}}$ [A]**	**Discharge current $I_{dischrage}$ [A]**	**Charging time t_{charge} [s]**	**Discharging time $t_{discharge}$ [s]**	**Expected charge/energy during charge Q_{Ah}, E_{Wh}**	**Expected charge/energy during discharge Q_{Ah}, E_{Wh}**	**Charge/energy during charge Q_{Ah}, E_{Wh}**	**Charge/energy during discharge Q_{Ah}, E_{Wh}**
2.2	1	1	7200	2800	1.578 Ah 6.212 Wh	-0.785 Ah -3.002 Wh	**1.578 Ah** **6.212 Wh**	**-0.785 Ah** **-3.002 Wh**
2.2	0.5	0.5	14400	5600	1.578 Ah 6.212 Wh	-0.785 Ah -3.002 Wh	**1.563 Ah** **6.094 Wh**	**-0.786 Ah** **-2.868 Wh**
2.2	1.5	1.5	4800	1867	1.578 Ah 6.212 Wh	-0.785 Ah -3.002 Wh	**1.579 Ah** **6.265 Wh**	**-0.783 Ah** **-3.008 Wh**
1.5	1	1	4909	1909	1.076 Ah 4.235 Wh	-0.535 Ah -2.047 Wh	**1.076 Ah** **4.235 Wh**	**-0.534 Ah** **-2.043 Wh**
1.5	0.5	0.5	9818	3818	1.076 Ah 4.235 Wh	-0.535 Ah -2.047 Wh	**1.065 Ah** **4.155 Wh**	**-0.535 Ah** **-1.954 Wh**
1	0.5	0.5	6545	2545	0.717 Ah 2.824 Wh	-0.357 Ah -1.365 Wh	**0.710 Ah** **2.770 Wh**	**-0.356 Ah** **-1.299 Wh**

The results show good scalability of the model. For the parameter Q_{Ah}, the maximum deviation from the expected value during charge is 0.015 Ah, which is an error of 0.95%. During discharge, the error is even smaller - 0.25%. For the parameter Q_{Wh}, the maximum deviation from the expected value during charge is 0.118 Wh, which is an error of 1.9 %. In the case of discharge, the maximum deviation from the expected value is 0.093 Wh, which is an error of 4.54%. These results confirm that cross-influence between model parameters has been minimized. It is important to note that in this model, the self-heating influence during battery charge has not been fully implemented, and this influence is not taken into account in the expected values.

The influence of the curve form control coefficient k_{form} is also studied on battery charge and discharge behavior. In Fig. 8 shows the time diagrams when charged at 3 different values of this coefficient.



(a) $k_{form} = 3$ (b) $k_{form} = 4$ (c) $k_{form} = 5$

Fig. 8. Results from verification of the battery model – charging curve. View from QUCS-S

Table 2 presents results from the quantitative evaluation of the impact of this parameter. The study was carried out under the following parameters: $C_{cell} = 2.2$ Ah, $I_{cell_{CC}} = I_{dischrage} = 1$ A, $V_{cell_{CV}} = 4.2$ V, $V_{batt_{OC}} = 3.47$ V.

Table 2. Results from a study of the influence of the curve form control coefficient on battery charge/discharge behavior

Curve form control coefficient, k_{form}	**Charge/energy during charge, Q_{Ah}, E_{Wh}**	**Charge/energy during discharge, Q_{Ah}, E_{Wh}**
3	**1.578 Ah, 6.217 Wh**	**-0.785 Ahc, -3.002 Wh**
4	**1.578 Ah, 6.212 Wh**	**-0.785 Ah, -3.002 Wh**
5	**1.591 Ah, 6.259 Wh**	**-0.785 Ah, -3.001 Wh**

As expected, this parameter only affects the behavior of the battery during charge. The effect on the charge/energy stored is very small, while the form of the voltage change changes quite a bit. Therefore, this parameter is more relevant to a more accurate modeling of the voltage change curve during charge, without significantly affecting the integral parameters Q_{Ah} и E_{Wh}.

5. CONCLUSION

The paper examines the possibility of SPICE modeling and simulation of the charge/discharge behavior of Li-ion battery cells using the open-source software product QUCS-S. A parametrized model has been developed, which can model the behavior of Li-ion battery cells with different capacities, at different values of the charging current, within certain limits. The steps in its development are presented, and the chosen modeling approaches are justified by simulation examples. The model still has a number of shortcomings, and there are opportunities for its improvement, which may be the subject of future research: a more detailed study of the dependencies between individual parameters, a study of the reasons for the loss of convergence of the simulation at some specific parameter values, and the improvement of methods for improving convergence.

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