Thevenin-based Battery Model with Ageing Effects in Modelica

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***Abstract*—In the era of transition to the renewable energy the importance of a good model of the battery cannot be overrated. This paper presents the Thevenin-based battery model with aging effects that is parameterized and validated with respect to the battery manufacturer's datasheets. The proposed model of the battery combines the Thevenin-based and runtime-based battery models that represent charging/discharging transient behavior of the battery. The model has been further improved by adding ageing effects using crack propagation model. Charging rate, depth of discharge and overcharge were used as main factors for capacity fading, while temperature effects were neglected as the temperature is not controllable parameter in the application the model is designed for. This allows to speed up the simulation getting an acceptable performance of a model-based optimization such as model predictive control or machine learning. The developed model was implemented using Modelica language, allowing to simulate the model in any software that supports Functional-Mockup Interface.**

***Index Terms*—lithium-ion battery, battery modelling, capacity fade, Thevenin model, runtime model, Modelica**

I. Introduction

Nowadays electrification is not possible to imagine without an energy storage that is ensured by batteries [1]. The Li-ion batteries that are widely used due to their high power density characteristic and lightweight are part of electronic devices. Moreover, the batteries that are integrated into electrical grids, allowing store large amount of energy and to balance the grid performing demand response. Among the loads that participate in the fluctuations the electric vehicles that charge/discharge their batteries from/into the grid [2]. Furthermore, prosumers utilizing solar panels to sell the produced electricity with higher price require a battery to store energy waiting for the best offer from the electricity market [3]. To decrease a cost of batteries and reduce a pollution of their recycling, exploitation of the batteries should be optimized, prolonging its operation as much as possible.

Previously, models that were developed to simulate Li-ion batteries differ by a modeling approach [4]–[6]. Among these models electrochemical models, which defined analytically with partial differential equations, are the most complex and complete ones, but they require a lot of computation power for simulation [7]. In the contrary, equivalent circuit-based models can be easily simulated using circuit analogy. These models are capable of giving current I and voltage V information. Therefore, these models are easily interpretable by electrical engineers [5]. However, such models cannot estimate State of Charge (SoC) of the battery, and do not contain ageing effects of the battery [8]. Nevertheless, Thevenin-based and runtime-based electrical models can be combined to achieve charging simulation as well as transient behavior of the battery, but such model cannot be implemented in circuit simulator, but rather should be done in modelling software [5]. Moreover, Thevenin-based battery was previously successfully combined with crack propagation model for modelling ageing effects [6]. Despite multiple implementations of the electrical circuit battery model with ageing effects, there are no open source library with implemented model, which can be used for simulation. As computation power becomes available allowing for modeling of complex systems as microgrids or interconnected power systems, open access of validated battery models can be later used to solve powers system tasks using model-based optimization algorithms, such as model predictive control (MPC) and reinforcement learning (RL). For this purpose in this work Modelica language is used. Another factor is growing research attention to reducing charging time of the battery without extra damage to the battery [9], [10], which also requires efficient battery model with capacity fading.

Modelica [11] is an object oriented equation-based language that is used for multi-domain modeling including power systems [12]. Being a high-level language to represent a model in a form of algebraic and differential equations, connect them as components using graphical user interface, Modelica translates its models into C code, in this way, allowing to simulate these models with a high performance. Furthermore, OpenModelica environment [13] allows to export models as a functional mockup unit (FMU). In FMU all information required to simulate the model (such as variables, equations, inputs, solver) is stored. Being a convenient model representation for an exchange between incompatible software, FMU can be imported and simulated in such software products as Simulink, OpenModelica, Dymola, and JModelica.org without loss of information [14]. To facilitate interaction with Model-

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ica models from Python, the PyFMI library [15] was developed to interface FMU from Python that is the most frequently used programming language for modern Machine Learning frameworks.

The contribution of this paper is:

- Combining Thevenin-based and runtime-based models for simulating charging/discharging dynamics of the battery. In addition, damage accumulation and crack propagation models were included for capacity fading simulation;
- Simplifying the developed battery model ignoring temperature effects for higher performance and easier control of the battery aiming to apply model-based optimization techniques;
- Implementation of the model in Modelica that can be used in any FMU-compatible software;
- Validation of the developed model comparing the battery characteristics for tree different test cycles with the commercial battery datasheets.

This paper is organized as follows: Section II presents the proposed methodology of the battery modeling and a description of the theoretical base used for modeling. In Section III a general overview of modeling architecture with the proposed battery model's parameters setup is presented. Section IV contains simulation results of the proposed battery model validation with respect to characteristics of batteries that are provided by manufactures. Paper ends with Section V where conclusions are summarized.

II. Battery Modeling Methodology

In this section, accurate and intuitive battery model, which is able to simulate a transient behavior of a typical Li-ion battery for particular State of Charge (SoC) with ability to charge and discharge, is introduced. As an improvement of the model, ageing effects that represent degradation of the battery with various exploitation conditions were added to the model originally presented in [5]. The ageing effects allow to represent the charging and discharging dynamics of the battery in time which is crucial for model-based optimization of battery usage. In the case of using batteries that are installed in a climate controlled premises the effects of temperature as well as calendar losses for capacity fading can be ignored. Another reason of neglecting of the aforementioned parameters is inability to control them. Thus, the combined model consists of three components (Figure 1):

- ***Thevenin-based component*** which models voltage response for particular SoC, and also able to represent transient dynamics of voltage.
- ***Runtime-based component*** which allows to control input current to change internal SoC, in this way, allowing to simulate charging and discharging of the battery.
- ***Capacity degradation component*** which combines damage accumulation and crack propagation models to simulate capacity fading depending on the working conditions of the battery.

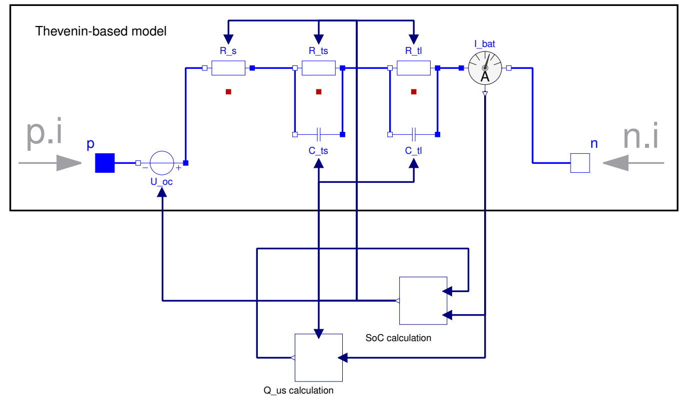

Fig. 1. The model of the battery implemented using Modelica

The main application of the proposed model is model-based optimization of battery operation. The optimization has to be performed fast and efficient, therefore, simplification of the battery model is required. Thus, the presented model in [4] and [6] that model the dependence of capacity fading and voltage response on the temperature were adapted to the needs of modeling for optimization. As generally the controller to optimize battery operation cannot effect the current temperature of the environment, equations were simplified to ignore temperature change, therefore, the constant $T = 20°C$ is assumed. Nevertheless if the temperature change modeling of thermally-induced processes is crucial for certain applications, Arrhenius relation is suggested to be used for temperature effects simulation:

$$A = A_0 \cdot e^{-\frac{E_a}{RT}} \tag{1}$$

where A is quantity of interest, A_0 - the pre-exponential term, E_a - the activation energy, R - the universal gas constant (the molar equivalent to the Boltzmann constant), and T - the temperature in Kelvin.

A. Thevenin-based component

Thevenin-based model with two RC circuits is used as the base to the developed battery model. This model is able to represent voltage and current dependency on a particular SoC and simulate short-term and long-term dynamics of the battery. The long-term dynamics is effectively modeled using the Thevenin-based model that has more than one RC circuit [4]. In this model the open-circuit voltage is used to represent the voltage response of the battery in the steady state and is assumed to be static. Also, the characteristics that represent dependence of RC elements on SoC were added to RC network components including series resistor (R_s) for the range of SoC values when high is $SoC > 0.8$ and low is $SoC < 0.2$ to simulate effects of the overcharge and undercharge of the battery. For this purpose equations from [4] are employed, but simplified for a condition of a constant temperature $T = 20°C$. Thus, all dependencies of the

Thevenin-based circuit parameters on SoC can be summarized as:

$$R_s(SoC) = R_{s_0} + \sum_{i=0}^{4} k_{R_{s,i}} \cdot SoC^i \tag{2}$$

$$R_{t,s}(SoC) = R_{t,s_0} + \sum_{i=0}^{4} k_{R_{ts,i}} \cdot SoC^i \tag{3}$$

$$C_{t,s}(SoC) = C_{t,s_0} + \sum_{i=0}^{6} k_{C_{ts,i}} \cdot SoC^i \tag{4}$$

$$R_{t,l}(SoC) = R_{t,l_0} + k_{R_{tl,1}} \cdot \exp^{k_{R_{tl,2}} \cdot SoC} + k_{R_{tl,3}} \cdot SoC \tag{5}$$

$$C_{t,l}(SoC) = C_{t,l_0} + \sum_{i=0}^{6} k_{C_{tl,i}} \cdot SoC^i \tag{6}$$

where $k_{R_s,i}, k_{R_{ts,i}}, k_{C_{ts,i}}, k_{C_{tl,i}}$ are parameters dependent on battery type, which were received as coefficients for polynomial fit with respect to SoC, and $R_{s_0}, R_{t,s_0}, C_{t,s_0}, R_{t,l_0}, C_{t,l_0}$ are initial parameter values of resistance, capacitance. Those parameters are different during charging and discharging and were previously found by fitting polynomials in [4]. The parameter values used in this work can be found in Table I.

B. Runtime-based component

To get a variation of SoC depending on the voltage of an open-circuit, the Thevenin-based model was combined with runtime-based model that was proposed in [5]. In such an approach, U_{oc} is a voltage that changes depending on the current SoC. We can express this dependency as:

$$U_{OC}(SoC) = k_0 + k_1 \cdot SoC + k_2 \cdot \exp^{k_3 \cdot SoC} + k_4 \cdot \exp^{\frac{k_5}{1-SoC}} \tag{7}$$

where $k_0, k_1, k_2, k_3, k_4, k_5$ - the coefficients which are calculated by curve fitting during parameter extraction. Thus, U_{oc} for different values of SoC is precalculated and included into the model's lookup table that is used to change the voltage depending on the current level of SoC (SoC calculation block in Figure 1). In this model Coulomb counting method is implemented to calculate the SoC of the battery:

$$SoC = SoC_0 - \frac{1}{Q_{us}} \int I_{bat}(t)dt \tag{8}$$

where SoC_0 is initial SoC, Q_{us} is the usable charge capacity, and I_{bat} is current in the battery.

C. Capacity degradation component

Due to aging effects, usable capacity of a battery is decreasing, therefore, a capacity fading ξ can be defined as:

$$\xi = Q_{nom} - Q_{us} \tag{9}$$

where Q_{nom} is nominal capacity of the battery.

The end of life condition depends on the type of a battery, but by convention is considered at 80% of the nominal capacity. In current work capacity fading is considered as unique State of Health (SoH) indicator, because self-discharge dynamics modeling is omitted due to inability to control it by optimization. Thus, SoH can be calculated, as:

$$SoH = 1 - \frac{\xi}{0.2 \cdot Q_{nom}} \tag{10}$$

Capacity fading can be divided into two losses: calendar and cycling. While the first one is mainly dependant on the battery's total working time and temperature, which affects electrode film growth [4], the second one is determined by the exploitation conditions. Therefore, for the cycling loss the main factors are:

- Temperature
- Depth of Discharge (DoD)
- Overcharge
- C-rate

Due to our task calendar losses and temperature effects were dropped and focus was shifted to DoD, Overcharge and C-rate. One of the approaches for capacity fading estimation is damage accumulation model, where battery's life cycle is divided into number of the events, during each capacity fading is calculated and then sum up.

In particular in the method [6] life cycle is divided into charged-discharged cycles and in each of those intervals capacity fading is estimated by crack propagation model. To differentiate high SoC and DoD, SoC_{avg} and SoC_{dev} are introduced. High SoC_{avg} indicates that battery operates on high SoC and high SoC_{dev} shows that DoD is high and SoC during one cycle varies a lot. Also, concept of number of effective cycles was introduced to count amount of the energy went through the battery. We can calculate these parameters for the event i as:

$$\begin{cases} SoC_{avg,i} = \frac{1}{t_{\Delta i}} \int_{t_{i-1}}^{t_i} SoC(t)dt \\ SoC_{dev,i} = 2\sqrt{3}\sqrt{\frac{1}{t_{\Delta i}} \int_{t_{i-1}}^{t_i} (SoC(t) - SoC_{avg,i})^2 dt} \\ N_{eff} = \int_{t_{i-1}}^{t_i} \frac{|I_{bat}(t)|}{2 \cdot Q_{nom}} dt \end{cases} \tag{11}$$

After discarding calendar loss and temperature effects, capacity fading formula from [6] is rewritten as:

$$\xi_i = K_{co} \cdot N_{eff} \cdot e^{\frac{SoC_{dev,i}-1}{K_{ex}}} \cdot e^{K_{soc} \frac{SoC_{avg,i}-0.5}{0.25}} \cdot (1 - L_i) \tag{12}$$

where K_{co}, K_{ex}, K_{soc} are battery specific constants, which are fitted to battery life data, and L is damage accumulation term which is defined as:

$$L_i = \sum_{i=1}^{E} \xi_i \tag{13}$$

For the proposed model it is important to have feedback on how SoH is changed each timepoint, in that way optimization algorithm will be able to take into account changes. Therefore, the capacity fading is calculated iteratively:

$$\begin{cases} \xi(t) = L_{n-1} + \xi_n(t) \\ L_{n-1} = \sum_{i=1}^{n} \xi_i \end{cases} \tag{14}$$

where n is the current charge-discharge cycle. Therefore, the total capacity fading can also decrease during a battery operation cycle. However, when charge-discharge cycle is ended, the changes to capacity fading ξ are irreversible.

III. THE PROPOSED BATTERY MODEL IN MODELICA

In this research the battery model was implemented using the Modelica language with a use of OpenModelica environment. In Figure 1 the general architecture of the battery model and its implementation is presented. Thevenin-based component is the basic model, where series resistor R_s is used for instant drop of voltage for particular SoC, and two RC networks (R_{ts}, C_{ts}) and (R_{tl}, C_{tl}) are included to represent the transient behavior. U_{oc} is an open-circuit voltage where output voltage depends on the SoC level according to the lookup table. $SoC\ calculation$ component calculates current SoC using Coulomb counting method 8 taking into account current capacity Q_{us} which is affected by the capacity fading. $Q_{us}\ calculation$ component in Figure 1 uses equations (11), (12), and (14) to calculate current Q_{us} and SoH.

The model's parameters identification requires a knowledge of the hardware characteristics (e.g. battery specification from the producer). In addition, the laboratory testing of the real equipment is time-consuming. Thus, the precise model of the battery allows to do simulations cheaper. In this work the parameters for the circuit components are used that are presented in [4]. These parameters correspond to the A123 APR18650M1 battery dynamics (parameters are available in Appendix A). The parameters for the capacity fading component of the model [6] correspond to the battery A123 ANR26650M1A.

IV. MODEL SIMULATION AND VALIDATION

The presented model (see Figure 1) is validated using several test scenarios:

- Test cycle of the battery with periodic charge, discharge, and rest time
- Capacity fading estimation test
- Advanced capacity fading estimation test

In these test scenarios the real battery characteristics and data were employed from the corresponding datasheets that are provided by a manufacturer.

A. Test cycle with periodic charge, discharge, and rest time

One of the typical test cycles that is presented in [4] is reproduced for the developed battery model in this work (see Figure 2). This test cycle includes time of charge, discharge and battery rest time. Battery is firstly discharged with 1C rate, during which every 0.05 Ah battery is rested for 1 minute. After battery is fully discharged, it is rested for 30 minutes, and charged in similar manner afterwards. Such test cycle is usually used for estimating parameters for the model [16]. The voltage output response is measured and evaluated as the result of the test cycle. To compare of voltage response, measurements from the A123 APR18650M1 battery that are presented in [4] served as reference. In Figure 3 the resulted voltage response of the battery model is very similar to the measured data. More specifically, mean average error (MAE) is 10 mV for charging and 13 mV for discharging cycle of the battery model. Maximum error is 11.5 mV, which is nearly the same, as results found in [4], where maximum error was 11 mV. Thus, the developed battery model passed the validation using this test cycle.

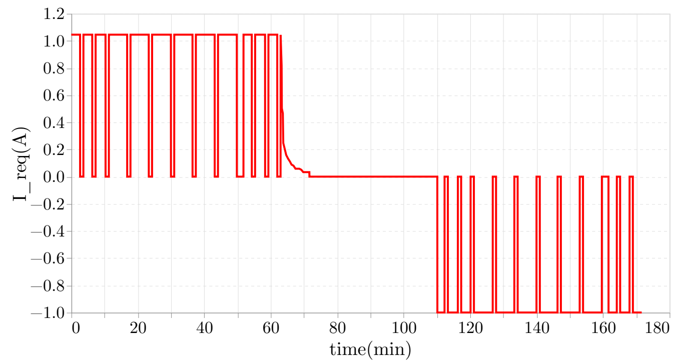

Fig. 2. Profile of the test cycle for determining the model parameters

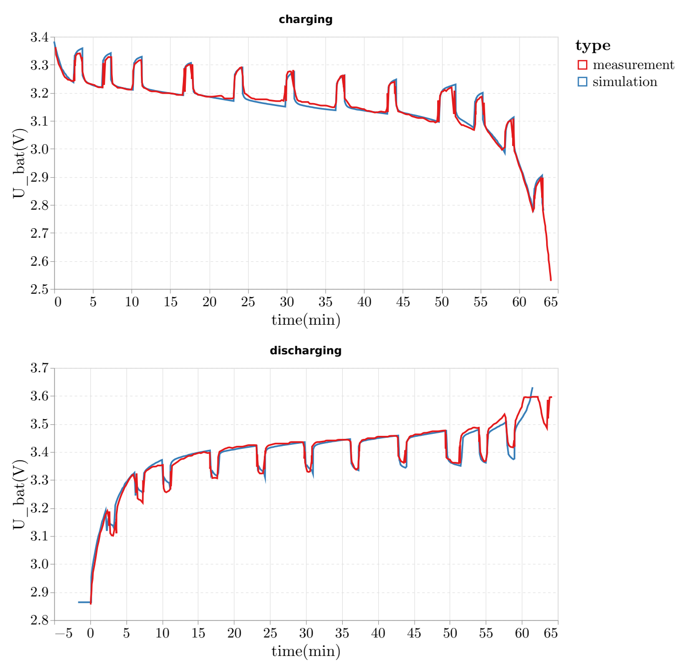

Fig. 3. Battery voltage response during test cycle

B. Capacity fading estimation test

Capacity fading estimation is another method to test the validity of the battery model. The result of this test is compared to the real battery (i.e. A123 AN26650M1A) characteristic. However, due to limited data availability, parameters for crack propagation model were taken for a different Li-ion battery. Thus, dynamics of SoH of the resulted battery model is not accurate when compared to the specific real battery. Thus, data for both batteries was extracted from respective datasheets [17]

[18]. Even though the batteries are different, in Figure 4 comparing the degradation of capacity for A123 ANR26650M1A and A123 APR18650M1 batteries, the resulted SoH in % for each battery and the developed model is very similar being a result of series of charging-discharging cycles with 1C rate[1] and 100 % depth of discharge.

Thus, even with imprecision induced by employing parameters of different batteries, the presented battery model is a good approximation in terms of this test, and therefore, can be used for simulations and battery representation as part of model-based optimization tasks. Nevertheless, in case of application when an exact model of the battery has to be reproduced, all the model's parameters should be reevaluated with respect to a specific battery model.

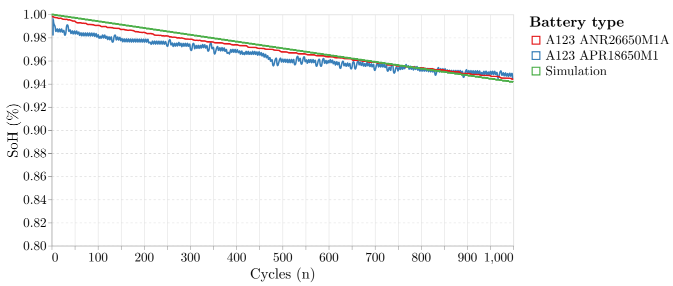

Fig. 4. Capacity fading for two types of batteries and the simulated model (Figure 1)

C. Advanced capacity fading estimation test

To ensure that the model of the battery corresponds to real characteristics, an advanced capacity fading estimation test is suggested. This test includes the battery operation cycles under different charging and discharging rates including dependency on temperature parameter in the datasheets. To evaluate performance of the capacity degradation component in the battery model, the data from the datasheet [17] was used as a reference. In the Figure 5 for 1C charging-discharging cycles SoH dynamics is nearly the same as the reference with MAE only 0.2%. However, for 1.3C charging/2.1C discharging the references that were available in the datasheet correspond to higher temperature operating conditions of the battery, therefore, the error is much bigger for such operating condition (see 5). Nevertheless, the capacity fading effectively increases for higher C-rates.

An important aspect of the resulted Modelica battery model is its high performance. In particular, the 1000 cycles with 1.3 charging/2.1 discharging C-rates for SoH evaluation, which corresponds to 556 hours of the battery operation, were complete only in 320 seconds. This fact makes the battery very attractive for fast model-based optimization.

V. Conclusion

In this paper the novel model of the Li-ion battery is presented. This model combines the Thevenin-based and runtime-based models that were further improved by adding ageing effects using crack propagation model. The original crack propagation model was modified to accumulate capacity damage iteratively on each step and to discard temperature effects, thus it can be efficiently used in model-based optimization algorithms. The resulted mathematical model is capable of simulating the charging and discharging of the battery with transient behavior and capacity degradation over multiple runs. The developed model was validated comparing to the characteristics of the real batteries that were provided by manufacturers. The simulations showed good validation results. However, for industrial applications parameters should be estimated for particular battery considering the temperature dynamics.

The model was implemented using Modelica language in OpenModelica environment resulting in high computational performance. Moreover, the battery model was exported/imported into FMU enabling the use in any FMI-compatible software.

The source code[2] of the developed model is publicly available and can be used for future work in other studies.

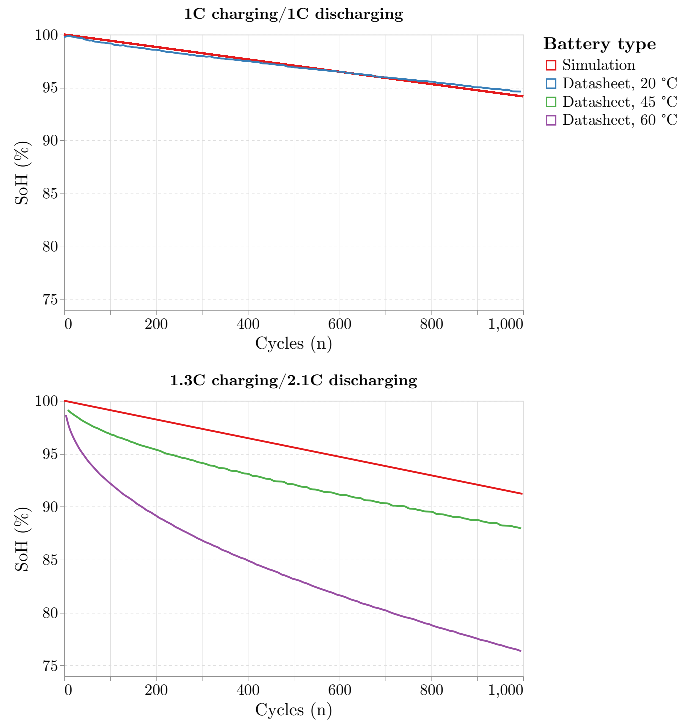

Fig. 5. Capacity fading for different load

Appendix

This appendix presents the parameters of the developed Li-ion battery model (see Table I) that is developed using Modelica language, and released as open source.

[1] C-rate is defined as the charge / discharge current divided by the nominally rated battery capacity.

[2] https://github.com/Midren/MPC_for_battery_operation

TABLE I
PARAMETERS OF THE DEVELOPED BATTERY MODEL

Parameter	Description	Charging	Discharging	Unit
Parameters of series resistor R_s [4]				
R_{s0}		8.98e-2	8.210e-2	Ohm
$k_{R_s,1}$		-7.216e-2	-4.1006e-2	Ohm
$k_{R_s,2}$		2.273e-1	1.609e-1	Ohm
$k_{R_s,3}$		-2.892e-1	-2.518e-1	Ohm
$k_{R_s,4}$		1.298e-1	1.369e-1	Ohm
Parameters of resistor $R_{t,s}$ for short-term transient behavior [4]				
$R_{t,s0}$		1.827e-2	1.4e-2	Ohm
$k_{R_{t,s1}}$		1.080e-2	7.13e-11	Ohm
$k_{R_{t,s2}}$		11.03	-21.11	Ohm
$k_{R_{t,s3}}$		-6.463e-3	03	Ohm
Parameters of resistor $R_{t,l}$ for long-term transient behavior [4]				
$R_{t,l0}$		4.722e-2	3.1e-2	Ohm
$k_{R_{t,l1}}$		2.95e-1	8.913e-15	Ohm
$k_{R_{t,l2}}$		20.00	-32.23	
$k_{R_{t,l3}}$		-2.420e-2	4.473e-3	Ohm
Parameters of capacitor $C_{t,s}$ for short-term transient behavior [4]				
$k_{C_{t,s0}}$		389.7	6.849e2	F
$k_{C_{t,s1}}$		1408	2.340e3	F
$k_{C_{t,s2}}$		-1007	-1.013e4	F
$k_{C_{t,s3}}$		169.7	1.723e4	F
$k_{C_{t,s4}}$		0	-1.026e4	F
$k_{C_{t,s5}}$		0	0	F
$k_{C_{t,s6}}$		0	0	F
Parameters of capacitor $C_{t,l}$ for long-term transient behavior [4]				
$k_{C_{t,l0}}$		2.232e3	7.144e3	F
$k_{C_{t,l1}}$		-3.102e4	2.283e4	F
$k_{C_{t,l2}}$		5.998e5	-8.124e4	F
$k_{C_{t,l3}}$		-2.958e6	-4.009e3	F
$k_{C_{t,l4}}$		6.271e6	2.042e5	F
$k_{C_{t,l5}}$		-6.007e6	-1.541e5	F
$k_{C_{t,l6}}$		2.130e6	0	F
Parameters for capacity fading simulation [6]				
K_{co}	the throughput coef.	3.66e-5		
K_{ex}	the exponent for DoD	0.717		
K_{soc}	the average SoC coef.	0.916		
Parameters for open-circuit voltage				
k_0		-5.863e-1		V
k_1		21.9		V
k_2		3.414		V
k_3		1.10e-1		
k_4		-1.718e-1		V
k_5		8e-3		

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This publication is dedicated to all Ukrainian people who are defending our freedom at the frontier of combat in the center of Europe.

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