UDC 621.355
DOI: 10.15587/2706-5448.2024.304400

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NUMERICAL MODELING OF ELECTRICAL PARAMETERS OF $LiFePO_4$ BATTERIES

The object of research is the physical processes of electric energy storage in Li-ion batteries. The problem being solved in the work is related to the lack of reliable mathematical models of storage batteries, which leads to the appearance of undesirable effects or emergency situations when changing operating modes.

In the course of the work, Li-ion battery models based on electrochemical theory and electrical circuits were considered. The six most common equivalent battery replacement schemes are presented. The advantages and disadvantages of the considered substitution schemes are given. The dual-polarization mathematical model was found to most accurately describe the performance of the battery at the end of the discharge and charge cycles compared to the first-order Thevenin model, the RC model, and the active resistance battery model. The physical processes in the storage battery during pulse discharge, which is the main part of electrical energy storage systems based on electrochemical technology, were studied. Mathematical modeling was carried out in the Matlab software package using the Simulink application program package. The dependence of the parameters of the equivalent lithium-ion battery replacement scheme according to the second-order Thevenin model on the ambient temperature and state of charge is considered. It was established that the value of EMF E depends more on the change in SOC than on temperature. In turn, the active resistance R_{OM} shows a greater dependence on temperature than on the change in SOC. At high temperatures, the resistance value decreases. The parameters R_1 and C_1 characterizing the electrochemical polarization vary in the range from 10 to 75 % SOC. The parameters R_2 and C_2, which depend on the concentration polarization, vary in the intervals from 0 to 25 % SOC and 75 to 100 % SOC.

The recommendations for choosing a Li-ion battery model developed in the work can be used in practice. The established dependencies will help to better design electrical energy storage systems based on electrochemical technology.

Keywords: *lithium-ion battery, electric model, parameters of the equivalent circuit of substitution, state of charge, temperature.*

Received date: 09.05.2024
Accepted date: 22.06.2024
Published date: 28.06.2024

How to cite

Buryk, M., Lobodzinsky, V., Buryk, I., Lisovyi, O. (2024). Numerical modeling of electrical parameters of $LiFePO_4$ batteries. Technology Audit and Production Reserves, 3 (1 (77)), 27–34. doi: https://doi.org/10.15587/2706-5448.2024.304400

1. Introduction

Renewable energy sources are used in electrical systems to ensure reliability, economy and environmental friendliness. Wind and solar power plants occupy two thirds of the total volume of alternative media [1]. The instability of electricity generation in renewable sources, which is associated with the possible lack of sufficient conditions, negatively affects the distribution of electricity. In order to take into account interruptions during the generation of electrical energy and ensure a balance between the produced and consumed electrical power, energy storage systems based on mechanical, chemical, thermal, electrochemical and other technologies are used [2]. The demand for the latter is growing rapidly in connection with the development of the ecological direction of energy generation and electric transport.

Batteries are electrochemical devices that convert chemical energy into electrical energy. They consist of separate cells, each of which has two electrodes (anode and cathode) and an electrolyte, and according to the principle of operation, they are divided into two groups. The first group (primary) includes batteries intended for one-time use. After complete consumption of active substances from the electrodes, they become inoperable. The second group (secondary) includes batteries that are intended for recharging. The latter, after the consumption of active masses in the solution, are transferred to the working state by means of the passage of an electric current through the element in the reverse direction.

Lithium-ion batteries (Li-ion) are one of the most used as an energy storage device in power plants with renewable energy sources, portable devices and electrical appliances. Among the main advantages, one should note their high energy density, small size, durability, low self-discharge, environmental friendliness, etc. [3].

One of the most important Li-ion electrical parameters is SOC (State of Charge) – a parameter that informs about the current remaining capacity of the battery. State of Charge is measured as a percentage of the total battery capacity. In order to increase battery life and performance, SOC needs

ISSN 2664-9969

constant monitoring. The next equally important parameter is SOE (State of Energy), which indicates the remaining energy in the battery. Some types of batteries include a BMS (Battery Management System) system that monitors the level of charge and discharge, keeping them from over-voltage, short-circuit, over-charge and over-discharge. The application of the latter for Li-ion can be considered and analyzed within the framework of the approach of equivalent electrical circuits [4]. The quantitative assessment of electrical parameters is the key to increasing the service life and effective control of the battery.

The Li-ion nomenclature is very broad, so it becomes increasingly difficult to estimate and predict their parameters. In this situation, the problem of choosing the optimal model that will fulfill the characteristics of individual types of batteries arises. As an example, $LiFePO_4$ has pronounced memory, hysteresis and relaxation effects. Neglect of phase transitions for the last constant is one of the main causes of numerical modeling errors [4].

This paper will consider existing electrical and «electrochemical» models of batteries.

The aim of research is to numerically model the dependence of Li-ion electrical parameters on temperature and state of charge.

2. Materials and Methods

The object of research is the physical processes of electric energy storage in Li-ion batteries. The lack of reliable models leads to the appearance of unwanted effects or emergency situations when changing operating modes.

Analytical and numerical methods based on the MATLAB software complex with the SIMULINK application program package were used to simulate Li-ion characteristics and parameters during pulse discharge and at different ambient temperatures.

3. Results and Discussion

The battery model based on the electrochemical theory is considered. A chemical energy source is an active element of an electrical circuit in which chemical energy is directly converted into electrical energy without a thermal stage, so the efficiency of this element is close to 95 %.

The electrochemical cell of the source consists of two electrodes, which are spatially separated by an electrolyte or an ionic conductor (conductor of the second kind). A conductor of the first kind that is in contact with a conductor of the second kind is called an electrode. An electrode potential arises at the interface between these conductors. The cathode is the electrode on which the reduction of the oxidizing agent takes place, and the anode is the electrode on which the oxidation of the reducing agent proceeds [5].

The thermodynamics of electrochemical elements allows to determine the theoretical potential difference between the positive and negative electrodes in the absence of current.

From the Gibbs-Helmholtz equation, let's determine the EMF value:

$$E=\frac{-\Delta G}{n\cdot F}=\frac{-(\Delta H-T\Delta S)}{n\cdot F}=$$
$$=\frac{-\Delta H}{n\cdot F}+T\cdot\frac{\Delta S}{n\cdot F}=\frac{-\Delta H}{n\cdot F}+T\cdot\frac{\Delta E}{\Delta T},\ \text{V}, \quad (1)$$

where E – electromotive force, V; ΔG – Gibbs energy, J/mol; n – the number of electrons involved in an electrochemical reaction; F=96500 – Faraday constant, Kl/mol or A sec; ΔH – change in enthalpy (thermal effect of chemical reaction), J/mol; $T\Delta S$ – bound energy, J/(mol); ΔS – change in entropy, J/(mol·K); T – temperature, K; $\Delta E/\Delta T$ – EMF temperature coefficient associated with the variation of the entropy of the reaction (current creation process), V/K.

EMF of chemical energy source E is equal to:

$$E=\varphi_+-\varphi_-,\ \text{V}, \quad (2)$$

where φ_+ – equilibrium electrode potential of the positive electrode (cathode), V; φ_- – equilibrium electrode potentials of the negative electrode (anode), V.

The equilibrium potential of the electrode depends on the temperature, the type of electrode reaction and the activity of gaseous and dissolved substances and is determined by the Nernst expression:

$$E=E_0+T\cdot\frac{R_y}{n\cdot F}\ln\left(\frac{Ox}{Red}\right),\ \text{V}, \quad (3)$$

where E_0 – standard equilibrium potential of the electrode, V; R_y = 8.314 – universal constant, J/(mol·K); Ox – concentration of the oxidized form; Red – concentration of the reduced form.

Voltage at the terminals of the power source at open circuit voltage U_{oc} (no load is connected to the battery poles (break)) is equal to the EMF value of the chemical source. But if side (harmful) reactions are observed and balanced potentials are not established on the electrodes, then the voltage decreases.

A conventional graphic representation of an electrochemical source is shown in Fig. 1, *a*, and the equivalent circuit for replacing a battery with internal resistance R_0 is presented in Fig. 1, *b*.

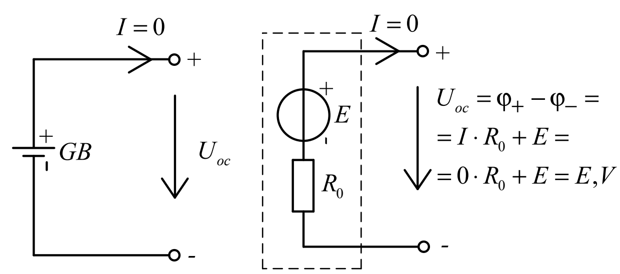

Fig. 1. Accumulator battery:
a – conventional graphic image; *b* – equivalent scheme of substitution at open circuit voltage

The volt-ampere characteristics (VAC) of batteries are non-linear. Let's show in Fig. 2 VAC in the discharge mode for a $LiFePO_4$ battery with a nominal power of 5.12 kWh, with a rated voltage of 51.2 V, with a rated capacity of 100 Ah, with a standard charge voltage of 56 V, with a maximum discharge current of 100 A, with a voltage of cut-off discharge 44.8 V at a temperature of 25 °C and a charge current of 20 A.

Let's write down the expressions for determining the values of the discharge and charge voltages of the battery when balanced potentials are not established on the electrodes:

$$U_{dis} = E - \Delta\varepsilon - I_{dis} \cdot R_{ohm} < U_{ch} = E + \Delta\varepsilon + I_{ch} \cdot R_{ohm},\ \text{V}, \qquad (4)$$

where U_{dis} – battery discharge voltage, V; $E = U_{oc}$ – EMF of a chemical element, V; $\Delta\varepsilon = \Delta\varepsilon_{ep} + \varepsilon_{chemp} + \varepsilon_{conp} = I \cdot R_p$ – element polarization, V; $\Delta\varepsilon_{ep}$ – electrochemical polarization, V; ε_{chemp} – chemical polarization, V; ε_{conp} – concentration polarization, V; I_{dis}, I_{ch} – electric currents of discharge and charge, respectively, A; R_{ohm} – the sum of the active resistances of the electrodes and other current-conducting elements, Ohm; R_p – polarization resistance, Ohm; U_{ch} – battery charge voltage, V.

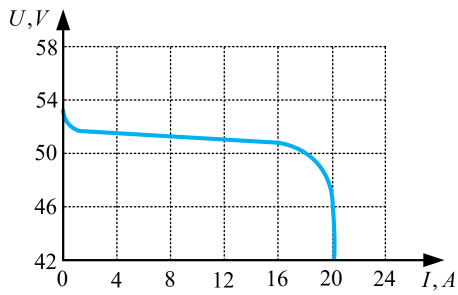

Fig. 2. VAC of the $LiFePO_4$ battery

Let's rewrite expressions (4) taking into account the polarization resistance R_p:

$$\begin{aligned} U_{dis} &= E - I_{dis} \cdot R_p - I_{dis} \cdot R_{ohm} = \\ &= E - I_{dis} \cdot \left(R_p + R_{ohm}\right) = E - I_{dis} \cdot R_{0dis},\ \text{V}; \\ U_{ch} &= E + I_{ch} \cdot R_p + I_{ch} \cdot R_{ohm} = \\ &= E + I_{ch} \cdot \left(R_p + R_{ohm}\right) = E + I_{ch} \cdot R_{0ch},\ \text{V}, \end{aligned} \qquad (5)$$

where R_0 – internal resistance of the chemical energy source, Ohm.

The internal resistance of the battery during its discharge is determined by the formula:

$$R_{0dis} = \frac{E - U_{dis}}{I_{dis}} = \frac{E - I_{dis} \cdot R_{load}}{I_{dis}},\ \text{Ohm}, \qquad (6)$$

where R_{load} – active load resistance, Ohm.

The internal resistance of the battery during its charge is calculated according to the expression:

$$R_{0ch} = \frac{U_{ch} - E}{I_{ch}} = \frac{I_{ch} \cdot R_{charger} - E}{I_{ch}},\ \text{Ohm}, \qquad (7)$$

where $R_{charger}$ – active resistance of the charger, Ohm.

The equivalent scheme of battery replacement is presented in Fig. 3 in load discharge mode, where U_{load} – load voltage.

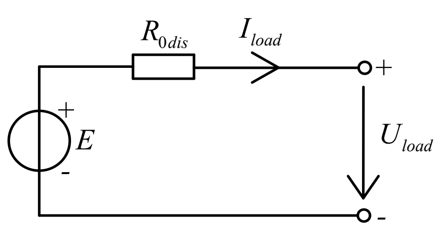

Fig. 3. Equivalent circuit for replacing a chemical energy source

Internal resistance battery model or active-internal resistance model described by a linear equation [6–8]:

$$U_{load} = E - I \cdot R_{ohm},\ \text{V}, \qquad (8)$$

where U_{load} – voltage on the battery terminals (voltage on loaded), V; $E = U_{oc}$ – EMF of the battery, V; I – amperage, A; R_{ohm} – internal resistance of the battery, Ohm.

Equivalent circuit of battery replacement according to the model with active internal resistance (R_{int}) coincides with the scheme of substitution of a chemical energy source based on the electrochemical theory, which is shown in Fig. 3.

To the advantages of the equivalent substitution scheme R_{int} belong to:

1. Simplicity (the substitution scheme consists of an internal resistance R_{ohm} and EMF $E = U_{oc}$).

2. The possibility of use for the purpose of predicting the behavior of the battery in various conditions.

Failure to take into account such factors as the level of degradation (aging), self-discharge and temperature, which can affect the behavior of the battery, is considered the main drawback of this scheme.

Resistor-capacitor battery model RC is a more progressive model than the model with active internal resistance. Equivalent circuit of battery replacement on the basis *RC* model is shown in Fig. 4. The substitution scheme includes: capacity C_b (total battery capacity) and C_c (surface effect capacity of the battery active resistances R_{ohm} (internal resistance), R_c (resistance of the capacitor C_c) and R_t (resistance of the battery terminals) [6]. Voltage U_{oc} determines the state of charge of the battery, and the voltage U_c is equal to the voltage across the capacitor C_c. Voltage U_{load} is the voltage across the battery terminals (load voltage). I_{load} – battery load current.

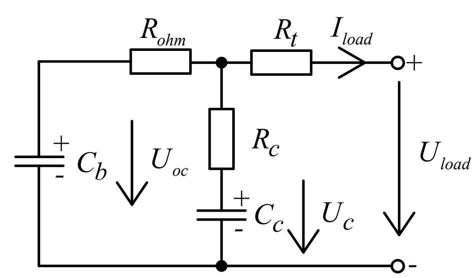

Fig. 4. Equivalent battery replacement scheme based on the *RC* model

The *RC* model can be used to determine battery condition and optimal discharge current. The corresponding model is also used to predict battery voltage. However, it should be remembered that the specified model may be inaccurate in non-standard modes and at high discharge currents.

An equivalent substitution scheme based on the Thevenin model is used to model the behavior of the battery (Fig. 5).

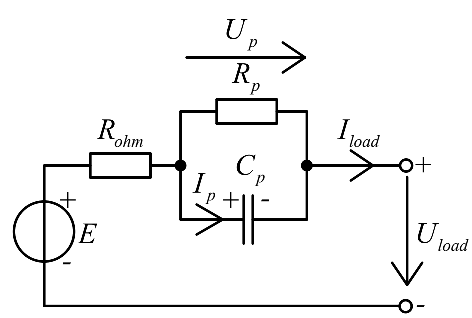

Fig. 5. Equivalent battery replacement scheme according to Thevenin model

Usually, the Thevenin model consists of 3 parts – equivalent capacity C_p, internal resistance R_0 and an EMF source E. Equivalent capacity C_p is used to take into account transient characteristics during charge and discharge. It includes the internal resistance of the battery include polarization resistance R_p and active resistance R_{ohm}. Thevenin model is used in the design of power systems, analysis of battery performance, development of battery control algorithms, and identification of battery malfunctions.

Determine the voltage at the battery terminals U_{load} and the Thevenin equivalent voltage U_p with parallel connection of active resistance R_p and capacity C_p it is possible according to the following equations:

$$\begin{cases} U_p + R_p C_p \dfrac{dU_p}{dt} = I_{load} \cdot R_p, \text{ V}, \\ U_{load} = E - U_p - I_{load} \cdot R_{ohm}, \text{ V}. \end{cases} \tag{9}$$

The Thevenin model, although easy to use, does not always give an accurate picture of the behavior of lithium-ion batteries. Its drawback is the inability to take into account two important polarization effects:

1. *Concentration polarization*: occurs when lithium ions do not have time to diffuse to the electrodes at the required speed, which leads to a decrease in voltage.
2. *Electrochemical polarization*: associated with the slowing down of chemical reactions on the electrode, which also negatively affects the voltage value.

Dual polarization model (DP) (Fig. 6) is designed to overcome these shortcomings. Another such substitution scheme is called the *second-order Thevenin model*. It splits the polarization into two separate components, allowing more accurate modeling of battery behavior, especially at the end of charge and discharge cycles.

The DP model battery consists of the following elements:

1. *Open circuit voltage U_{oc}:* the voltage produced by the battery when there is no load.
2. *Internal resistances:* active resistance R_{ohm}, which describes the energy losses due to the resistive elements of the battery; *polarization resistances* – R_{ep} and R_{conp}, which characterize electrochemical and concentration polarization.
3. *Effective capacities:* C_{ep} and C_{conp}, which are used to describe transient reactions occurring during energy transfer. Capacity C_{ep} is used to describe electrochemical polarization, a C_{conp} to describe concentration polarization.

Voltages U_{ep} and U_{conp} describe the stresses arising on capacities C_{ep} and C_{conp}. I_{ep}, I_{conp} are the generated currents C_{ep} and C_{conp}. Thanks to equation (9), it is possible to describe the principle of operation of the DP dual polarization model battery:

$$\begin{cases} U_{ep} + R_{ep} C_{ep} \dfrac{dU_{ep}}{dt} = I_{load} \cdot R_{ep}, \\ U_{conp} + R_{conp} C_{conp} \dfrac{dU_{conp}}{dt} = I_{load} \cdot R_{conp}, \\ U_{load} = E - U_{ep} - U_{conp} - I_{load} \cdot R_{ohm}, \text{ V}. \end{cases} \tag{10}$$

The DP battery model is used to simulate and predict the behavior of different types of electrochemical batteries. It is used in research and development of new types of batteries, optimization of energy storage systems, modeling of electric vehicles, as well as in the analysis of power supply systems.

The simulated DP lithium cell model with temperature dependence and controlled current source is shown in Fig. 7. Stray circuit or self-discharge currents are not considered in this model, but this equivalent circuit is a compromise between complexity and accuracy [9]. The simulation model of the equivalent battery cell replacement circuit is built on the basis of SIMSCAPE blocks, as shown in Fig. 8.

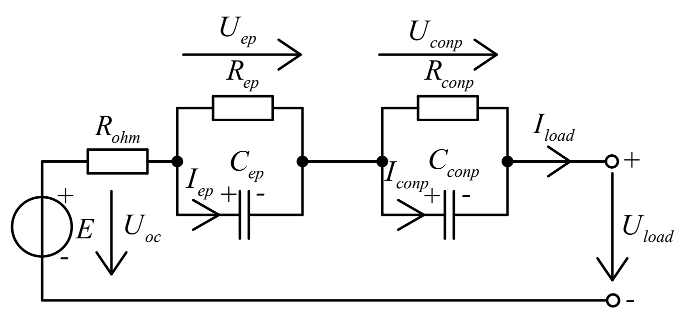

Fig. 6. Equivalent battery replacement scheme according to the DP model

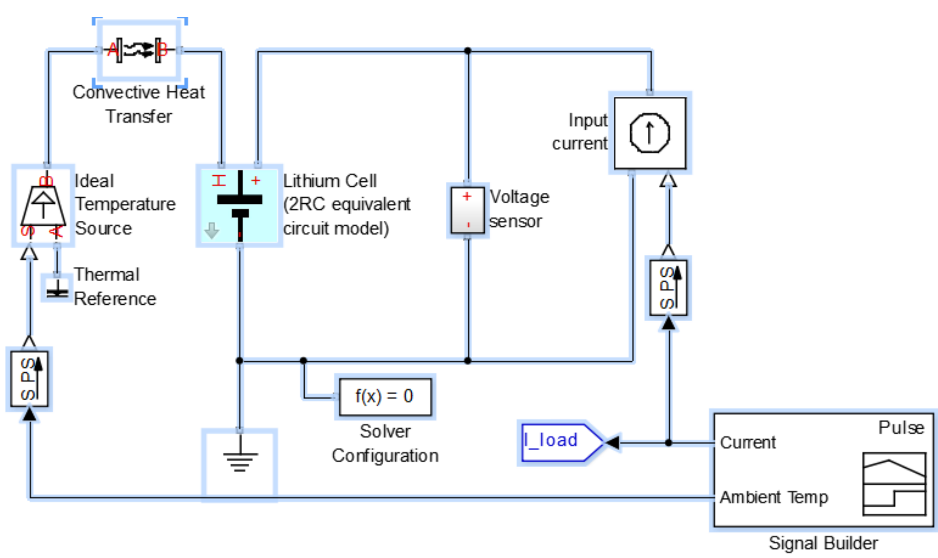

Fig. 7. Simulation model of a battery with a controlled current source

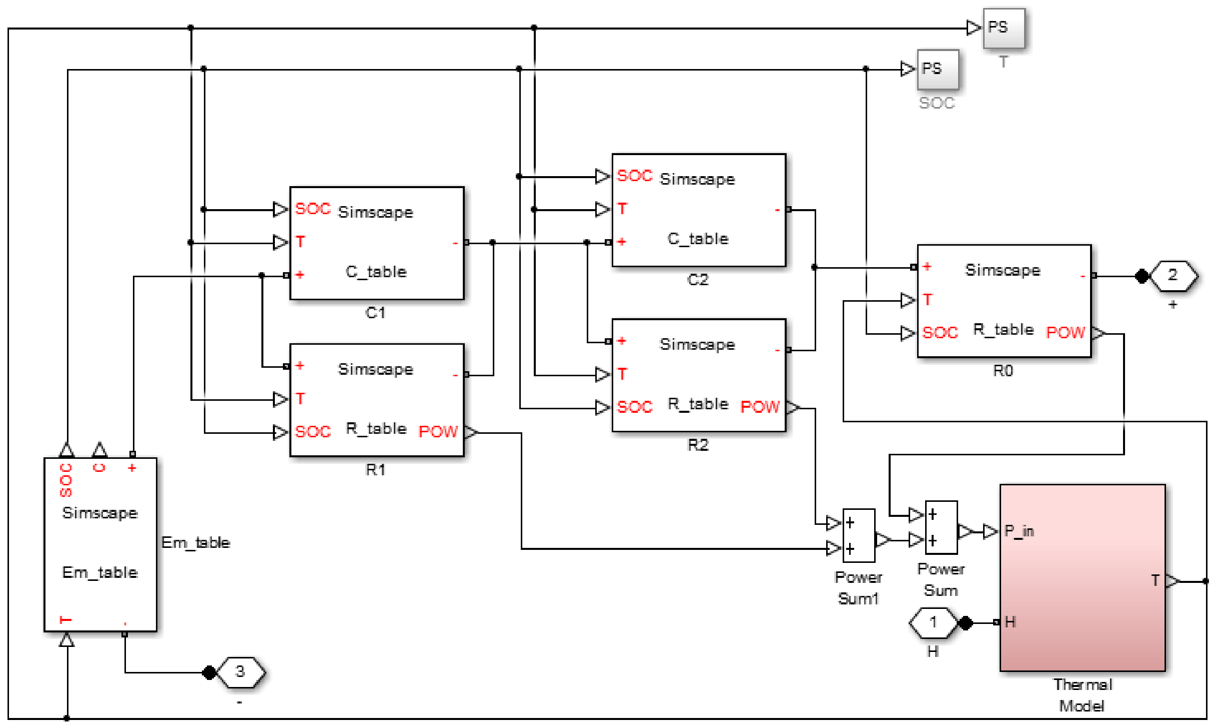

Fig. 8. Simulation model of the equivalent battery replacement scheme

Modeling of pulse discharge characteristics was performed on 4.18 Ah cells at six different temperatures. The battery cell was initially charged to 3.53 V, and then subjected to cycles of the partial discharge-rest phase. The results of the study show that the cell potential drops with decreasing SOC, as the cell discharges with a set of 4.18 A (Fig. 9). Battery discharge pulses lead to a slight increase in temperature by 0.4 °C from 20 °C.

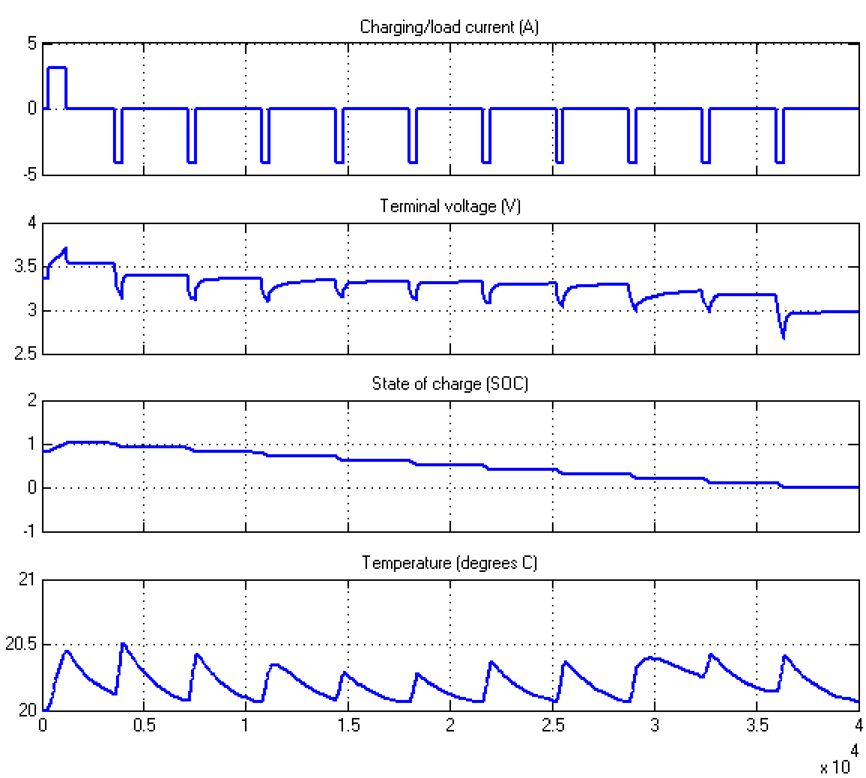

Fig. 9. Discharge curve for a lithium cell 4.18 Ah at a temperature of 20 °C

SOC is determined based on the Coulomb current count:

$$\mathrm{SOC} = 1 - \left(\int_0^t \frac{I_m}{C_Q} \mathrm{d}t \right), \ \%, \tag{11}$$

where I_m – the strength of the electric discharge current, A; $C_Q(I,T)$ – cell capacity, Ah; T – temperature, K.

The internal temperature of the cell is determined by the equation of thermal conductivity of a homogeneous body that exchanges heat with the environment:

$$T + C_T \cdot R_T \cdot \frac{dT}{dt} = T_a + R_T \cdot P_S, \tag{12}$$

where T – temperature, K; C_T – heat capacity of the cell, J·m^{-3}/K; R_T – coefficient of convective heat exchange between the cell and the environment, W·m^{-2}/K; T_a – absolute temperature, K; P_S – power of the internal heat source, W.

Fig. 10 shows the dependence of EMF E on SOC at different temperatures (–20 °C, –15 °C, –10 °C, 0, +20 °C, +40 °C).

The graphs E(SOC, T) show that electromotive force is more affected by state of charge than temperature. The highest value of E of a battery cell in the range of SOC change from 20 to 90 % is observed at a temperature of +20 °C.

Graphs R_{ohm}(SOC, T) are shown in Fig. 11. The internal resistance R_{ohm} shows a greater dependence on temperature than on the change in SOC

ISSN 2664-9969

due to the movement of ions through the separator. At high temperatures, the resistance value decreases [10].

Dependencies of the resistive component $R_1(\mathrm{SOC},T)$ characterizing the electrochemical polarization are shown in Fig. 12. The value of the active resistance $R_1 = R_{ep}$ is inversely proportional to the temperature. At temperatures −20 °C, +20 °C and +40 °C an increase in value is observed R_1.

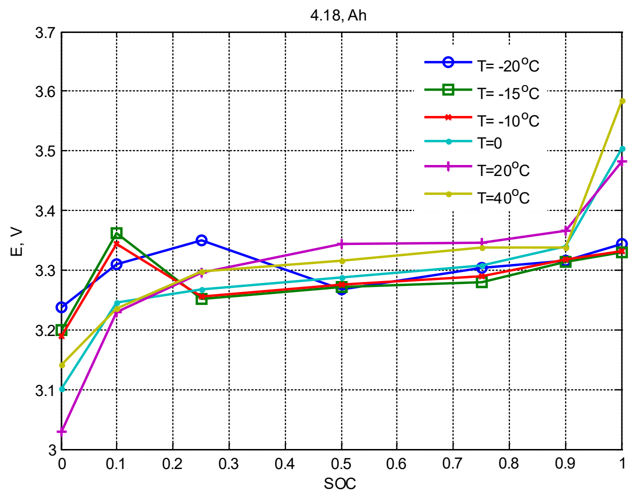

Fig. 10. Dependence $E(\mathrm{SOC},\ T)$

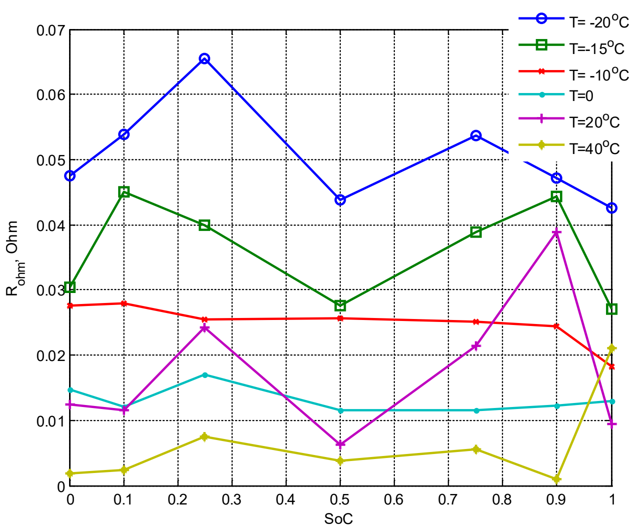

Fig. 11. Dependence $R_{ohm}(\mathrm{SOC},\ T)$

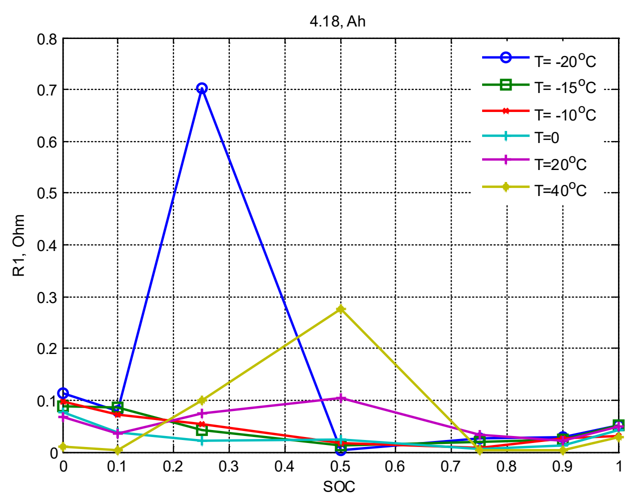

Fig. 12. Dependence $R_1(\mathrm{SOC},\ T)$

Fig. 13 shows the graphs of the capacitive component dependencies $C_1(\mathrm{SOC},T)$. Capacity $C_1 = C_{ep}$ and increases as the temperature increases 0.5 SOC.

Graphs of dependence of the resistive component $R_2(\mathrm{SOC},T)$ that characterize the concentration polarization are shown in Fig. 14.

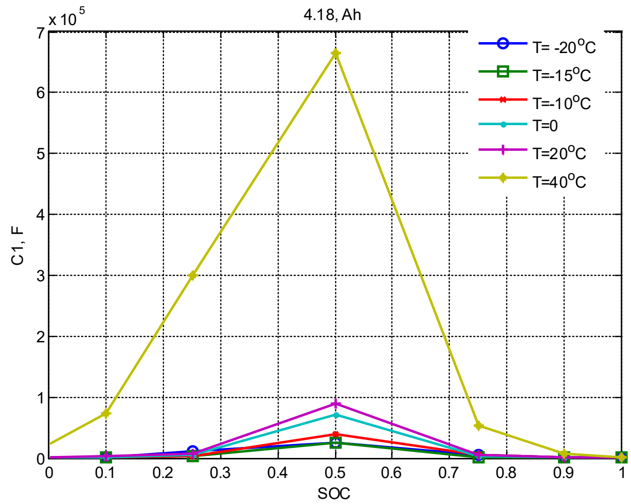

Fig. 13. Dependence $C_1(\mathrm{SOC},\ T)$

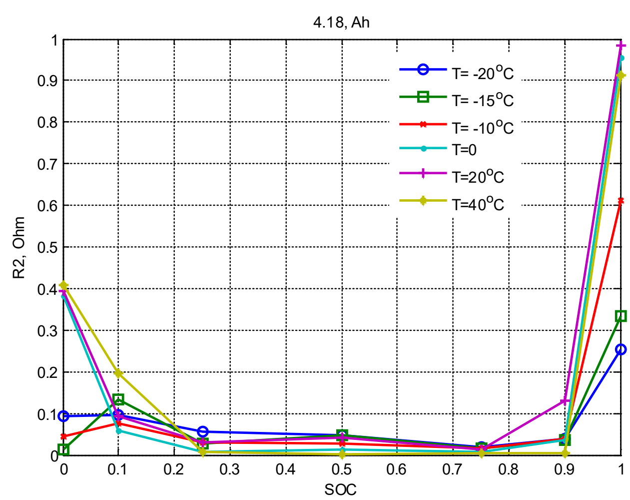

Fig. 14. Dependence $R_2(\mathrm{SOC},\ T)$

Active resistance $R_2 = R_{conp}$ and at different temperatures does not change in the range from 90 to 20 % SOC during discharge. For temperatures 0, +20 °C and +40 °C at 20–0 % SOC an increase in resistance is observed R_2 up to 4 times. As a result, the voltage on the battery terminals decreases in magnitude (Fig. 10). In the range of 100–90 % SOC a decrease in the resistance value is observed R_2. In Fig. 15 graphs of the capacitance component $C_2(\mathrm{SOC},T)$ are presented. Capacity $C_2 = C_{conp}$ and increases with an increase in temperature by 10 % SOC and decreases when decreased SOC from 100 to 75 %.

There are many models for predicting the performance of different types of batteries.

The classification of battery models is based on two groups: mathematical and physical. Physical models include electrical devices that modulate the operation of the battery as a whole or some of its properties.

In turn, mathematical models are divided into two groups and consist of systems of equations describing the operation of specific batteries.

The first group includes models that describe the processes of charging and discharging batteries in real installations at operating currents.

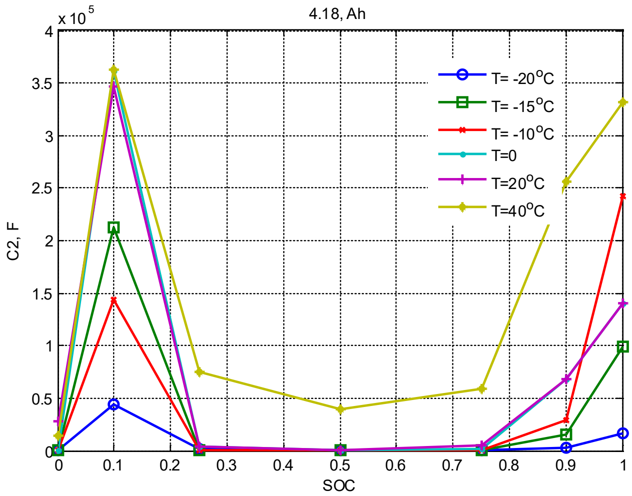

Fig. 15. Dependence C_2(SOC, T)

When building the models of the first group, four approaches are used:

1) static approach based on the class of degree polynomials;

2) phenomenological approach, which is built on the basis of experimental dependencies;

3) a dynamic approach based on known physical and chemical laws (electrotechnical model);

4) a constructive approach that uses «smart» suggestions using experimental dependencies.

Models of static, dynamic and constructive approaches are further divided into two groups:

1) models that determine the behavior of the battery as an element of an electric circuit;

2) models reflecting the influence of technological factors on the electrical characteristics of batteries.

The second group includes impedance models that describe the operation of batteries at low currents and polarizations in the linear region. They are divided into two groups: classical and structural models.

The model from the first group based on dual polarization takes into account polarization effects and more accurately shows the behavior of lithium-ion batteries and is a compromise between complexity and accuracy. These models can be used when researching electrical energy storage systems.

The equation in operator form describing the principle of operation of a Li-ion battery has the following form:

$$U_{load}(p) = E(p) - U_{ep}(p) - U_{conp}(p) - I_{load}(p)\cdot R_{ohm} =$$

$$= E(p) - \frac{I_{load}(p)\cdot R_{ep}}{\tau_{ep}p+1} - \frac{I_{load}(p)\cdot R_{conp}}{\tau_{conp}p+1} - I_{load}(p)\cdot R_{ohm} =$$

$$= E(p) - I_{load}(p)\left(\frac{R_{ep}}{\tau_{ep}p+1} + \frac{R_{conp}}{\tau_{conp}p+1} + R_{ohm}\right), \text{ V}, \qquad (13)$$

where $\tau_{ep} = R_{ep}\cdot C_{ep}$, $\tau_{conp} = R_{conp}\cdot C_{conp}$ – time constants characterizing electrochemical and concentration polarization, respectively, sec.

As can be seen from the expression, the internal resistance of the battery is non-linear:

$$R_0(p) = \frac{R_{ep}}{\tau_{ep}p+1} + \frac{R_{conp}}{\tau_{conp}p+1} + R_{ohm}.$$

Reducing the value of internal resistance R_0 makes the VAC of the battery more rigid. Increasing capacity values C_{ep}, C_{conp} leads to slowing down of electrochemical and concentration polarizations.

The practical use of the proposed mathematical model of the battery in energy systems allows to identify features that do not appear during modeling.

Prolonged air alarms or emergency power outages during martial law in Ukraine make it difficult to conduct experimental studies that take into account the effects of unmodeled dynamics and parametric uncertainties of the battery at different states of its charge and ambient temperature.

The further development of the proposed topic, which is connected with the verification of theoretical provisions with experimental data, is the next stage of the research.

4. Conclusions

Li-ion battery models based on electrochemical theory and electrical circuits are considered. The dual-polarization mathematical model was found to most accurately describe the performance of the battery at the end of the discharge cycle compared to the first-order Thevenin model, the *RC* model, and the active resistance battery model.

The physical processes in the battery during pulse discharge, which is the main part of electrical energy storage systems based on electrochemical technology, were studied. The dependence of the parameters of the equivalent lithium-ion battery replacement scheme according to the second-order Thevenin model on the ambient temperature and SOC state of charge is considered. It was established that the value of E depends more on the change in SOC than on temperature. In turn, active resistance R_{ohm} shows a greater dependence on temperature than on SOC change. At high temperatures, the resistance value decreases. Parameters R_1 and C_1, that characterize electrochemical polarization vary in the range from 10 to 75 % SOC. Parameters R_2 and C_2, which depend on the concentration polarization, change at intervals from 0 to 25 % SOC and 75 to 100 % SOC.

Conflict of interest

The authors declare that they have no conflict of interest in relation to this study, including financial, personal, authorship, or any other, that could affect the study and its results presented in this article.

Financing

The study was conducted without financial support.

Data availability

The manuscript has no associated data.

Use of artificial intelligence

The authors confirm that they did not use artificial intelligence technologies when creating the presented work.

 ISSN 2664-9969

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