The Development of a Mathematical Model of Lithium-Ion Battery Discharge Characteristics

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***Abstract*—This paper is devoted to obtaining a mathematical model of the lithium-ion battery discharge capacity at a constant current discharge from the system of physical and chemical processes in a lithium-ion battery equations obtained earlier by the authors. The input of this model is the discharge capacity of a particular instance of a lithium-ion battery and a constant discharge current at which the discharge capacity is determined. The output of the model is determined by the discharge capacity of the considered instance of the lithium-ion battery. The model under consideration for the discharge capacities of a lithium-ion battery is obtained by excluding dynamic variables and unknown constant coefficients from the system of physical and chemical processes in lithium-ion battery equations. This exclusion of dynamic variables is carried out numerically by calculating different dynamics of physical and chemical processes in a lithium-ion battery corresponding to different values of constant coefficients and further approximation of the desired model on these calculated dynamics. The obtained model is tested experimentally.**

Keywords—discharge capacity of lithium-ion battery, physical and chemical processes in lithium-ion battery, mathematical model

I. Introduction

High specific characteristics of lithium-ion batteries make it advisable to use them on the board of aircraft [1]. One of the most important characteristics of a lithium-ion battery is its discharge capacity. This capacity is determined by the DC discharge current and varies from instance to instance of the battery. Therefore, the discharge capacity of a lithium ion battery, defined by a constant discharge current shall be calculated as using this discharge current, and through some tell-tale characteristics of a lithium-ion battery obtained from the control discharge curves of a lithium ion battery, remove the control level. For example, during discharges with control currents of discharge 0.2C, 1.0C, 2.0C. This paper is devoted to obtaining a model of the discharge capacity of a lithium-ion battery.

II. Problem Statement

The tasks solved in this paper are:

- obtaining the dependence of the discharge capacity C_{I_p} of the lithium-ion battery on the current I_p, nominal capacity C_{nom} and control discharge currents of 0.2C, 1.0C, 2.0C discharge capacities $Q_{0.2C}^{(contr)}$:

$$\frac{Q_I^p}{C_{nom}} = \hat{Q}_I^p \left(\frac{I_k}{K_I C_{nom}}, \frac{Q_{0.2C}^{(contr)}}{C_{nom}}, \frac{Q_{1.0C}^{(contr)}}{C_{nom}}, \frac{Q_{2.0C}^{(contr)}}{C_{nom}} \right), \quad (1)$$

where $K_I = const$, $K_I > 0$.

- experimental verification of the reduced dependence (1) using experimentally captured discharge curves of a specific lithium-ion battery.

III. Research Methods

The dependence (1) of the discharge capacity of the lithium-ion battery is obtained from the system of equations of physical and chemical processes in the battery obtained by the authors earlier in [2] by excluding dynamic variables and unknown constant coefficients from this system.

In General, the exclusion of the described values from the system of dynamic equations is carried out as:

- analytically, by simplifying the system of physical and chemical processes equations and further analytical transformation of simplified expressions;
- numerically using Monte Carlo methods, by specifying randomly (from a set of possible values) the coefficients included in the equations of physical and chemical processes, and the initial values of dynamic variables, further calculation of the corresponding dynamics of physical and chemical processes and obtaining the desired dependence (including dependence (1)) by approximation methods [2]-[4].

In the case of analytical exclusion of dynamic variables and unknown constants in the vast majority of cases, the system of physical and chemical processes equations is simplified. Each subset of the set (possible values) of the

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initial values of dynamic variables and unknown constant coefficients has its own simplification of the system of physical and chemical processes equations. Thus, we have a set of models, each of which corresponds to a subset of the set (possible values) of initial values and unknown coefficients. Each subset of the described values corresponds to a specific brand of the simulated technical object. Hence, from the obtained set of models, we choose for each brand of the simulated technical object the model that best describes the experimentally obtained test results of this object with the required accuracy.

Similarly, in the case of numerical receipt of a mathematical model of a technical object, we also break down into subsets many (possible values) of the initial values of dynamic variables and coefficient values, each of which build (numerically, using Monte Carlo methods and approximation methods) the corresponding mathematical model of the object in question. And then for each instance of the object in question, using the test results of these objects, we select a mathematical model that best describes these test results.

In the case of lithium-ion batteries, dependence (1) will be used to use the system of equations of physical and chemical processes in batteries by numerical methods. The initial values of dynamic variables, which are included in the system of equations of physical and chemical processes in lithium-ion batteries, are determined from the equilibrium conditions (thermodynamic) of these physical and chemical processes. Thus, to obtain dependence (1) we set the possible values of constant coefficients, included in the system of equations of physical and chemical processes in the lithium-ion battery, break into subsets, on each of which we build dependence (1). Then we test each dependence (1) experimentally for a specific brand of lithium-ion battery and choose the dependence (1), best describing the test results of these lithium-ion batteries (with the required accuracy).

IV. Equations Of Physical And Chemical Processes In A Lithium-Ion Battery

Earlier, the authors obtained a system of equations of physical and chemical processes in a lithium-ion battery, given in [2]. The coefficients with indices included in this system of equations are the setting ones. They depend on the individual parameters of lithium-ion batteries. These parameters vary from instance to instance of the lithium-ion battery of the model in question. Other coefficients included in this system are approximations. They are the same for all instances of the model in question.

V. Obtaining A Mathematical Model For Lithium-Ion Battery Discharge Capacities

In this paper, we will give only one such subset of coefficients, which are part of the above-mentioned system of physical-chemical equations, to illustrate the given method of obtaining dependence of lithium-ion battery (Fig. 1). Moreover, we will set the values given in [2] to the approximation coefficients, since at these values we obtain a discharge voltage curve coinciding with the experimental one (relative error of 6%) [2].

A. *Calculation of the set of possible dynamics of physical and chemical processes in a lithium-ion battery*

Generating different sets of possible values of the setting coefficients included in the equations of physical and chemical processes in lithium-ion batteries, we obtain a set of corresponding possible discharge voltage curves at different constant discharge currents [2]. The discharge capacities corresponding to these possible dynamics are given in Tables I (will be used to obtain the dependence (1)) and II (will be used to verify the correctness of obtaining the dependence (1) from the system of equations of physical and chemical processes in a lithium-ion battery given in [2]).

TABLE I. CAPACITIES AT VARIOUS DISCHARGE CURRENTS, % C

№№	Control capacities			Reference capacities	
	Discharge current of 1.0C	*Discharge current of 2.0C*	*Discharge current of 0.2C*	*Discharge current of 0.5C*	*Discharge current of 1.5C*
1	129.3	108.3	134.43	132.63	123.3
2	127.23	102.3	134.1	131.83	119.1
3	125.79	97.35	133.5	131.43	115.53
4	125.1	94.83	133.5	131.43	112.5
5	124.95	94.23	133.5	131.13	112.5
6	128.793	105.00	134.25	132.45	122.1
7	127.53	103.5	134.7	132.3	119.1
8	126.45	98.7	134.7	132.15	115.53
9	124.23	92.37	133.95	131.067	110.75
10	128.43	111.963	134.31	131.981	123.15
11	125.31	95.73	134.183	131.49	113.55

TABLE II. CAPACITIES AT VARIOUS DISCHARGE CURRENTS, % C

№№		1	2	3	4	5
Control capacities	*Discharge current =1.0C*	128.43	129.3	128.31	129.9	128.73
	Discharge current = 2.0C	103.35	108.3	109.93	111.3	105.81
	Discharge current = 0.2C	134.43	134.67	134.37	134.67	134.67
Reference capacities	*Discharge current = 0.4C*	133.05	133.35	132.75	133.35	133.35
	Discharge current = 0.5C	132.45	132.81	131.97	132.81	132.75
	Discharge current = 0.8C	130.35	130.71	130.083	131.25	130.65
	Discharge current = 1.2C	126.3	127.47	126.27	128.13	126.63
	Discharge current = 1.5C	121.5	123.15	122.49	124.53	122.1
	Discharge current = 1.8C	111.63	116.31	116.01	118.11	113.7

B. *Obtaining the Li-ion battery discharge capacity dependence*

Having obtained the discharge capacities of a lithium-ion battery for various possible dynamics of physical and chemical processes in a lithium-ion battery, we will obtain dependence (1) for these discharge capacities. As can be easily seen from Tables I and II, the discharge capacity of the lithium-ion battery also decreases as the reference discharge capacity of the lithium-ion battery decreases. Hence, it is expedient to search for the dependence (1) on the control discharge capacitances in a quadratic form:

$$
\begin{aligned}
\frac{Q_I^p}{C_{nom}} &= \tilde{Q}_I^{p(0)}\left(\bar{I}_k\right)+\tilde{Q}^{p(1)}_{I,Q^{(contr)}_{0.2C}}\left(\bar{I}_k\right)\frac{Q^{(contr)}_{0.2C}}{C_{nom}}+ \\
&+\tilde{Q}^{p(1)}_{I,Q^{(contr)}_{1.0C}}\left(\bar{I}_k\right)\frac{Q^{(contr)}_{1.0C}}{C_{nom}}+\tilde{Q}^{p(1)}_{I,Q^{(contr)}_{2.0C}}\left(\bar{I}_k\right)\frac{Q^{(contr)}_{2.0C}}{C_{nom}}+ \\
&+\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{0.2C},Q^{(contr)}_{0.2C}}\left(\bar{I}_k\right)\left(\frac{Q^{(contr)}_{0.2C}}{C_{nom}}\right)^2+ \\
&+\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{0.2C},Q^{(contr)}_{1.0C}}\left(\bar{I}_k\right)\frac{Q^{(contr)}_{0.2C}}{C_{nom}}\frac{Q^{(contr)}_{1.0C}}{C_{nom}}+ \\
&+\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{1.0C},Q^{(contr)}_{1.0C}}\left(\bar{I}_k\right)\left(\frac{Q^{(contr)}_{1.0C}}{C_{nom}}\right)^2+ \\
&+\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{0.2C},Q^{(contr)}_{2.0C}}\left(\bar{I}_k\right)\frac{Q^{(contr)}_{0.2C}}{C_{nom}}\frac{Q^{(contr)}_{2.0C}}{C_{nom}}+ \\
&+\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{2.0C},Q^{(contr)}_{2.0C}}\left(\bar{I}_k\right)\left(\frac{Q^{(contr)}_{2.0C}}{C_{nom}}\right)^2+ \\
&+\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{1.0C},Q^{(contr)}_{2.0C}}\left(\bar{I}_k\right)\frac{Q^{(contr)}_{1.0C}}{C_{nom}}\frac{Q^{(contr)}_{2.0C}}{C_{nom}}, \bar{I}_k=\frac{I_k}{K_I C_{nom}},
\end{aligned}
\tag{2}
$$

where dependencies $\tilde{Q}_I^{p(0)}\left(\bar{I}_k\right)$, $\tilde{Q}^{p(1)}_{I,Q^{(contr)}_{0.2C}}\left(\bar{I}_k\right)$, $\tilde{Q}^{p(1)}_{I,Q^{(contr)}_{1.0C}}\left(\bar{I}_k\right)$, $\tilde{Q}^{p(1)}_{I,Q^{(contr)}_{2.0C}}\left(\bar{I}_k\right)$, $\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{0.2C},Q^{(contr)}_{0.2C}}\left(\bar{I}_k\right)$, $\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{0.2C},Q^{(contr)}_{1.0C}}\left(\bar{I}_k\right)$, $\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{1.0C},Q^{(contr)}_{1.0C}}\left(\bar{I}_k\right)$, $\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{0.2C},Q^{(contr)}_{2.0C}}\left(\bar{I}_k\right)$, $\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{2.0C},Q^{(contr)}_{2.0C}}\left(\bar{I}_k\right)$, $\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{1.0C},Q^{(contr)}_{2.0C}}\left(\bar{I}_k\right)$ are searched from the data given in Table I.

These dependences for some discharge currents are given in Table III (determined for reference capacitances as a percentage of the rated capacitance divided by 100). The value of the current coefficient is taken equal to 1/1.17 h^{-1} for convenience reasons.

TABLE III. DEPENDENCES FOR DISCHARGE CURRENTS

	Current 0.5C	**Current 1.5C**	**Current 1.0C**	**Current 2.0C**	**Current 0.2C**
$\tilde{Q}_I^{p(0)}\left(\bar{I}_k\right)$	2.363	-7.9614	0.28092	-0.0742	0.35425
$\tilde{Q}^{p(1)}_{I,Q^{(contr)}_{1.0C}}\left(\bar{I}_k\right)$	1.41126	-5.1178	0.31619	0.12328	0.13608
$\tilde{Q}^{p(1)}_{I,Q^{(contr)}_{2.0C}}\left(\bar{I}_k\right)$	-4.6089	22.4280	0.12381	0.97771	0.00955
$\tilde{Q}^{p(1)}_{I,Q^{(contr)}_{0.2C}}\left(\bar{I}_k\right)$	-0.4059	1.99463	0.13640	0.00949	0.33579
$\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{1.0C},Q^{(contr)}_{1.0C}}\left(\bar{I}_k\right)$	-0.5099	3.46674	0.23504	-0.0019	-0.0859
$\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{1.0C},Q^{(contr)}_{2.0C}}\left(\bar{I}_k\right)$	-2.1439	9.89820	-0.1033	0.00226	0.04727
$\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{0.2C},Q^{(contr)}_{1.0C}}\left(\bar{I}_k\right)$	1.94123	-9.7385	0.14148	-0.0898	0.02576
$\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{2.0C},Q^{(contr)}_{2.0C}}\left(\bar{I}_k\right)$	0.47742	-3.4434	0.00787	-0.0002	-0.0046
$\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{0.2C},Q^{(contr)}_{2.0C}}\left(\bar{I}_k\right)$	4.66861	-20.410	-0.0060	0.01479	-0.0448
$\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{0.2C},Q^{(contr)}_{0.2C}}\left(\bar{I}_k\right)$	-2.3247	10.9935	-0.1155	0.03388	0.25218

Using the reference values of dependencies calculated from a variety of possible dynamics of physical and chemical processes in a lithium-ion battery $\tilde{Q}_I^{p(0)}\left(\bar{I}_k\right)$, $\tilde{Q}^{p(1)}_{I,Q^{(contr)}_{0.2C}}\left(\bar{I}_k\right)$, $\tilde{Q}^{p(1)}_{I,Q^{(contr)}_{1.0C}}\left(\bar{I}_k\right)$, $\tilde{Q}^{p(1)}_{I,Q^{(contr)}_{2.0C}}\left(\bar{I}_k\right)$, $\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{0.2C},Q^{(contr)}_{0.2C}}\left(\bar{I}_k\right)$, $\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{0.2C},Q^{(contr)}_{1.0C}}\left(\bar{I}_k\right)$, $\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{1.0C},Q^{(contr)}_{1.0C}}\left(\bar{I}_k\right)$, $\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{0.2C},Q^{(contr)}_{2.0C}}\left(\bar{I}_k\right)$, $\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{2.0C},Q^{(contr)}_{2.0C}}\left(\bar{I}_k\right)$, $\tilde{Q}^{p(2)}_{I,Q^{(contr)}_{1.0C},Q^{(contr)}_{2.0C}}\left(\bar{I}_k\right)$ at the corresponding reference points, as well as interpolation by cubic splines, we obtain the required dependence (1) in the form of (2) with a given cubic interpolation of these coefficients. The discharge capacities of the lithium-ion battery calculated from this obtained dependence are shown in Table IV. Comparing these calculated according to the model of the discharge capacity are shown in Table IV discharge capacity with the discharge capacity shown in Table III, we get the relative error (in %) receipt from the system of equations of physico-chemical processes in lithium-ion battery models for discharge capacities given in Table IV (in parentheses).

TABLE IV. DISCHARGE CAPACITY OF A LITHIUM-ION BATTERY, % C

№№	**1**	**2**	**3**	**4**	**5**
Current = 0.2C	134.42944 (0.000413)	134.67028 (0.000211)	134.36969 (0.000229)	134.67086 (0.000641)	134.67002 (0.000017)
Current = 0.4C	133.23683 (0.140421)	133.39567 (0.034245)	132.80279 (0.03977)	133.4067 (0.042516)	133.36119 (0.008395)
Current = 0.5C	132.61509 (0.124646)	132.79085 (0.014422)	132.06604 (0.072773)	132.84502 (0.02637)	132.7178 (0.024255)
Current = 0.8C	130.40187 (0.039793)	130.86884 (0.121524)	129.88077 (0.15546)	131.18898 (0.046489)	130.56753 (0.063122)
Current = 1.0C	128.43112 (0.000875)	129.29996 (0.000031)	128.30996 (0.000032)	129.89856 (0.001108)	128.73046 (0.000359)
Current = 1.2C	125.84759 (0.3582)	127.28617 (0.144213)	126.48124 (0.167293)	128.23377 (0.080985)	126.34678 (0.223659)
Current = 1.5C	120.18278 (1.084129)	122.74593 (0.328109)	122.55846 (0.055889)	124.34282 (0.150309)	121.15524 (0.773758)
Current = 1.8C	111.42779 (0.181145)	115.36482 (0.81264)	116.16014 (0.129419)	117.7567 (0.299129)	113.16675 (0.468996)
Current = 2.0C	103.3506 (0.000576)	108.30058 (0.000537)	109.93047 (0.000423)	111.30048 (0.00043)	105.81071 (0.000674)

Table IV shows that the relative error of obtaining a model for the discharge charge capacity of a lithium-ion battery from the system of equations of physical and chemical processes in a lithium-ion battery does not exceed 1.1%.

VI. Experimental Verification Of The Model For The Discharge Charge Capacity Of A Lithium-Ion Battery

Now let's check the obtained model on the experimentally removed discharge voltage curves (discharge by direct currents of 0.2C, 0.5C, 1.0C, 1.5C, 2.0C) of a lithium-ion battery (Fig. 1) [5]. The discharge capacities obtained from these experimental curves (Fig. 1), calculated from the model (2) for discharge capacities, as well as the relative error of calculation of these capacities are given in Table V.

Table V shows that the relative error in calculating the discharge capacity of the lithium-ion battery according to the obtained model for the discharge capacity of the lithium-ion battery in comparison with the experimental data does not exceed 4%.

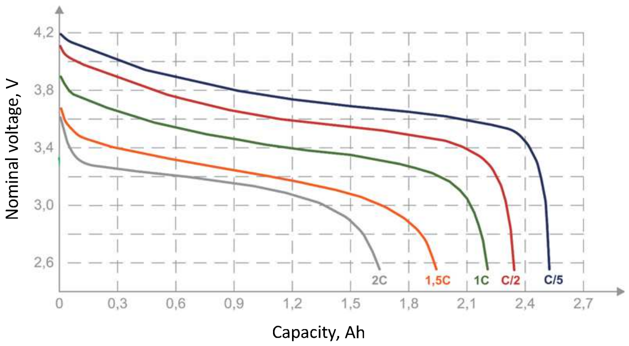

Fig. 1. Dependence of nominal voltage on the capacity

TABLE V. Comparison of Calculated Capacity with the Experimental Data

	Current =0.2C, %	***Current =0.5C, %***	***Current =1.0C, %***	***Current =1.5C, %***	***Current =2.0C, %***
Calculated capacity, % C	126.78452	121.97429	111.06694	100.90241	82.58582
Experimental capacity, % C	126.78392	117.63819	110.60302	97.18593	82.66332
Relative error	0.0004721	3.6859624	0.4194521	3.8240955	0.0937507

Conclusion

In this paper, a mathematical model was obtained for the discharge capacity of a lithium-ion battery from the system of equations of physical and chemical processes by excluding dynamic variables and unknown constant coefficients from this system. The elimination of these values was carried out numerically by generating random values of these coefficients, calculating the corresponding dynamics of physical and chemical processes in a lithium-ion battery and approximating the desired model on these dynamics. These random values were taken for a subset of the set of possible values of the constant coefficients of the system of equations of physical and chemical processes in a lithium-ion battery. And for this subset, a model of discharge characteristics of a lithium-ion battery was built. This model was tested experimentally, and it was shown that the relative error of deviation of the calculated values of the discharge capacity from the corresponding experimental model does not exceed 4%.

Since the model of discharge capacity of lithium-ion batteries obtained in this paper was obtained only for one subset of the set of possible values of the constant coefficients of the system of equations of physical and chemical processes in a lithium-ion battery, this model is not valid for all brands of lithium-ion batteries. For other brands of lithium-ion batteries, the described model must be obtained in the manner described in this paper for the remaining subsets of the set of possible values of the constant coefficients of the system of equations of physical and chemical processes in a lithium-ion battery. To allocate such appropriate considering Marche lithium-ion battery, you can also subset by matching the calculated curves of voltages and temperatures on the system of equations of physico-chemical processes in the battery with the corresponding experimentally removed for a specific brand of battery curves, stress and temperature [2], [4].

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