

Computer Simulation of Active Layers in Double-Layer Supercapacitors: Galvanostatics, Determination of Effective Coefficients, and Calculation of Overall Characteristics

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Received October 10, 2012

Abstract—A computer simulation of the structure and modes of functioning of biporous active layers (activated carbon) in double-layer capacitors (DLCs) was performed. The charging of DLCs in a galvanostatic mode was studied. The main characteristics of DLCs (charging time, specific capacity, stored energy, and power) were calculated. DLCs with aqueous electrolyte of different types were studied: active layer with the “ideal” structure (type 1), active layer with a monoporous structure (2), and biporous active layer (3). A computer simulation of biporous active layers of DLCs involves the formulation of a model of the structure of the active layer, percolation evaluation, and calculation of the effective ion conductivities of both highly porous carbon grains and the whole active layer. When calculating the characteristics of the active layers of DLC, we analyzed the effect of the main parameters (charge current density and active layer thickness) on the charging process and overall characteristics. The central problem of calculation of a DLC with a real, nonmonoporous structure was formulated. In active layers generally having pores of three types (micro-, meso-, and macropores) in the galvanostatic mode of DLC charging, the wide pores are polarized first. In this case, the limiting acceptable potential is achieved, and galvanostatic charging should be stopped and changed to potentiostatic charging. As a result, a large number of micropores can remain unpolarized. Therefore, it is important to perform a theoretical search for means to carry out complete adsorption of ions in micropores and obtain high specific capacities of DLCs.

Keywords: computer simulation, double-layer capacitor, galvanostatics, active layer with a biporous structure, aqueous electrolyte

DOI: 10.1134/S1023193514010030

1. STATEMENT OF THE PROBLEM

In the last two decades, electrochemical capacitors or supercapacitors have attracted considerable attention of researchers. These rechargeable power sources use recharging of the electric double layer on porous active layers with a high specific surface area of micropores [1]. They can provide specific capacities of 100 F/g and energies of the order of 50 kJ/kg [2].

Supercapacitors include double-layer capacitors (DLCs), pseudocapacitors, and hybrid capacitors [3]. In contrast to studies of the effect of side reactions [4] or studies that took into account Faraday processes [5], this study is concerned only with DLCs. A DLC consists of two porous polarizable electrodes (two active layers) immersed in an aqueous or nonaqueous electrolyte solution [6].

The goal of this study was to demonstrate a computer simulation of the structure and functioning of

biporous active layers (highly disperse activated carbon) during galvanostatic charging of DLCs. The structural and effective parameters of the model were determined and the main characteristics (charging time, potentials, specific capacities, energies, and power) were calculated. The central problem of calculating the characteristics of active layers of DLCs was formulated.

Let us explain what is meant under the “computer simulation of active layers.”

The active layer of a porous electrode (not only in DLCs, but also in fuel cells with polymer electrolyte, lithium ion batteries, etc.) is a complex structural formation. Due to this complex structure, high specific surface (cm^2/cm^3) is created in the active layer for a definite electrochemical process to occur on it and optimum channels appear for supplying electrons, ions, and gas molecules (for the fuel cell) to this surface. High currents (A/cm^2) and specific capacities (F/g for the active layer of DLC) or a sufficient

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amount of the desired product (electrosynthesis) can be obtained only under this condition.

The structure of the active layer can be described by at least four parameters. For example, in the active layers of DLCs, this is the active layer thickness (L , cm), the mean radii of small (ρ_1 , cm) and large (ρ_2 , cm) pores, and the fraction of the volume of the active layer (g) in a small pore (obviously, the proportion of volume in large pores is $1 - g$). The charging current density should be added to these four parameters (galvanostatics, I , A/cm²). A number of parameters that characterize the active layer but cannot be varied should also be added.

The challenge for the researcher is to analyze how this whole large set of parameters affects the characteristics of the active layers of DLCs (the charging time and the specific capacity, energy, and power). This problem cannot be adequately solved by experimental methods. Therefore, here we have to resort to computer simulation.

A computer simulation (using the active layer of DLC as an example) involves the following steps.

First of all, a computer model of the active layer of DLC that is adequate to real samples is created and all the parameters of the structure of the active layer in this model are determined.

Then the parameters of the structure of the active layer are correlated with the effective coefficients in the set of equations that describe the charging of the active layer of DLC.

Thereafter calculations by the set of equations that describe the charging are performed and the characteristics of the active layers of DLCs are evaluated.

A series of computer simulations can give an answer to many questions concerning the mechanism of the operation of the active layer of DLCs. We can finally optimize the parameters of the structure of the active layers of DLCs and obtain the maximum values of overall characteristics.

This program is implemented as described below.

2. CALCULATED EQUATIONS

The galvanostatic charging of the surface of porous electrodes was first studied by O.S. Ksenzhek (Ukraine) half a century ago [7–9]. The same problems were simultaneously studied by other authors [10, 11]. The potentiostatic charging of porous electrodes was also investigated in [12]. The goal of these studies, however, was not reduced to attempts to achieve high specific capacity of the double layer in active layers.

The properties of porous electrodes designed for use in fuel cells also started to be actively studied at that time. The charging of porous electrodes at constant current allowed kinetic studies of electrochemical processes not distorted by macrokinetic effects [13–15]. The concept of the porous space in elec-

trodes remained very simplified at that time. The pores in electrodes mostly had the form of identical nonintersecting cylindrical capillaries.

The differential equation that describes the charge conservation law for ion adsorption from an electrolyte during galvanostatic charging was proposed in [16]:

$$kd^2E/dx^2 = gSC_s dE/dt, \quad (1)$$

where $0 \leq x \leq L$ is the active layer of a finely divided carbon material, x is the coordinate, L is the thickness of the active layer, k (S cm⁻¹) is the effective specific conductivity of the active layer, $E(x, t)$ (V) is the potential, t is time, S (cm⁻¹) is the specific surface area of the porous material, C_s (F/cm²) is the specific capacity of the electric double layer on this material, and g is the proportion of the active part of the surface of the material.

The boundary conditions (galvanostatic charging mode) are

$$-k(dE/dx)|_{x=L} = I, \quad (2)$$

where I (A/cm²) is the charge current density, and

$$(dE/dx)|_{x=0} = 0. \quad (3)$$

The initial condition is

$$E|_{x,t=0} = E_0. \quad (4)$$

Equation (1) with boundary and initial conditions (2)–(4) can be recorded in a different way. We introduce a new notation: $x^* = x/L$ is the reduced coordinate; $E^* = E/E_0$ is the reduced potential; and t^* is the reduced time ($t^* = t/\tau$), where τ has the meaning of the characteristic charging time,

$$\tau = gSC_s L^2/k. \quad (5)$$

Then instead of (1) we have

$$d^2E^*/dx^{*2} = dE^*/dt^*. \quad (6)$$

The boundary conditions are

$$-dE^*/dx^*|_{x^*=1} = I^*, \quad (7)$$

where $I^* = I/J$ is the reduced charge current density ($J = kE_0/L$ is the characteristic charging current density), and

$$dE^*/dx^*|_{x^*=0} = 0. \quad (8)$$

The initial condition is

$$E^*|_{x^*,t^*=0} = 1. \quad (9)$$

The solution of (6) has the form

$$E^*(x^*, t^*) = 1 + I^* \left[t^* + \frac{3x^{*2} - 1}{6} + \frac{2}{\pi^2} \sum_{m=1}^{+\infty} (-1)^{m+1} \frac{\exp(-m^2 \pi^2 t^*)}{m^2} \cos(m\pi x^*) \right]. \quad (10)$$

Figure 1 shows how the character of the distribution of the reduced potential $E^* = E/E_0$ changes

throughout the active layer thickness at different moments of reduced time t^* at a charge current density $I^* = 1$ if t^* is gradually increased from 0.01 to 1.0.

3. THE "IDEAL" ACTIVE LAYER

Let us now calculate how the basic characteristics of the active layer of DLC change with time. The equations for calculating the overall characteristics (potential, specific capacity, specific stored energy, and specific power) are given in the Appendix (at the end of the paper).

The main equations for the overall characteristics are summarized below:

The potential of the active layer is

$$E(L,t) = E_0 + \frac{I}{k} \left[\frac{kt}{gSC_s L} + \frac{L}{3} - \frac{2L}{\pi^2} \sum_{m=1}^{+\infty} \frac{\exp\left(-\frac{m^2 \pi^2 k t}{L^2 SC_s}\right)}{m^2} \right]$$

The specific capacity of the active layer is

$$\frac{C(t)}{L} = \frac{kt}{L^2 \left[\frac{kt}{gSC_s L^2} + \frac{1}{3} - \frac{2}{\pi^2} \sum_{m=1}^{+\infty} \frac{\exp\left(-\frac{m^2 \pi^2 k t}{L^2 SC_s}\right)}{m^2} \right]}, \text{ F/cm}^3.$$

In the limit of $t \rightarrow \infty$,

$$\frac{C}{L} = gSC_s, \text{ F/cm}^3. \quad (11)$$

The specific energy of the active layer is

$$\frac{W}{L} = \frac{I^2}{k} \left[\frac{kt^2}{2gSC_s L^2} + \frac{t}{3} + \frac{L^2 SC_s}{k} \right] \times \left[\frac{2}{\pi^4} \sum_{m=1}^{+\infty} \frac{\exp\left(-\frac{m^2 \pi^2 k t}{L^2 SC_s}\right)}{m^4} - \frac{1}{45} \right]$$

The specific capacity of the active layer is

$$\frac{P(t)}{L} = \frac{I \Delta \varphi(t)}{L} = \frac{I^2}{k} \times \left[\frac{kt}{gSC_s L^2} + \frac{1}{3} - \frac{2}{\pi^2} \sum_{m=1}^{+\infty} \frac{\exp\left(-\frac{m^2 \pi^2 k t}{L^2 SC_s}\right)}{m^2} \right]$$

The structure of the active layer of DLC is initially assumed to be "ideal." All the pores are identical cyl-

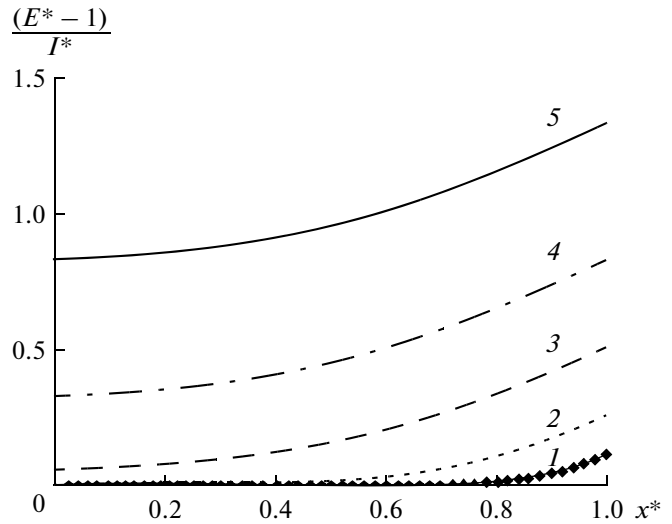


Fig. 1. Distribution of the deviation of the reduced potentials from the reduced initial potential $(E^* - 1)/I^*$ over the active layer thickness in a double-layer capacitor at different moments of the reduced time t^* at a reduced charging current density $I^* = 1$, t^* : (1) 0.01, (2) 0.05, (3) 0.2, (4) 0.5, and (5) 1.0.

inders arranged uniformly in space and filled with an electrolyte.

The parameters of the "ideal" active layer are: Ω is the porosity of the active layer, D is the diameter of the cylindrical pores, and S (cm^{-1}) is the specific pore surface area. If n is the number of pores at 1 cm^2 of the active layer surface, then, obviously,

$$\Omega = \pi(D/2)^2 n, \quad (12)$$

$$S = \pi D n. \quad (13)$$

Eliminating n from (12) and (13), we obtain

$$S = 4\Omega/D. \quad (14)$$

It should also be added that in all of the above equations in the "ideal" active layer model, the effective ion conductivity of the active layer should be calculated by the equation

$$k = k_0 \Omega, \quad (15)$$

where k_0 is the ion conductivity in the electrolyte.

4. CHARACTERISTICS OF DLCs WITH THE "IDEAL" ACTIVE LAYER

Below it is assumed that the porosity of the active layer is $\Omega = 0.5$, the specific conductivity of the aqueous electrolyte solution (30% H_2SO_4 + water [17]) is $k_0 = 0.8 \text{ S cm}^{-1}$, and the initial potential is $E_0 = 0.5 \text{ V}$ [6]. Then, obviously, $k = k_0 \Omega = 0.4 \text{ S cm}^{-1}$; the specific surface area is $S = 2 \times 10^4 \text{ cm}^{-1}$.

The potential difference $E(L, t) - E_0$ can actually increase only by a relatively small value. The electrolyte in DLC can be either aqueous or nonaqueous (organic). The devices based on aqueous electrolytes

Table 1. DLC, “ideal” active layer, aqueous electrolyte (30% H₂SO₄ + water). Dependence of the charging time t , specific capacity C/L , energy W/L , and power P/L on the charging current density I and active layer thickness L : $\Omega=0.5$, $D = 10^{-4}$ cm, $S = 2 \times 10^4$ cm⁻¹, $k_0 = 0.8$ S cm⁻¹, $k = 0.4$ S cm⁻¹, $E_0 = 0.5$ V, and $E^*(L) = 1.5$ V

I , A/cm ²	L , cm	t , s	C/L , F/cm ³	W/L , J/cm ³	P/L , W/cm ³
1.0	0.001	0.0004	0.4	0.2	1000
	0.01	0.004	0.4	0.2	100
	0.1	0.037	0.37	0.198	10
	1.0	0.13	0.13	0.084	1
0.1	0.001	0.004	0.4	0.2	100
	0.01	0.04	0.4	0.2	10
	0.1	0.4	0.4	0.2	1
	1.0	3.7	0.37	0.198	0.1
0.01	0.001	0.04	0.4	0.2	10
	0.01	0.4	0.4	0.2	1
	0.1	4	0.4	0.2	0.1
	1.0	39.7	0.4	0.2	0.01

Table 2. DLC, “ideal” active layer, aqueous electrolyte (30% H₂SO₄ + water). Dependence of the charging time t , specific capacity C/L , energy W/L , and power P/L on the charging current density I and active layer thickness L : $\Omega = 0.5$, $D = 10^{-7}$ cm, $S = 2 \times 10^7$ cm⁻¹, $k_0 = 0.8$ S cm⁻¹, $k = 0.4$ S cm⁻¹, $E_0 = 0.5$ V, and $E^*(L) = 1.5$ V

I , A/cm ²	L , cm	t , s	C/L , F/cm ³	W/L , J/cm ³	P/L , W/cm ³
1.0	0.001	0.4	399.7	200	1000
	0.01	3.97	396.7	200	100
	0.1	36.7	366.7	198	10
	1.0	125.7	125.7	84	1
0.1	0.001	4	400	200	100
	0.01	40	399.7	200	10
	0.1	396.7	396.7	200	1
	1.0	3670	366.7	198	0.1
0.01	0.001	40	400	200	10
	0.01	400	400	200	1
	0.1	3997	399.7	200	0.1
	1.0	39660	396.7	200	0.01

have low internal resistance, but the charging voltage $E(L, t) - E_0$ for them is limited to about 1 V. The DLCs based on nonaqueous electrolytes, however, have high internal resistance but provide a charging voltage of 2–3 V.

The maximum admissible capacity in the active layer was assumed to be $E^*(L) = E(L, t) = 1.5$ V.

The problem under study has two main parameters: the charging current density I and the active layer thickness L . Let us analyze how the variation of these parameters affects the DLC charging time t ,

specific capacity C/L , specific energy W/L , and specific power P/L .

The calculated data are presented in Tables 1 and 2. The data of Table 1 differ from those of Table 2 only in variation of the pore diameter D . Two values were chosen for this parameter: 10^{-4} (Table 1) and 10^{-7} (Table 2) cm. All other parameters of the active layers were assumed to be identical.

The formulas given in Section 3 indicate that the specific power and specific energy of the active layer are proportional to the square of the charging current density I^2 , the potential difference $E(L, t) - E_0$ is proportional to the charge current density I , and the specific capacity is independent of the charge current density. Therefore, knowing the overall characteristics at $I = 1$ A/cm², we can easily evaluate them for the case when I changes. The dependence of the overall characteristics of DLC on the active layer thickness L is more complicated.

The data of Tables 1 and 2 show that the potential difference $E^*(L) - E_0 = 1.5 - 0.5 = 1$ V is sufficient for the charging of the active layer surface to be nearly completed. The specific capacity can be determined by Eq. (11).

The limiting specific capacity in Table 1 is naturally three orders of magnitude smaller than the corresponding values given in Table 2. This is due to the fact that, according to (11), the limiting capacity is proportional to the specific surface area S .

The charging times t in Table 1 are three orders of magnitude smaller than the charging times in Table 2 as they must be in accordance with Eq. (5) because the charging surface area S increases by three orders of magnitude when the pore radius D decreases.

The situation is similar for the specific capacity C/L . According to (11), the limiting specific capacities in Tables 1 and 2 should differ by three orders of magnitude. At large charging currents I and active layer thicknesses L , the limiting capacity does not set in throughout the whole thickness of the active layer, in contrast to the case with low charging currents.

According to the data of Tables 1 and 2, the specific energy W/L is virtually independent of I and L . This is explained by the fact that in the equation for the specific energy of the active layer given in Section 3, W/L is proportional to the square of the charging current I and the square of the charging time t . Therefore, t increases by one order of magnitude when I decreases by the same value. As a result of this mutual compensation, the specific energy remains almost constant, as demonstrated by the data of Tables 1 and 2.

In contrast to the specific energy, the specific power P/L depends significantly on the charging current. In the formula given in Section 3, the specific power is proportional to the square of the charging current I and depends linearly on the charging time t .

Thus, as the charging current I decreases and the charging time increases, both by one order of magni-

tude, the specific power should decrease by one order of magnitude in contrast to the specific energy. This is confirmed by the data of Tables 1 and 2, which show that the specific power decreases by one order of magnitude when I decreases by the same value. Evidently, the specific power decreases with the active layer thickness in direct proportion.

It is also useful to analyze how the characteristics of DLCs with the “ideal” active layer change when the porosity of the active layer g changes. These data are presented in Table 3.

In the “ideal” active layer model, the specific surface area S (14) increases with porosity along with the effective ion conductivity of the active layer k (15). As a result, at fixed current density I , active layer thickness L , and pore diameter D , the limiting specific capacity starts to rapidly increase along with the charging time.

In the “ideal” active layers with 1 nm pores, it is possible to obtain very high specific capacity, 720 F/cm³ (the last line, Table 3).

The analysis of the characteristics of DLCs with the “ideal” active layer is certainly of pure methodological interest because it demonstrates how to perform calculations of the main characteristics of DLCs and what results are to be expected. However, clearly, it is hardly possible to create “ideal” porous media with a set of cylindrical pores even 1 μ m in diameter.

Therefore, based on previous formulations we now consider the model of active layers which are more real in character.

5. BIPOROUS ACTIVE LAYER: A COMPUTER MODEL

For high performance of DLCs, active layers with high specific surface areas (finely divided activated carbons and tissues) of the order of hundreds or thousands m²/g are generally used [18–21]. Carbon as an active electrode material is used today in the majority of commercial systems (~95% of the market [22]). The advantages of carbon materials are their high electron conductivity (10⁵ S cm⁻¹) and moderate cost.

The effective functioning of the active layer requires that at least two clusters should be formed in it for a continuous supply or removal of ions and electrons. Therefore, a theoretical study of the mechanism of the action of active layers should concentrate on a study of connectivity in the space of different structural elements involved in the organization of the electrochemical process. Thus it becomes necessary to use the percolation theory [23].

The program of a computer simulation of the active layer of a definite type consists of a chain of steps listed at the end of Section 1.

This study presents a computer simulation of the operation of the active layers of DLCs from this viewpoint. The goal of this study is a comprehensive under-

Table 3. DLC, “ideal” active layer, aqueous electrolyte (30% H₂SO₄ + water). Dependence of the charging time t , specific capacity C/L , energy W/L , and power P/L on the active layer porosity Ω and pore diameter D . $k_0 = 0.8$ S cm⁻¹, $k = 0.4$ S cm⁻¹, $E_0 = 0.5$ V, $E^*(L) = 1.5$ V, $I = 0.1$ A/cm², and $L = 0.1$ cm

Ω	D , cm	t , s	C/L , F/cm ³
0.1	10 ⁻⁴	0.077	0.077
	10 ⁻⁷	76.67	77
0.5	10 ⁻⁴	0.397	0.4
	10 ⁻⁷	396.66	400
0.9	10 ⁻⁴	0.717	0.72
	10 ⁻⁷	716.64	720

standing of the mechanism of functioning of active layers and DLCs in general and calculation of the basic characteristics of active layers: charging time, potential, specific capacity, energy, and power.

We will now formulate the model of the active layer of DLC.

The carbon materials have been used by the mankind since the ancient times and are finding more and more applications in practice [24].

Activated carbons are obtained by carbonization of organic substances or fossil coals (heating to high temperatures without contact with air to obtain products with high carbon contents). The next step is activation: the partial oxidation of coal is carried out in an atmosphere of water vapor or carbon dioxide, which leads to burnout of some part of carbon, tar, and other substances, resulting in further development of porosity and increased accessibility of pores [25].

The activated carbons usually contain all three types of pores: micro (less than 2 nm), meso (2–50 nm), and macropores (this classification was first proposed in [26]), the ratio of which can vary for different types of activated carbon.

There are large-pore activated carbons, which always contain micropores, and finely porous activated carbons, which contain large pores in addition to micropores. Active coke is a specific product with a uniform distribution of pores of all types [27].

Obviously, for DLC, it is important to have a combination of micropores, mesopores, and macropores, which provides both high specific surface area (micropores) and an access to the enormous surface of micropores through the system of larger pores. To avoid complication of the DLC model, we assumed that mesopores were absent, with only micro- and macropores present.

Let us consider the biporous structure of an active layer in which the large pore voids filled with the electrolyte are randomly mixed with agglomerates of many very fine carbon particles on whose surface the charge adsorption should occur.

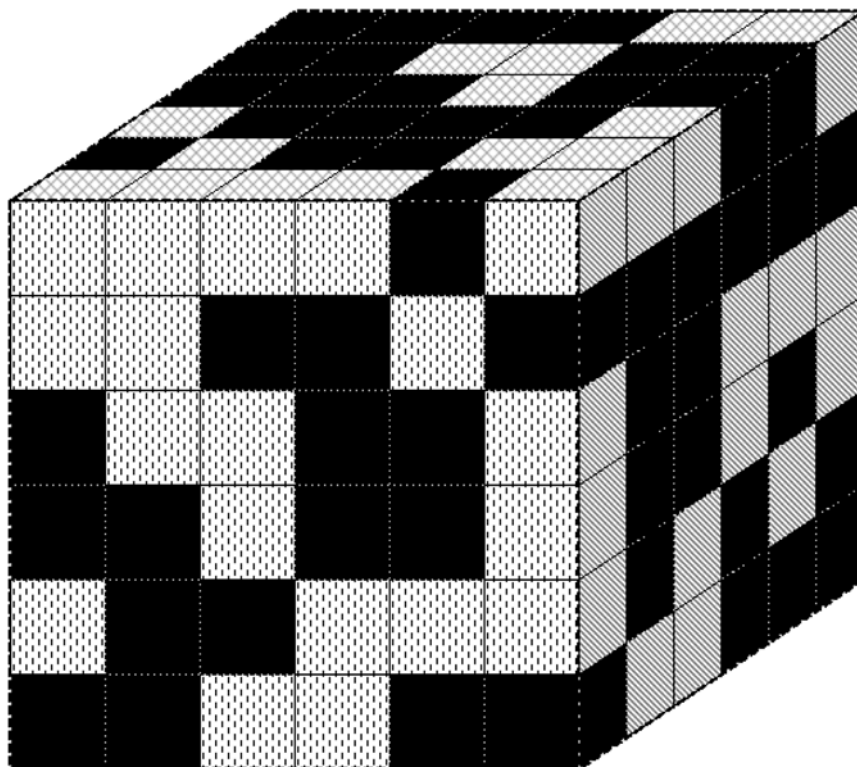


Fig. 2. Sample of the active layer model of a double-layer capacitor (model with equal-sized cubic grains of two types). Black cubes: porous carbon grains, light cubes: electrolyte grains; $g = 0.5$.

The voids with the electrolyte and the agglomerates of fine carbon particles wetted with the electrolyte are called grains (electrolyte and carbon grains). We assumed that these grains of two types were equal in size and shaped as cubes with an edge length D^* . The fine carbon particles that partially fill the carbon grains were also modeled by porous microcubes with the same edge length d .

Thus, to describe the structure of the active layer of model DLCs, we chose the model of equal-sized grains of two types. The model is partially shown in Fig. 2. Clearly, we have

$$g + g_1 = 1, \quad (16)$$

where g is the volume concentration (proportion) of porous carbon grains, and g_1 is the volume concentration (proportion) of electrolyte grains.

As a three-dimensional model of the active layer of DLC, we took a model cube with dimensions $N_s \times N_s \times N_s = N_s^3$.

The model cube should have macroscopic dimensions. This means that the active layer thickness L should be much larger than the size of the individual grain D^* , as indeed takes place in reality (the active

layers have thicknesses of dozens and hundreds of microns). The following inequality should be valid:

$$D^* \ll L. \quad (17)$$

As a matter of fact, the percolation curves are stabilized and do not experience any changes at sufficiently large N_s values [28]. This can be achieved by taking that $N_s = 100$. Below the model cube under study accommodates $100 \times 100 \times 100 = 10^6$ grains of two types.

6. PERCOLATION CALCULATIONS

For the reversible adsorption of ions of appropriate sign to occur in carbon grains, ions should be continuously fed along the coupled chains of electrolyte grains and (porous) carbon grains partially wetted with electrolyte and electrons should be fed along the coupled chains of carbon grains. Two percolation clusters should be distinguished in the active layer [23]: ionic (from electrolyte grains) and electronic (from carbon grains). Each of these clusters is a set of directly bonded grains of a definite type. The percolation clusters permeate the entire active layer along its thickness.

Percolation clusters are formed at the percolation threshold if the volume concentrations of the corre-

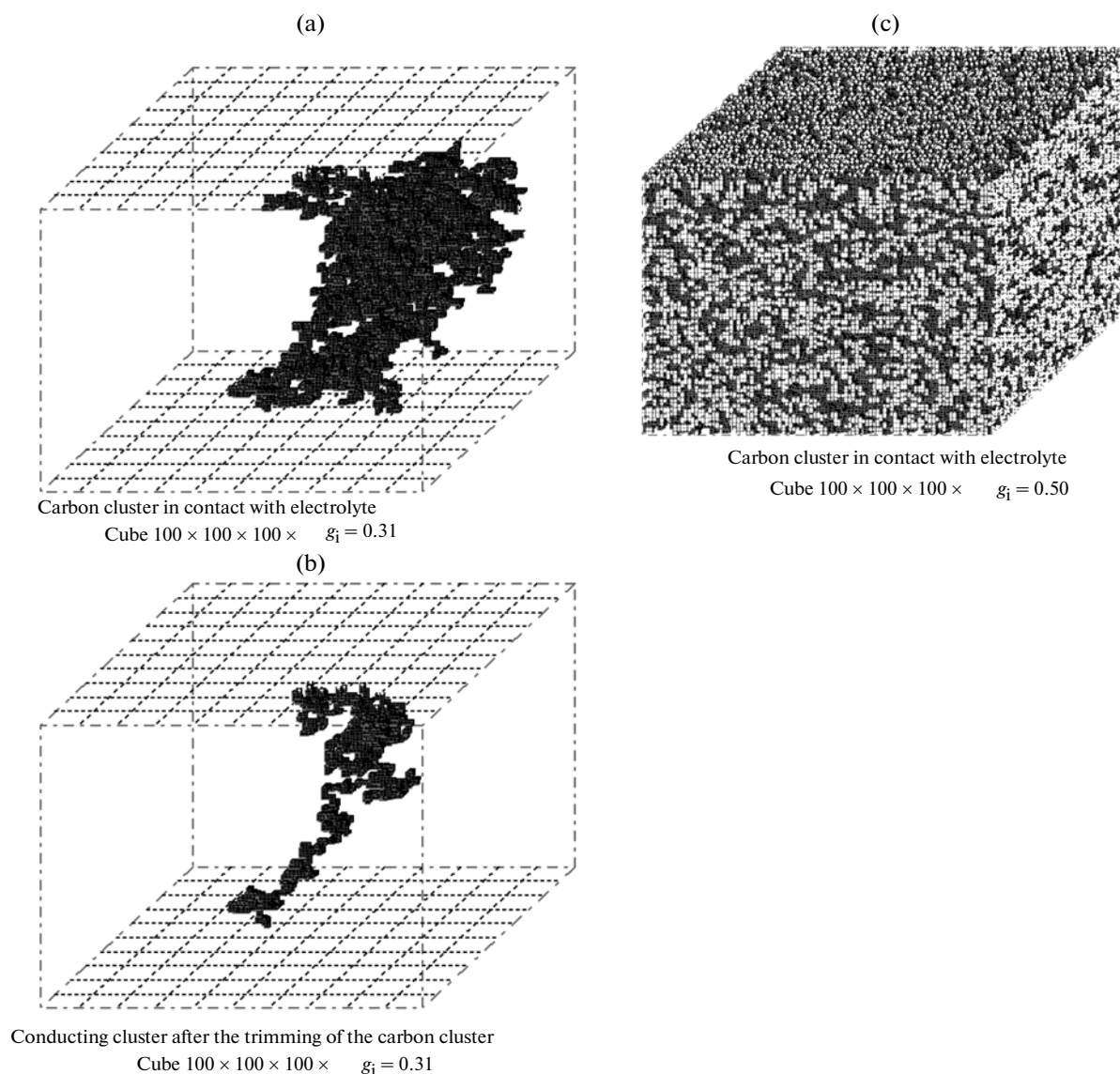


Fig. 3. Sample of the structure of the active layer in a double-layer capacitor: (a) percolation carbon cluster; the fraction of carbon grains in the active layer is $g = 0.31$; the particles of the carbon cluster are black; the remaining volume of the active layer is filled with the electrolyte; (b) “skeleton” of the percolation carbon cluster, along which electron transport is effected in the active layer (the deadlock elements of the percolation carbon cluster are omitted); and (c) structure of the active layer at $g = 0.5$.

sponding grains reached a certain critical value g^* or g_i^* . In the cubic lattice [23] with which we are concerned, the percolation threshold is [29]

$$g^* = g_i^* = [(1 + 2^{1/2})^{1/3} + (1 - 2^{1/2})^{1/3}]/2 = 0.298. \quad (18)$$

Thus, for normal functioning of the active layer (ion conductivity in carbon grains cannot be high, as shown below), it is required that at least two conditions should be fulfilled simultaneously:

$$g \geq 0.30, \quad g_i \geq 0.30. \quad (19)$$

Conditions (16) and (19) together indicate that the proportion of carbon grains in the active layer should lie the range

$$0.3 \leq g \leq 0.7, \quad (20)$$

if we want ions to flow to the active layer mainly through the large electrolyte pores (the case of the biporous active layer). However, the monoporous active layer (e.g., the activated carbon tissues) with small electrolyte pores in carbon grains are also of interest; the proportion of carbon grains should be set as $g = 1$.

Figure 3a shows an example of the structure of the active layer of DLC for the proportion carbon grains in the active layer $g = 0.31$. We can see a percolation carbon cluster whose particles are colored black. The remaining volume of the active layer is filled with the electrolyte. Clearly, this active layer is not yet functional, with only some part of the volume of the cube model involved in charge storage. Therefore, the con-

Table 4. Dependence of the reduced specific surface area of contact between the carbon and electrolyte percolation clusters S^* on the volume concentration of carbon grains g in the active layer of DLC

g	S^*
0.31	0.049
0.32	0.395
0.33	0.619
0.35	0.885
0.40	1.189
0.45	1.320
0.50	1.359
0.55	1.320
0.60	1.189
0.65	0.885
0.67	0.619
0.68	0.395
0.69	0.049

centration of carbon grains in the active layer should be increased.

Talking about ion transport in electrolyte, we can state that, like any percolation cluster, the percolation ion cluster (consisting entirely of electrolyte grains and shown in Fig. 3a) contains not only flow-through elements through which ions can flow, but also dead-end elements closed for ion transport.

Let us remove all ballast dead-end elements in Fig. 3a. The resulting reduced percolation cluster (or, rather, the skeleton of the initial percolation cluster) is

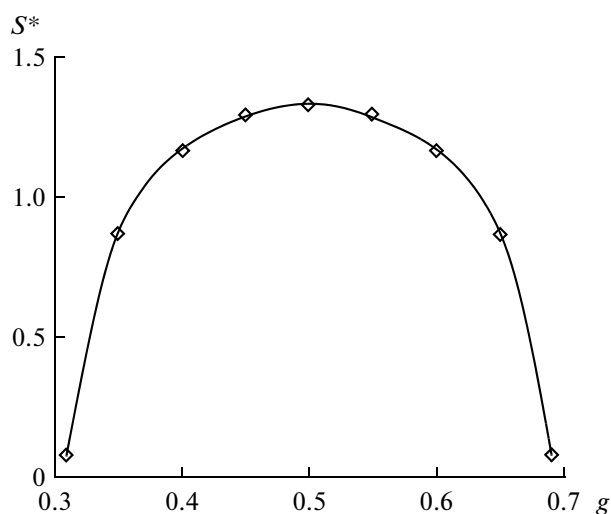


Fig. 4. Dependence of the reduced specific surface area of the contact between the carbon and electrolyte percolation clusters S^* in the active layer of a double-layer capacitor on the volume concentration of carbon grains g .

shown in Fig. 3b. Only these clusters are effective for transport of both ions and electrons (in the carbon percolation cluster) in the active layer of DLC. This should be taken into account in calculations of the effective specific conductivity of the active layer.

The active layer of DLC at $g = 0.5$ can be visualized in Fig. 3c. The carbon grains in it are black and the electrolyte grains are gray.

Let us now return to the problem of choosing the optimum proportion of carbon grains from the values allowed by condition (20). What value of g should be taken? To answer this question, at least partially, we perform a computer calculation of the dependence of the reduced specific surface area of the contact between two (carbon and electrolyte) percolation clusters S^* on the volume concentration of carbon grains g . The calculated data are shown in Table 4 and Fig. 4.

S^* reaches a maximum at $g = 0.5$. Here, the carbon and electrolyte percolation clusters are equivalent and most closely intertwined. The specific surface area of the contact between two clusters S^{**} can be calculated by the equation

$$S^{**} = S^*/D^*. \quad (21)$$

7. ION CONDUCTIVITY OF THE ACTIVE LAYER

To calculate the overall characteristics of DLCs, we need the effective ion conductivity of the active layer. Note that ion conductivity is characteristic not only of electrolyte grains, but also of carbon grains as they are filled with carbon particles only partially.

The algorithms for computations of effective ion conductivity are found in [30, 31]. The following should be noted. First, we are naturally concerned with carbon grains with high specific surface area. For this, the edge length d of carbon microcubes should be selected sufficiently small. That is, the inequality

$$d \ll D^* \quad (22)$$

should be valid. Second, there is clear similarity between the distribution of the carbon and electrolyte grains in the active layer and the void microcubes in the individual carbon grains. Therefore, the specific surface area of carbon microcubes in carbon grains can be evaluated by the equation

$$S = S^*/d. \quad (23)$$

The S^* value can be taken from Table 4 if we take g^{**} instead of g in it.

The calculated dependence of the reduced effective specific ion conductivity k^* on the volume concentration of carbon particles (carbon microcubes) g^{**} is presented in Table 5 and Fig. 5.

We can see that the conductivity k^* decreases rapidly as g^{**} increases. Note that at the optimum concentration $g^{**} = 0.5$ (according to Fig. 3, the specific

Table 5. Dependence of the reduced effective specific ion conductivity k^* on the volume concentration of carbon particles g^{**} in carbon grains

g^{**}	k^*
0.31	0.363
0.33	0.324
0.35	0.295
0.40	0.230
0.45	0.171
0.50	0.110
0.55	0.060
0.60	0.026
0.65	0.005
0.69	9.3×10^{-5}

Table 6. Dependence of the reduced effective specific ion conductivity k^{**} on the volume concentration of carbon grains g in the active layer of DLC (at $g^{**} = 0.5$)

g	k^{**}
0.1	0.819
0.2	0.677
0.3	0.552
0.4	0.430
0.5	0.346
0.6	0.268
0.7	0.206
0.8	0.155
0.9	0.129
1.0	0.110

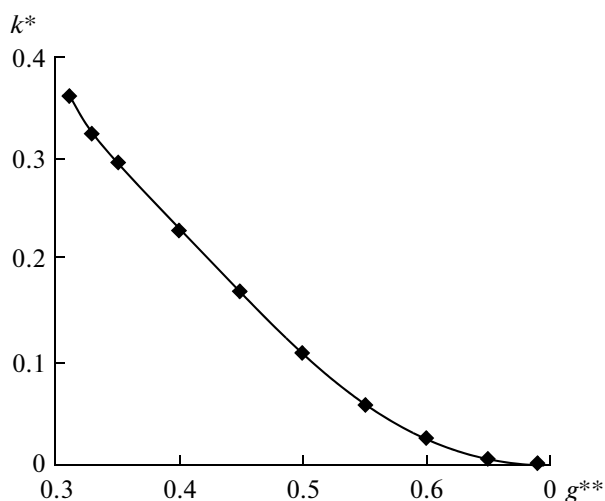
surface area of fine carbon particles in carbon grains is maximum possible), the conductivity $k^* = 0.11$.

Now we have to calculate the dependence of the reduced effective specific ion conductivity k^{**} on the volume concentration of carbon grains g in the active layer of DLC. The active layer consists of a mixture of electrolyte grains with conductivity 1 and carbon grains with conductivity k^* (Table 5). The calculated values of k^{**} are shown in Table 6 and Fig. 6 on an assumption that $g^{**} = 0.5$. Naturally, $k^{**} = 0.11$ when $g = 1.0$ (active layer with a monoporous structure).

Finally, the effective specific ion conductivity of the active layer k can be determined by the equation

$$k = k_0 k^{**}, \quad (24)$$

where k_0 is the specific ion conductivity of the chosen electrolyte.

**Fig. 5.** Dependence of the reduced effective specific ion conductivity k^* in the carbon grains of a double-layer capacitor on the volume concentration in the carbon grains of carbon particles g^{**} .

8. THE CENTRAL PROBLEM OF DLCs

It seems that we can now calculate the characteristics of DLCs with an aqueous electrolyte and biporous active layers containing highly dispersed agglomerates of fine carbon particles (Fig. 2). However, this is difficult because it is not clear how to correctly determine the real polarized part of the specific surface area S in the right-hand side of Eq. (1).

The fact is that a biporous active layer has a set of electrolyte pores of two types: wide (voids filled with electrolyte) and small (in carbon grains). Sections 3 and 4 that described the “ideal” active layer of DLC showed that during galvanostatic charging of the active layer of DLC, the wide pores filled with electrolyte are the first to be quickly polarized, while polarization of small pores starts much later.

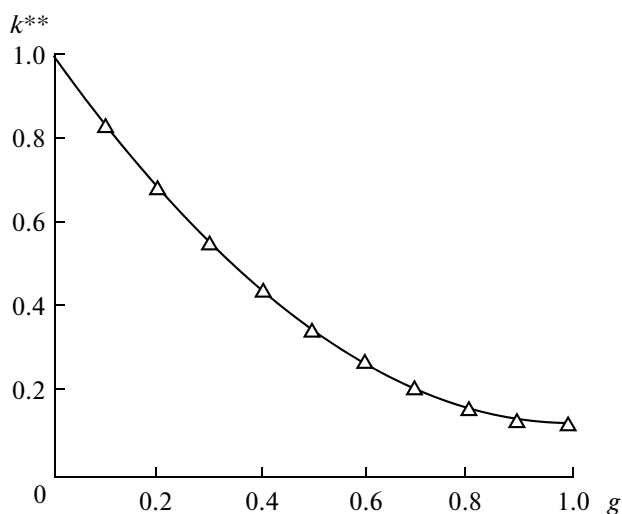
**Fig. 6.** Dependence of the reduced effective specific ion conductivity k^{**} in the active layer of a double-layer capacitor on the volume concentration of carbon grains g .

Table 7. Parameters of structure and galvanostatic charging of the biporous active layer in DLCs

Parameter	Quantity
Carbon particle concentration in carbon grains	$g^{**} = 0.5$
Fraction of carbon grains in the active layer	$g: 1.0$
Edge length of the carbon microcube	$d = 1 \text{ nm}$
Specific surface area in carbon grains	$S = 1.36 \times 10^7 \text{ cm}^{-1}$
Initial potential of the active layer	$E_0 = 0.5 \text{ V}$
Specific capacity of the carbon surface	$C_s = 2 \times 10^{-5} \text{ F/cm}^2$
Conductivity of the aqueous electrolyte	$k_0 = 0.8 \text{ S cm}^{-1}$ (30% H_2SO_4 + water)
Specific conductivity of the active layer	$k = k_0 k^{**}$ (at $g = 0.5$ $k^{**} = 0.11$) = 0.088 S cm^{-1}

Thus, strictly speaking, in the given biporous model of the active layer of DLC, galvanostatic charging can be performed only for one limiting case, namely, at $g = 1$ when the whole active layer consists of 100% carbon grains (of agglomerates of small particles impregnated with the electrolyte solution). It is assumed here that all pores in the active layer of DLC are of approximately the same size.

Let us perform the following calculation. Let us adopt the following parameters (shown in Table 7).

The results of these calculations are presented in Table 8.

Because of considerable ohmic limitations ($k = 0.088 \text{ S cm}^{-1}$; $k = 0.4 \text{ S cm}^{-1}$ in Tables 1 and 2) and low maximum possible potential ($E^*(L) - E_0 = 1 \text{ V}$), the specific capacity does not reach the limit of 272 F/cm^3 set by Eq. (11). The maximum specific capacity in Table 8 does not exceed $\sim 82 \text{ F/cm}^3$. The specific energy and specific power are significant.

Table 8. DLC, aqueous electrolyte ($g = 1.0$, $k = 0.088 \text{ S cm}^{-1}$): dependence of the charging time t , specific capacity C/L , specific energy W/L , and specific power P/L on the charging current density I and active layer thickness L . Initial potential $E_0 = 0.5 \text{ V}$, the limiting possible potential $E^*(L) = 1.5 \text{ V}$

$I, \text{ A/cm}^2$	$L, \text{ cm}$	$t, \text{ s}$	$C/L, \text{ F/cm}^3$	$W/L, \text{ J/cm}^3$	$P/L, \text{ W/cm}^3$
1.0	0.001	0.27	271	128.2	1000
	0.01	2.62	261.7	127.9	100
	0.1	16.93	169.3	108.9	10
0.1	0.001	2.72	271.9	135.9	100
	0.01	27.1	271	135.9	10
	0.1	261.7	261.7	135.7	1
0.01	0.001	27.2	272	136	10
	0.01	271.9	271.9	136	1
	0.1	2710	271	136	0.1

Unfortunately, it is hardly possible to form an active layer of DLC impregnated with electrolyte and consisting only of finely dispersed carbon particles.

It was already mentioned that the active layers of DLCs are mainly prepared from activated carbon materials. They are based on wood, mineral and brown coals, peat, fruit kernels and nutshells, synthetic resins, and polymers.

The activation of carbon materials involves two stages: carbonization and activation. The goal is to develop meso- and macroporosity, which allows an increase in the accessibility of micropores.

Carbonization and heating to high temperatures are inevitably accompanied by a release of volatile products. The solid residue (coal) formed in the vessel is a highly porous carbon material. It has high porosity (85%) [25] but low adsorption capacity because the micropores are blocked with the pyrolysis products.

This disadvantage can be eliminated by further activation, when some part of carbon, tar, and other substances are burnt out at temperatures slightly lower 1000°C , which eventually makes the micropores accessible.

Thus we have a vicious cycle. The presence of large pores in the active layers is the result of the use of traditional technologies for the production of activated carbon materials. The wide pores open up access to the smallest pores and seemingly provide high characteristics of DLCs (specific capacity, energy, and power). The same quickly polarizable wide pores, however, become a barrier for polarization of micropores and high overall characteristics of DLCs.

This is the central problem for DLCs. It is necessary to find ways to alleviate the problems and seek end runs to enhance ion adsorption in micropores. This will lead to high specific capacity of DLCs with active layers based on activated carbon materials.

9. CONCLUSIONS

Thus we performed a computer simulation of the structure of active layers and studied various ways of functioning of carbon double-layer capacitors. The

charging of DLCs in a galvanostatic mode was studied. The basic overall characteristics of DLCs (charging time and specific capacity, stored energy, and power) were calculated. The effect of two external parameters (charging current density and active layer thickness of DLCs) on the charging was analyzed.

The active layers of DLCs with aqueous electrolytes of different types were studied: (1) the “ideal” active layers (a set of parallel cylindrical pores of the same radius filled with electrolyte), (2) biporous active layers (a set of wide and small pores), and (3) monoporous active layers (no wide pores and the small pores are filled with electrolyte).

A computer simulation of biporous active layers of DLCs was performed according to a complete program of research. A model of the structure of active layers was formulated. Then percolation calculations were carried out. The effective ion conductivities were calculated for both highly porous carbon grains whose fine pores are filled with electrolyte and the whole active layer. The specific surface areas of the carbon mass on which the reversible adsorption of the corresponding ions occurs were also evaluated.

The biporous active layer was modeled by grains of two types which imitated a set of voids randomly distributed in space and filled with electrolyte (electrolyte grains) and porous agglomerates of very fine carbon particles on the surface of which the charge can be stored (carbon grains). The grains of these two types were regarded as equal-sized and shaped as cubes. The carbon particles that partially filled the volume of carbon grains were also modeled by microcubes with the same edge length. The model cube that imitated the biporous active layer of DLCs generally was macroscopic and could accommodate one million of grains of the two types.

A computer simulation of DLCs is useful for several reasons. Firstly, it leads to better understanding of the functioning of DLCs. Secondly, since the number of parameters of DLCs is large, it is necessary to optimize the structure and parameters of active layers. All this can be done by means of a computer simulation. Thirdly, series of computer experiments can be performed, which allows quick answers to many questions of interest for researchers and practitioners.

This paper formulated the central problem of calculating the characteristics of DLCs with a real non-monoporous (“ideal” active layers) structure of the active layer. The fact is that wide pores are the first to be polarized in active layers that generally have pores of three types (micro-, meso-, and macropores) in a galvanostatic mode of DLC. They quickly reach the maximum admissible potential; therefore, the galvanostatic charging should be stopped to pass to the potentiostatic charging.

As a result, many micropores remain nonpolarized. The specific capacity of DLCs will not reach the desired level.

This is some kind of vicious cycle. The presence of large pores in the active layers is the result of the use of traditional technologies for the preparation of activated carbon materials (carbonization and subsequent activation of the carbon material). The wide pores open up access to the smallest pores and seemingly to high characteristics of DLCs (high specific capacity, energy, and power). The same quickly polarizable wide pores, however, become an obstacle to the polarization of micropores.

This is the central problem for DLCs. It is necessary to find ways to alleviate the problems and seek end runs to enhance ion adsorption in micropores. This will lead to high specific capacity of DLCs with active layers based on activated carbon materials.

APPENDIX 1

Algorithm for Calculating the Reduced Specific Surface of Contact between the Electrolyte and Carbon Percolation Clusters

Let us consider a model cube consisting of 10^6 unit cells with dimensions $100 \times 100 \times 100$. Each cell is assigned an element of a three-dimensional matrix $A_{(i,j,k)}$. The carbon phase is randomly distributed over the cells, while the matrix elements are assigned $A_{i,j,k} = “1”$; the electrolyte phase is distributed with the label $A_{i,j,k} = “0”$. The relative number of cells labeled with “1” equals the g parameter (the proportion of carbon grains).

On one of the cube faces we select the cells with the label “0”, labeling them with “E” (electrolyte phase). Then we examine the adjacent cells and if there are cells labeled with “0” among them, the corresponding matrix elements are assigned a new value of $A_{i,j,k} = “E”$ and the cell coordinates are remembered. A set of these cells is considered to be a new front of the wave of electrolyte percolation through the pores. Each cell of the front then becomes the start of electrolyte movement to the adjacent accessible cells (by analogy with the Huygens–Fresnel principle in optics). The wave propagates along the cells labeled with “0” and allows them to be assigned a new label “E”. If the wave reaches the opposite face, this points to the presence of a percolation electrolyte cluster. The chains of cells marked with “E” that start on the front face but have no exit to the rear face are excluded from further consideration by returning the cells to the original state with the label “0”. Likewise, a carbon cluster is isolated and labeled with “C”.

To calculate the reduced specific surface area of the contact between the electrolyte and carbon percolation clusters, we search through all “C” cells in series and calculate the number of faces that contact with “E” cells in each cell. Dividing the total number of contacts by 10^6 unit cells, we obtain the reduced specific surface area S^* .

APPENDIX 2

Derivation of Basic Equations for the Overall Characteristics

The galvanostatic mode of operation of the porous electrode is considered. This mode is described by the differential equation in partial derivatives.

A solution of (1) with boundary conditions (2) and (3) and initial condition (4) is sought in the form

$$E(x, t) = v(x, t) + \psi(x, t)$$

with the requirement that the function $\psi(x, t) = \frac{I x^2}{k 2L} + E_0$ should satisfy boundary conditions (2) and (3).

For the function $v(x, t)$, we obtain the boundary value problem:

$$a^2 \frac{\partial^2 v(x, t)}{\partial x^2} + \frac{I a^2}{k L} = \frac{\partial v(x, t)}{\partial t}, \quad (A.1)$$

$$0 \leq x \leq L, \quad 0 \leq t \leq \infty,$$

where $a^2 = \frac{k}{g S C_s}$,

with the boundary conditions

$$\frac{dv(0, t)}{dx} = 0 \quad \frac{dv(L, t)}{dx} = 0, \quad (A.2)$$

and the initial condition

$$v(x, 0) = E_0 - \psi(x, 0) = -\frac{I x^2}{k 2L}. \quad (A.3)$$

The solution of the boundary value problem (A.1)–(A.3) is sought by the variable separation method in the form of

$$v(x, t) = \sum_n v_n(t) X_n(x), \quad (A.4)$$

where $X_n = \cos(n\pi x/L)$ $n = 0, 1, \dots$ are the eigenfunctions of the boundary value problem

$$X''(x) + \lambda^2 X(x) = 0 \quad X'(0) = 0 \quad X'(L) = 0. \quad (A.5)$$

The functions $v_n(t)$ are to be determined. The function $v(x, t)$ already satisfies the boundary conditions (A.2). If we require that $v(x, t)$ should also satisfy (A.1) and initial condition (A.3), the $v_n(t)$ functions are determined from this. For this, the left-hand side of (A.1) and the right-hand side of (A.3) are expanded in a series of eigenfunctions $X_n(x)$. Substituting (A.4) into (A.1), we obtain the equality

$$\sum_{m=0}^{\infty} \left[\frac{\partial}{\partial t} v_m(t) + a^2 \lambda_m^2 v_m(t) - \theta_m(t) \right] X_m(x) = 0, \quad (A.6)$$

where $\theta_m(t) = \frac{1}{\|X_m^2\|} \int_0^L \frac{I a^2}{k L} X_m(x) dx \quad \|X_m^2\| = \int_0^L X_m^2(x) dx =$

$$\int_0^L \cos^2(\lambda_m x) dx = \frac{L}{2}, \quad \text{but } \|X_0^2\| = L.$$

For equality (A.6) to be satisfied, it is sufficient that the equalities

$$\frac{\partial}{\partial t} v_m(t) + a^2 \lambda_m^2 v_m(t) = \theta_m(t) \quad m = 0, 1, \dots \quad (A.7)$$

should be valid. At $m = 0$ $\theta_0(t) = \frac{I a^2}{k L}$ and $\frac{\partial}{\partial t} v_0(t) = \frac{I a^2}{k L}$.

Hence it follows that

$$v_0(t) = v_0(0) + \frac{I a^2}{k L} t. \quad (A.8)$$

For $m > 0$ $\theta_m(t) = \frac{2}{L} \int_0^L \frac{I a^2}{k L} \cos(m\pi x/L) dx = \frac{2 I a^2}{L k L} \times$
 $\left(\frac{\sin(0) - \sin(m\pi)}{m\pi} L \right) = 0$, and the solution of (A.7) is of the form

$$v_m(t) = v_m(0) \exp(-a^2 \lambda_m^2 t). \quad (A.9)$$

Now we use the initial condition (A.3) and (A.4)

$$\sum_{m=0}^{\infty} v_m(0) X_m(x) = -\frac{I x^2}{k 2L}.$$

Expanding the right-hand side of this equality in the eigenfunctions $X_n(x)$, we obtain

$$v_0(0) = -\int_0^L \frac{I x^2}{k 2L} dx = -\frac{I L}{k 6} \quad v_m(0) = \frac{1}{\|X_m^2\|} \int_0^L -\frac{I x^2}{k 2L} \times \cos(\lambda_m x) dx = -\frac{2 L I}{k \lambda_m^2} \cos(\lambda_m L) = -\frac{2 L I}{k \lambda_m^2} (-1)^m. \quad (A.10)$$

Taking (A.9) and (A.10) into account, we obtain

$$E(x, t) = v(x, t) + \psi(x, t) = v_0(0) + \sum_{m=1}^{\infty} v_m(0) e^{-a^2 \lambda_m^2 t} \cos(\lambda_m x) + \frac{I x^2}{k 2L} + E_0.$$

As a result, the solution of (1) has the form

$$E(x, t) = E_0 + \frac{I}{k} \left[\frac{kt}{g S C_s L} + \frac{3x^2 - L^2}{6L} + \frac{2L}{\pi^2} \times \sum_{m=1}^{+\infty} (-1)^{m+1} \frac{\exp\left(-\frac{m^2 \pi^2 k t}{L^2 S C_s}\right)}{m^2} \cos(m\pi x/L) \right]. \quad (A.11)$$

The capacity of the active layer is

$$C = \frac{q}{\Delta\phi} \quad (A.12)$$

by definition.

If the capacitor charging current is constant, $I = \text{const}$, the charge on the electrode is $q = It$. We assume that the increment of the potential on the front side of the electrode during charging is $\Delta\varphi = E(L,t) - E_0$.

According to (A.11), the potential on the front side of the electrode is

$$E(L,t) = E_0 + \frac{I}{k} \times \left[\frac{kt}{gSC_s L} + \frac{L}{3} - \frac{2L}{\pi^2} \sum_{m=1}^{+\infty} \frac{\exp\left(-\frac{m^2 \pi^2 k t}{L^2 SC_s}\right)}{m^2} \right] \quad (\text{A.13})$$

Consequently,

$$C = \frac{kt}{L \left[\frac{kt}{gSC_s L^2} + \frac{1}{3} - \frac{2}{\pi^2} \sum_{m=1}^{+\infty} \frac{\exp\left(-\frac{m^2 \pi^2 k t}{L^2 SC_s}\right)}{m^2} \right]} \quad (\text{A.14})$$

The energy of the active layer is

$$W = \int_0^t \{I\Delta\varphi(t)\} dt = \frac{I^2 L}{k} \left[\frac{kt^2}{2gSC_s L^2} + \frac{t}{3} + \frac{2L^2 SC_s}{k\pi^4} \sum_{m=1}^{+\infty} \frac{\exp\left(-\frac{m^2 \pi^2 k t}{L^2 SC_s}\right) - 1}{m^4} \right] \quad (\text{A.15})$$

Since $\sum_{m=1}^{\infty} \frac{1}{m^{2n}} = \frac{2^{2n-1} \pi^{2n}}{(2n)!} |B_{2n}|$, where B_{2n} are the Bernoulli numbers [32], then, if we take into account the equality $\sum_{m=1}^{\infty} \frac{1}{m^4} = \frac{2^3 \pi^4}{4!} \left| -\frac{1}{30} \right|$, the expression for the energy can be transformed into

$$W = \frac{I^2 L}{k} \left[\frac{kt^2}{2gSC_s L^2} + \frac{t}{3} + \frac{L^2 SC_s}{k} \times \left\{ \frac{2}{\pi^4} \sum_{m=1}^{+\infty} \frac{\exp\left(-\frac{m^2 \pi^2 k t}{L^2 SC_s}\right)}{m^4} - \frac{1}{45} \right\} \right] \quad (\text{A.16})$$

The specific power of the active layer is

$$\frac{P(t)}{L} = \frac{I\Delta\varphi(t)}{L} = \frac{I^2}{k} \times \left[\frac{kt}{gSC_s L^2} + \frac{1}{3} - \frac{2}{\pi^2} \sum_{m=1}^{+\infty} \frac{\exp\left(-\frac{m^2 \pi^2 k t}{L^2 SC_s}\right)}{m^2} \right] \quad (\text{A.17})$$

Notation for the Parameters of the Active Layer of the Carbon Double-Layer Capacitor (DLC)

L (cm) is the thickness of the active layer

x is the coordinate in the active layer ($0 \leq x \leq L$)

$x^* = x/L$ is the reduced coordinate in the active layer ($0 \leq x^* \leq 1$)

$E(x, t)$ (V) is the potential in the active layer

t is the charging time

$t^* = t/\tau$ is the reduced charging time

$\tau = gSC_s L^2/k$ is the characteristic charging time

$E_0(x, t = 0)$ (V) is the initial potential of the active layer

$E^* = E/E_0$ is the reduced potential in the active layer

S^* is the reduced specific surface area of the contact between the electron and ion percolation clusters in the active layer (dimensionless)

S^{**} ($\text{cm}^2/\text{cm}^3 = \text{cm}^{-1}$) is the specific surface of the contact between the electron and ion percolation clusters in the active layer

k_0 (S cm^{-1}) is the specific ion conductivity in the electrolyte

k^* is the reduced effective specific ion conductivity in carbon grains

k^{**} is the reduced effective specific ion conductivity in the active layer

$k = k_0 k^{**}$ (S cm^{-1}) is the effective specific ion conductivity in the active layer

$I, \text{A}/\text{cm}^2$ is the charging current density of the carbon DLC

I/J is the reduced charging current density of the carbon DLC

$J = kE_0/L$ is the characteristic charging current density of the carbon DLC

g is the volume concentration (proportion) of carbon grains in the active layer of DLC

g_i is the volume concentration (proportion) of electrolyte grains in the active layer of DLC

g^{**} is the volume concentration of carbon particles in carbon grains

D is the diameter of cylindrical pores in the "ideal" active layer

D^* is the edge length of cubic grains in the active layer

d is the edge length of cubic carbon particles in carbon grains

S (cm^{-1}) is the specific surface area of carbon particles in carbon grains

C_s (F/cm^2) is the specific capacity of the double electric layer on the carbon material

$a = gSC_s$ is the characteristic specific capacity of carbon grains

C (F/cm^2) is the specific capacity of the active layer in the carbon DLC

C/L (F/cm^3) is the volumetric specific overall capacity of the active layer in the carbon DLC

W (J/cm^2) is the specific energy of the active layer in the carbon DLC

W/L (J/cm^3) is the volumetric specific overall energy of the active layer in the carbon DLC

P (W/cm^2) is the specific power of the active layer in the carbon DLC

P/L (W/cm^3) is the volumetric specific overall power of the active layer in the carbon DLC

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Translated by L. Smolina