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**THEORETICAL ASPECTS OF PROCESSES OF METAL PARTICLES ADSORPTION INSIDE CHANNELS AND ON SURFACE OF CARBON SORBENTS****T. Marsagishvili, M. Machavariani**

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**Abstract:** *The paper gives a brief analysis of experimental work on the production of sorbents from various biological wastes in one process. The obtained sorbents are used without additional activation.*

*In connection with such experimental material, the theoretical aspects of various processes in the channels and on the surface of the sorbent are considered. The processes of solvation of metal particles in an aqueous medium are considered in the framework of the quantum theory of inhomogeneous condensed media with a redistribution of the electron density of the system. The processes of adsorption on the walls and in the channels of the sorbent are considered taking into account the effects of spatial dispersion of the system.*

**Keywords:** *sorbent, adsorption, solvation, metal particle, aqueous solution*

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**Introduction**

The processes of extracting metal particles from various solutions require the use of special filters, sorbents, and, depending on the required conditions for a specific task (purity of the solution, sizes of metal particles extracted from solutions, concentrations of dissolved particles, etc.) there can be varying complexity. Moreover, for a particular process of extracting particles from solutions, it is important to know what processes are carried out in this case, what materials can be used in this case in order to ensure the best adsorption of the extracted particles on the surface and in the channels of the adsorbent.

To carry out such processes, it is necessary to use filters obtained using, in particular, carbon materials [1-12]. The full cycle of the extraction process requires consideration of the separate stages. These stages of the complete process include: solvation of metal particles by solvent molecules in which metal particles are located, processes of adsorption and desorption of these particles on the walls of channels, movement of solvated impurities in the liquid between filter particles. Each of these processes can be

considered within the framework of a general approach.

First of all, it is necessary to define a model for describing the system, namely, the particles that should be extracted from the liquid, the properties and materials of the filter, with the help of which certain particles will be extracted from the solution.

An experimental study of the processes of adsorption of metal impurities on the surface and in the channels of sorbents is of great interest for various processes both in chemical technology and in ecology. With the use of sorbents, of course, the cost of obtaining high-quality materials increases, and therefore obtaining cheap and accessible sorbents from the point of view of the technology for obtaining sorbents is essential. Cheap methods for obtaining sorbents within the framework of a single-phase technological process from recycled materials proposed in works [4-9], is a constantly urgent task. At the same time, the experimental studies carried out by the authors of works [4-9] show the need to develop theoretical models, within which it will be possible to evaluate, at least qualitatively, some

parameters of the purification process of a liquid (solution) from certain impurity particles. For example, the sorption material obtained by technology from hazelnut shells (production waste) within the process without additional activation has a specific surface of  $637.33 \text{ m}^2/\text{g}$ , and a similar product from activated carbon  $708.70 \text{ m}^2/\text{g}$  [6]. The area of micropores is  $427 \text{ m}^2/\text{g}$  and  $473 \text{ m}^2/\text{g}$ ; the volume of micropores is  $0.20 \text{ m}^3/\text{g}$  and  $0.21 \text{ m}^3/\text{g}$ ; measurements were carried out using device - Gemini 7 [6].

Studies using an electron microscope make it possible to obtain sufficiently accurate elemental composition of sorbents, for example, for nectarine we have about 91 - 92% carbon, 6 - 7% oxygen, and about 10 impurity elements - S, Ca, metals.

Theoretical calculations for such complex systems are too cumbersome and difficult to compare with real experiments, but some general calculations can be made.

Below, theoretical calculations will be presented for model processes for extracting certain metal particles from solutions using sorbents.

When developing theoretical models for the processes of adsorption of particles on the surface of a solid (sorbent - filter) from a solution, the quantum apparatus of temperature Green's functions for non-regular inhomogeneous non-isotropic systems will be used. To describe the medium (sorbents and liquids), solvation and fluctuation mechanisms will be used [10-12].

When moving inside liquid-filled sorbent channels, several mechanisms should be considered:

1. A solvated particle (a metal particle covered with a solvate shell) can move almost freely along the channel cavity.
2. When a solvated particle moves inside the channel, it can stop and be adsorbed on the channel wall.
3. In the latter case, the adsorbed solvated particle can become the center of the creation of a large accumulation of particles (a kind of thrombus in the channel) and block the movement of other particles.

The solvation energies of metal particles in a polar (aqueous) medium can be calculated or estimated using various models. The simplest

model is the calculation by the Born formulas, within the framework of models without taking into account the effects of frequency and spatial dispersion of an infinite (in terms of the size of the cavity for the medium in which the particle is located) medium.

More complex models taking into account the effects of frequency and spatial dispersion of the system can also be presented. In any case, when moving solvated particles, one should take into account the various mechanisms of interaction of such particles both with the medium and with other particles. Some primary results can be obtained from the thermodynamic analysis of non-regular polar systems with impurity particles.

For the system under study, it should be taken into account that there are two types of particles in the solution - sorbent particles, on which metal particles are adsorbed, and metal particles that are solvated by molecules of solvent - water.

The main cause of adsorption on the surface of metal particles is the presence of an electric dipole field, which characterizes precisely metal particles in which the electron cloud of metal atoms "goes" beyond the surface of the particle. As a result, this field promotes solvation on the surface of solvent (water) molecules. At the same time, the presence of such a field also contributes to the process of deposition of a metal particle on the surface of the sorbent. It is natural that the pattern of solvation of metal particles, on the one hand, and the deposition of solvated metal particles on the surface of the sorbent, on the other hand, are dependent on the ratio of various effects of interactions within such a system. Numerous experimental studies show that these processes actually occur in the systems under study [5-6, 9].

Besides, it can be noted that the adsorption of metal solvated particles takes place both on the surface of the sorbent and in the channels of similar materials.

When analyzing the processes occurring in such sorbents, it is of interest to theoretically interpret these processes, i.e., how adequately can adsorption processes in sorbents be described from the point of view of modern

quantum theory of processes in non-regular condensed systems.

As the channels of the sorbent are filled with metal particles, they will also move in the channels (exchange of location) near the walls or in the volume of the sorbent. Exact calculations using quantum methods are impossible given the diversity and complex structure of real sorbents. Nevertheless, some general analytical models may be of interest from the point of view of the dependence of the system on certain process conditions in sorbents. Moreover, as the properties of such systems are studied, it is possible to purposefully create systems with certain properties, for example, in terms of electrical

conductivity in various external electromagnetic fields, and use these data without measurements by complex devices.

### Hamiltonian of System

To correctly write the Hamiltonian of the system, it is necessary to take into account several factors that affect the system as a whole. First of all, the presence of several types of reacting particles, in particular, metal particles, particles of carbon sorbents, and the solvent - water.

We represent the Hamiltonian of the system in the form [13-15]:

$$H = H_m^0 + H_s^0 + H_p^0 + H_{ad}^0, \quad (1)$$

where  $H_m^0$  is the Hamiltonian of the medium, which assumes both water and the presence in it of sorbents and solvated metal particles that do not take part in the process of adsorption of a particular particle (adsorbing particle);

$H_s^0$  is the Hamiltonian of the sorbent involved in the adsorption process,

$H_p^0$  is the Hamiltonian of a metal particle,

$H_{ad}^0$  is the Hamiltonian of the interaction of a metal adsorbing particle with a sorbent

In the process of interaction in the system, the metal particle is solvated by water molecules, and the sorbents are also solvated by water molecules. The interaction leading to the adsorption of solvated metal particles on the sorbent surface has the character of a dipole-dipole interaction and is rather weak.

The Hamiltonian of the system may be represented as follows:

$$H = H_m + H_p + H_s - \frac{1}{2} \int \langle \vec{P}(\vec{r}) \rangle_0 \vec{E}(\vec{r}, Q_0) d\vec{r} - \int \delta \vec{P}(\vec{r}) \vec{E}(\vec{r}, Q_0) d\vec{r}, \quad (2)$$

where  $H_m$  is the Hamiltonian of the polarized medium;  $H_p$  - Hamiltonian of a solvated metal particle;  $H_s$  is the Hamiltonian of the sorbent particle involved in the adsorption process.  $Q_0$  is a set of coordinates of a metal particle;

$\langle \vec{P}(\vec{r}) \rangle_0$  is the average value of the water polarization operator on the sorbent surface over the states of the zero Hamiltonian (without taking into account the interaction of the

sorbent, metal particles, and medium;

$\vec{E}(\vec{r}, Q_0)$  - is the electric field strength of a solvated metal particle in the dipole approximation,  $\delta \vec{P}(\vec{r})$  - is the fluctuation of water polarization on the surface of the sorbent.

The last term in formula (2) leads to the adsorption process.

According to the fluctuation - dissipative theorem [16]:

$$\langle P_i(\vec{r}, t) \rangle_0 = - \int d\vec{r}' \int dt' G_{P_i P_k}^R(\vec{r}, \vec{r}'; t - t') E_k(\vec{r}', t'), \quad (3)$$

where  $G_{PP}^R$  is the retarded Green's function at non-zero temperature of operators of the medium polarization [13-15].

For the intensity of the electric field of solvated metal particle in dipole approximation the following expression may be used:

$$E_{\alpha}(\vec{r}) = - \int d\vec{r}' G_{E_{\alpha}E_{\beta}}(\vec{r}, \vec{r}') \sum_{i=1}^N \mu_{\beta}^i(\vec{R}_i) \delta(\vec{r} - \vec{R}_i) + G_{E_{\alpha}\phi}(\vec{r}, R) \rho(R). \quad (4)$$

Here  $G_{EE}$  and  $G_{E_{\phi}}$  - are Green's functions of operators of the intensity of the electric field and the scalar potential of the condensed medium, they may be expressed by Greens' functions  $G_{\phi\phi}$ , which may be simply defined from the solution of an electrostatic task.  $\mu^i$  - is the dipole moment of the  $i$ -th bond of a particle. Depending on the configuration of the particle, its structure and size, several dipoles can be distinguished to characterize the electric field of the particle. Such a procedure requires consideration of the particle configuration and

their sorting by structure. If the particles are with different configurations, then the task becomes more complicated and it is necessary to introduce several types of metal solvated particles.  $\vec{R}_i$  - is a radius-vector of the  $i$ -th dipole of the particle;  $\rho, \vec{R}$  - are the charge of the particle and the radius-vector of the charge localization point.

For a polarizable particle the value of  $\mu^i$  differs from the corresponding vacuum value,  $\mu^i$  could be determined through:

$$\mu_{\alpha}^i = \mu_{\alpha}^i + \sum_{j=1}^N \alpha_{\alpha\beta}^i \left\{ G_{E_{\beta}E_{\gamma}} \mu_{\gamma}^i + G_{E_{\alpha}\phi} \rho \right\}, \quad (5)$$

where  $\alpha_{\alpha\beta}^i$  - is the polarizability tensor of the  $i$ -th bond of a particle. It is obvious that if all components of the polarizability tensor and vacuum values of the dipole moment of the bond are known, then all  $3N$  values of  $\mu$  may be found from the system (5). The corresponding solutions of electrostatic tasks of model functions may be used as Green's functions, which allows to take into account the effects of

the spatial dispersion of the medium. Further, substituting the found values  $\mu_{\alpha}^i$  into the correlation (4), we define the electric field intensity of the system  $E_{\alpha}(\vec{r})$  and from (3) we find the polarization of the medium  $\langle P(\vec{r}) \rangle_0$ .

Substituting (3) into (2) we rewrite the Hamiltonian of the system in the following form:

$$H = H_m + H_p + H_s + \frac{1}{2} \int \vec{E}(\vec{r}, Q) G_{PP}^R(\vec{r}, \vec{r}') \vec{E}(\vec{r}, Q) d\vec{r} d\vec{r}' - \int \delta\vec{P}(\vec{r}) \vec{E}(\vec{r}, Q) d\vec{r}. \quad (6)$$

In this formula, we expand the electric field intensity into series by  $Q^0$  up to linear terms,

$$H = \delta\Omega_0 + H_p + H_m + H_s - \int d\vec{r} \delta\vec{P}(\vec{r}) \vec{E}(\vec{r}, Q). \quad (7)$$

In (7)  $\delta\Omega_0$  is the free energy of the solvated particle, which has the following form:

$$\delta\Omega_0 = \frac{1}{2} \int dt dt' \int d\vec{r} d\vec{r}' E_{\alpha}(\vec{r}, Q_0^0) G_{P_{\alpha}P_{\beta}}^R(\vec{r}, \vec{r}', t - t') E_{\beta}(\vec{r}', Q_0^0) \quad (8),$$

where  $Q_0^0$  is the equilibrium value of the coordinate  $Q_0$ .

### Calculation of free energies of solution $\delta\Omega_0$

In the formula (8), we will obtain the following expression for  $\delta\Omega_0$ :

$$\delta\Omega_0 = \frac{1}{2} \int d\vec{r} d\vec{r}' E_{\alpha}^0(\vec{r}) G_{P_{\alpha}P_{\beta}}^R(\vec{r}, \vec{r}'; \omega = 0) E_{\beta}^0(\vec{r}'). \quad (9)$$

For a homogeneous local isotropic medium, for which

$$G_{P_{\alpha}P_{\beta}}(\vec{r}, \vec{r}'; \omega = 0) = -\frac{1}{4\pi} \left(1 - \frac{1}{\varepsilon}\right) \delta_{\alpha\beta} \delta(\vec{r} - \vec{r}'). \quad (10)$$

the free energy of the solution  $\delta\Omega_0$  takes the following form:

$$\delta\Omega_0 = -\frac{c}{8\pi} \left(1 - \frac{1}{\varepsilon}\right) \int d\vec{r} (\vec{E}^0(\vec{r}))^2 \quad (11)$$

Here  $\varepsilon$  is static value of the dielectric permeability for water solution with metal particles and particles of sorbent.

If solvated metal particle has an equilibrium dipole moment, then for spherically symmetric particles we will obtain:

$$\delta\Omega_0 = -\left(1 - \frac{1}{\varepsilon}\right) \frac{\mu^2}{3r_0^3} \quad (12)$$

where  $r_0$  is the radius of the metal particle.

### Effects of medium spatial dispersion

Taking into account the spatial dispersion of the medium let us rewrite free energies of solution

$\delta\Omega_0$  (9) in the following form:

$$\delta\Omega_0 = -\frac{1}{2} \int \rho(\vec{r}) G_{\varphi\varphi}(\vec{r}, \vec{r}') \rho(\vec{r}') d\vec{r} d\vec{r}' \quad (13)$$

where  $G_{\varphi\varphi}$  is Green's function (GF) of the medium scalar potential operators,  $\rho$  – is the charge density of the solvated metal particle, which creates the electric field with the intensity  $E_0$ .

The effects of spatial dispersion of the medium (water with metal particles and particles of sorbent) may be considered in the process of the calculation of the free energy change of the system in case where some model functions will be used as Green's functions of

operators of the polarization fluctuation or the charge density or the medium scalar potential. To determine GF  $G_{\varphi\varphi}(\vec{r}, \vec{r}')$  we may use the results of the solution of electrostatic tasks: the GF  $G_{\varphi\varphi}(\vec{r}, \vec{r}')$  coincides with the magnitude of the electrostatic potential in point  $\vec{r}$  of the system, if in point  $\vec{r}'$  a unit charge will be placed. In consideration of the above mentioned it must be expected that behavior of GF  $G_{\varphi\varphi}(\vec{r}, \vec{r}')$  will be of type:

$$G_{\phi\phi}(r, r') = C(r) \frac{1}{|r-r'|} \quad (14)$$

In this case the behavior of GF  $G_{\varphi\varphi}$  and  $G_{\rho\varphi}$  will be of the following type:

$$G_{\phi\rho}(\vec{r}, \vec{r}') = G_{\rho\phi}(\vec{r}, \vec{r}') = -f(\vec{r}) \delta(\vec{r} - \vec{r}') \quad (15)$$

Fourier component of  $f(\vec{r})$  function may be connected with the longitudinal component of the dielectric permeability  $\varepsilon^l(k)$ . After standard conversions we will obtain:

$$f(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \int e^{i\vec{k}\cdot\vec{r}} f(\vec{k}) d\vec{k} \quad (16)$$

and

$$f(\vec{k}) = \frac{1}{4\pi} \left(1 - \frac{1}{\varepsilon^l(k)}\right) \quad (17)$$

Hereby, for Fourier components we have the following correlation:

$$G_{\phi\rho}(\vec{k}, \vec{k}') = -\frac{1}{4\pi} \left(1 - \frac{1}{\varepsilon^l(k)}\right) \delta_{\vec{k}, \vec{k}'} \quad (18)$$

In case of a local homogeneous medium from the previous formula we will obtain:

$$G_{\phi\rho}(\vec{k}, \vec{k}') = -\frac{1}{4\pi} \left(1 - \frac{1}{\varepsilon^l(k)}\right) \delta_{\vec{k}, \vec{k}'} = -\frac{C_0}{4\pi} \delta_{\vec{k}, \vec{k}'} \quad (19)$$

In  $\vec{r}$  space the last formula has the form:

$$G_{\phi\rho}(\vec{r}, \vec{r}') = -\frac{1}{4\pi} C_0 \delta(\vec{r} - \vec{r}') \quad (20)$$

To consider the space dispersion effects instead of  $\delta$ -function in formula (20) the following function may be used:

$$G_{\phi\rho}^{(\lambda)}(\vec{r}, \vec{r}') = -\frac{C_0}{4\pi} \Delta_\lambda(|\vec{r} - \vec{r}'|) \quad (21)$$

In the capacity of  $\Delta_\lambda(|\vec{r} - \vec{r}'|)$  function an exponentially damped function normalized on unity may be selected:

$$\Delta_\lambda(|\vec{r} - \vec{r}'|) = \frac{1}{8\pi\lambda^2} e^{-\frac{|\vec{r} - \vec{r}'|}{\lambda}} \quad (22)$$

If for the charge density of the impurity particle localization coincides with origin of  $\rho^{\text{ex}}$  a classic approximation will be used and if coordinates, then we assume that the point of the  $q$  charge

$$\rho^{\text{ex}}(\vec{r}) = q\delta(\vec{r}) \quad (23)$$

In this case for  $\delta\Omega_1$  we have:

$$\delta\Omega_1 = -\frac{C_0 q^2}{16\pi\lambda} = -\frac{q^2}{16\pi\lambda} \left(1 - \frac{1}{\varepsilon}\right) \quad (24)$$

Similarly, the change of free energies of the system may be calculated, where the space dispersion effects of the medium are described by more complicated functions.

Thus, for the free energy change of the system, when the introduction of a polyatomic polarizable non-dipole charged particle in a condensed medium, the calculations may be carried out with different degree of precision with due regard for various effects: in case of quantum or classic behavior of the degrees of

freedom of the solvate layer of metal particle on the surface of the sorbent the effects of spatial dispersion of a medium, which may be described by a set of different model functions; interactions of vibrations of solvate layer around metal particle on the surface of the sorbent with polarization fluctuations of a medium.

Let us view an impurity particle in a local homogeneous isotropic medium. We have the following expression for the free energy change:

$$\delta\Omega_1^d = -\int d\vec{r} d\vec{r}' (\vec{E}(\vec{r}) \vec{E}(\vec{r}')) \delta(\vec{r} - \vec{r}') \frac{C_0}{4\pi} \quad (25)$$

If the equilibrium dipole moment and the charge density of a particle equals zero, after the corresponding integration we obtain:

$$\delta\Omega_1^d = -[8\pi C_0 / (3r_0^3)] (\partial d / \partial Q)^2 \quad (26)$$

where  $r_0$  is the particle's radius.

As for allowance of space dispersion of the medium for the dipole particles, the expression for the free energy change of the system in one of the following forms is more convenient:

$$\delta\Omega_1 = \int d\vec{r} d\vec{r}' \nabla_{r\alpha} \nabla_{r'\beta} G_{\varphi\varphi}(\vec{r}, \vec{r}') P_\alpha^{ex}(\vec{r}) P_\beta^{ex}(\vec{r}') = \int G_{E_\alpha E_\beta}(\vec{r}, \vec{r}') P_\alpha^{ex}(\vec{r}) P_\beta^{ex}(\vec{r}') d\vec{r} d\vec{r}' \quad (27)$$

For the particle's polarization  $\rho^{ex}$  may be used point approximation:

$$\vec{\rho}^{ex}(\vec{r}) = \vec{d}\delta(\vec{r}) \quad (28)$$

For GF  $G_{\varphi\varphi}$  and  $G_{EE}$  may be used different model functions.

The most acceptable way to calculate of  $\delta\Omega_1$  for the charge density of the charged dipole particle in quantum approximation is to use correctly selected wave functions  $\Psi_d$  for various types of  $\Delta_\lambda$  functions.

Further analysis of the obtained relations is acceptable only for specific cases, with the solution of problems in digital format.

### Adsorption of particles in the channels of sorbents

First of all let's consider the process of physical adsorption of the particle on the channel's surface of sorbent from liquid. It will be assumed at that, that additional vibrating degree of freedom doesn't appear in the system in adsorption state. It is assumed that number of vibrating degrees of freedom in the beginning and that at the end of the process is equal. Therefore, we present the results for a simple case, following which only the medium (water

with impurity particles) is reorganized while the adsorption process does not change the structure of the particle. Even at this assumption the general expression for rate constant has rather bulky character.

Omitting cumbersome specific calculations, we give an expression for the rate constant of the adsorption process without taking into account the oscillatory subsystem [13-15]:

$$K_\alpha = \frac{|V_{fi}(\vec{R}^*, \psi^*)|^2}{\sqrt{|\psi''_{\theta\theta}|}} \Phi(\vec{R}^*, \psi^*) \exp\{-\beta\theta^* \Delta F - \psi^m(\vec{R}^*, \psi^*; \theta)\} \quad (29)$$

Here  $\vec{R}^*$ ,  $\psi^*$  are the coordinates of the adsorbed solvated metal particle,  $\Delta F$  is the free energy of the adsorption process,  $\Phi(\vec{R}^*, \psi^*)$  is the distribution function of the metal solvated particles.  $V_{fi}(\vec{R}^*, \psi^*)$  is the interaction of a

solvated metal particle with the sorbent surface leading to adsorption;  $\psi''_{\theta\theta}$  is width of integral over  $\theta$ , and point of inflection  $\theta^*$  may be found from equation:

$$\beta \Delta F + \frac{\partial \psi^m(\vec{R}^*, \psi^*; \theta)}{\partial \theta} = 0 \quad (30)$$

Matrix element  $V_{fi}(\vec{R}^*, \psi^*)$  is calculated with use of wave functions in frames of concrete model for amorphous solid, and can be considered as some phenomenological

parameter. Arguments of  $V_{fi}(\vec{R}^*, \psi^*)$  provide geometric characteristics of the process, distance to surface, spatial orientation of the particle at adsorption. Function  $\Phi(\vec{R}^*, \psi^*)$  is

distribution function of adsorbing particles. Model function may be selected as this function. If geometric dimension of the channel is big enough for motion of the particles along the channel, distribution of particles will be approximately uniform. If channel dimension doesn't allow free passing of particles, then distribution will be determined by mechanism

$$\Psi^m(\vec{R}^*, \psi^*, \theta) = E_r^m \frac{2}{k} \int_{-\infty}^{\infty} d\omega f(\omega) \frac{sh \frac{\beta\omega(1-\theta)}{2} sh \frac{\beta\omega\theta}{2}}{\omega^2 sh \frac{\beta\omega}{2}} \quad (31)$$

Where  $E_r^m$  is medium reorganization energy for charge adsorption processes,  $f(\omega)$  function

of transfer of particles along the channel. Note that  $\Psi^m(\vec{R}^*, \psi^*; \theta)$  is function of medium reorganization. It includes reorganization of two subsystems: sorbent (amorphous solid), on wall of which takes place adsorption, and liquid, where is placed adsorbing particle. It's formal expression is [15]:

describes the frequency spectrum of the medium.

### Conclusion

Theoretical aspects of the processes of adsorption of metal particles on the surface and in the channels of sorbents are considered. Sorbents obtained from various wastes using a special one-stage technology make it possible to purify solutions containing metal particles.

Theoretical issues of solution processes in

such systems are also considered, taking into account the effects of frequency and spatial dispersion of the medium - an aqueous solution containing metal and sorbent particles. The calculations were carried out for various model systems.

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## ТЕОРЕТИЧЕСКИЕ АСПЕКТЫ ПРОЦЕССОВ АДСОРБЦИИ МЕТАЛЛИЧЕСКИХ ЧАСТИЦ ВНУТРИ КАНАЛОВ И НА ПОВЕРХНОСТИ УГЛЕРОДНЫХ СОРБЕНТОВ

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**Аннотация:** В работе приведен краткий анализ экспериментальных работ по получению в одном процессе сорбентов из различных биологических отходов. При этом полученные сорбенты используются без дополнительной активации. В связи с подобным экспериментальным материалом рассмотрены теоретические аспекты различных процессов в каналах и на поверхности сорбента. Рассмотрены процессы сольватации металлических

частиц в водной среде в рамках квантовой теории неоднородных конденсированных сред с перераспределением электронной плотности системы. Рассмотрены процессы адсорбции на стенках и в каналах сорбента с учетом эффектов пространственной дисперсии системы.

**Ключевые слова:** сорбент, адсорбция, сольватация, металлическая частица, водный раствор

## KARBON SORBENTLƏRİN SƏTHİNDƏ VƏ KANALLARINDA METAL HİSSƏCİKLƏRİNİN ADSORBSİYA PROSESLƏRİNİN NƏZƏRİ ASPEKTLƏRİ

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**Xülasə:** Məqalədə bir prosesdə müxtəlif bioloji tullantılardan sorbentlərin alınması üzrə eksperimental işlərin qısa təhlili verilmişdir. Bu zaman alınan sorbentlər əlavə aktivləşdirmədən istifadə edilir. Belə təcrübə materialı ilə əlaqədar olaraq sorbentin kanallarında və səthində müxtəlif proseslərin nəzəri aspektləri nəzərdən keçirilir. Metal hissəciklərinin sulu mühitdə solvatlaşma prosesinə qeyri-homogen kondensasiya olunmuş mühitin elektron sıxlığının yenidən paylanması kvant nəzəriyyəsi çərçivəsində baxılır. Sorbentin divarlarında və kanallarında adsorbsiya proseslərinə sistemin faza dispersiyasının təsirləri nəzərə alınmaqla baxılır.

**Açar sözlər:** sorbent, adsorbsiya, metal hissəcik, sulu məhlul