Modeling the Structure and Diffusion of Porous Layers

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Abstract: The aim of this work is to develop an adsorber with a fixed bed of adsorbent and a mathematical model of the adsorption bed. On the basis of the theory of fractal clusters, an equation for calculating the layer porosity that takes into account the average cluster radius, the fractal dimension of the cluster structure and the anisotropy index of the adsorbent layer is proposed. The adsorption mechanism in the layer was established, and the proportionality coefficients were estimated based on the tetrahedral packing of grains in the layer. Based on the analysis of the movement of the carrier through the adsorption layer and its deformation, an equation that describes the change in the porosity of the granular layer when the water flow moves through it, depending on the proportionality coefficients, is proposed. An equation that made it possible to calculate the change in the porosity of the layer in comparison with the porosity of the stationary stacking was obtained. An effective design for the adsorber that made it possible to increase the efficiency of using the structure of porous adsorption layers was developed. Equations of the heat and mass transfer taking into account the granule shape coefficient, effective diffusion coefficient and mass transfer coefficient were derived. These equations establish the relationship between the average distance between active centers on the adsorption surface and the degree of filling of the adsorption surface with the adsorbed component.

Keywords: adsorption; diffusion; adsorbent; fractal clusters; layer porosity; adsorber; heat and mass exchange; active centers

1. Introduction

To prevent environmental pollution, modern water purification technologies are being introduced [1]. Adsorbents, especially modified activated carbons, play a significant role in the purification of drinking water sources and wastewater [2]. Fundamental and practical principles for the use of adsorbents are currently being developed depending on the specific surface area, adsorbent dose, contact time and temperature in water treatment processes [3]. To study adsorption processes, theoretical and numerical methods for studying the emergence of fractal clusters have been proposed [4]. The phase transition that separates an almost homogeneous phase and a phase exhibiting strong clustering was determined, and the fractal dimension of the clusters was calculated. In [5], a three-phase model for calculating thermal conductivity based on a capillary structure was created considering the peculiarities of the porous structure of building materials using fractal theory. The dependence of the quantitative influence of parameters such as the porosity, pore diameter distribution, moisture content and fractal structure on the thermal conductivity of wet porous materials was analyzed. The results obtained provide a theoretical basis for correcting the thermal conductivity of wet building materials. In [6], a fractal model of permeability for biodispersed porous media based on the fractal characteristics of pores in these media was developed. It was established that the fractal permeability model is a function of the fractal dimension of tortuosity; the fractal dimension of the pore area and
particle and cluster sizes; the microporosity within clusters; and the effective porosity of the medium. The fractal dimension of the pore area and the fractal dimension of the tortuosity of porous samples were determined. Good agreement was found between the fractal model for predicting permeability and the experimental data. This confirms the correctness of the presented fractal model of permeability for bidispersed porous media. A mathematical model was created to describe the flow of liquid in fractal dense porous media [7]. To solve this problem, four fractal measurements were used: the fractal measurement of pore size $D_f$, the geometric and hydraulic fractal sizes of tortuosities $D_{\tau g}$ and $D_{\tau}$, and the fractal dimension $D_{\lambda}$ characterizing the hydraulic distribution of diameter numbers. The relationship between these fractal measurements was analyzed, and $D_f$ was found to be equal to $D_{\lambda} + D_{\tau g}$. Then, a unified model connecting the porosity and $D_f$ was deduced for arbitrary fractal tight porous media. Based on its assumed scale-invariant behavior, a fractal mathematical model for estimating permeability was developed only according to the fundamental and clearly defined physical properties $D_f$ and $D_{\tau g}$, the scaling lacunarity $P_{\lambda}$, the range of pore sizes and the porosity of the fractal generator $\phi_0$. In [8], the Monte Carlo method was used to model the permeability of fractal porous media. Based on the fractal nature of the pore size distribution in porous media, probabilistic models of pore diameter and permeability were obtained. The results showed that the developed simulations represented good agreement compared to the existing fractal analytical solution in the general porosity range of interest. In [9], a mathematical model of the conjugate heat and mass transfer in porous media based on the fractal nature of the pore size distribution was developed. According to Darcy’s law and the Hagen–Poiseuille law for liquid flows, the diffusion coefficient of liquid water, which is a function of the fractal dimension, was theoretically obtained. This model considers the fluid flow to be influenced by surface tension and gravity, water vapor sorption/desorption by fibers, water vapor diffusion and phase changes. The influence of the porosity of porous fibrous media on the heat and mass transfer was analyzed. The theoretical predictions were compared with experimental data, and there was good agreement between them, indicating that the fractal model was satisfactory. A mathematical model of adsorption on a cluster with a fractal structure with an average fractal number was proposed [10]. The relationship between the structure of the cluster and the number of free centers on which adsorption can occur was considered. The concept of the coordination number of a fractal particle was introduced. An equation for the kinetics of irreversible adsorption on fractals was proposed. Studies of gas diffusion into pore networks have confirmed the existence of a fractal structure in the system [11]. Based on the analysis of the two fractal identities of the surface and the tortuosity of the pores, a fractal model of permeability was proposed and calculated in comparison to the modern Kozeny–Karman equation.

The main theoretical and practical difficulty when working with heterogeneous porous media is the problem of correlating laboratory data with industrial data [12]. To study adsorption characteristics, a numerical analysis of spherical adsorbent particles packed in an adsorption layer was proposed [13]. Numerical results have shown the influence of the shape of a rectangular, compacted adsorption layer on the amount of water vapor adsorption. Another article has proposed a method for averaging the volume to ordered and disordered spatially periodic porous media in two dimensions [14]. The predicted coefficient of longitudinal dispersion in disordered porous media was less than what was found in the experimental data. However, the predicted transverse dispersion coefficient was consistent with the experimental data. Another paper analyzed the phenomenon of channeling flow in the fill layers, as well as the phenomenon of channel formation when liquid flows through a packing layer [15]. The solution was obtained using the exponential distribution of porosity typical for packed layers. It was shown that the obtained expression for the velocity was convenient for analyzing other characteristics of the packed layer, such as the effective permeability of the layer. With the help of the Ergun equation, a one-dimensional formulation of the flow of liquids through packed layers was presented, considering the change in porosity along the radial direction [16]. It was found
that there is a relationship between the numerical and experimental results, and it was observed that the change in porosity with a radial position had a greater effect on the velocity channeling near the walls. It was found that the density profiles are characterized by the presence of one to three maxima that reflect the positional order of molecules in the adsorption layers, that is, the layered structure of the adsorbate [17]. The local density profiles in the Lennard–Jones adsorption layers, as well as the excess (Gibbs) and absolute adsorption values, were calculated via the density functional method (an approximation of the weight coefficient). The equilibrium in an ideal adsorption layer was investigated for the adsorption of a substance’s mixture [18]. The shape of the isotherm for multiplet adsorption depends on the distribution of elementary regions on the surface. A method [19] for the thermodynamic formalization of the selection of the parameters of the adsorption layer was proposed. The optimal parameters of the adsorption layer were determined during the adsorption of binary solutions on adsorbents with different structures. A study [20] showed the possibility of modeling adsorption in the pore space of slit or cylindrical geometry. This mathematical model has led to useful methods for extracting pore size distribution information from experimental adsorption isotherms. The method of [21] was based on the comparison of the adsorption isotherm on a porous solid with the isotherm measured on a reference nonporous absorbent. It was proven that the proposed approach made it possible to divide the total excess adsorption into min to partial and other characteristics for micro- and mesopores. A typical relationship between the accumulated liquid, temperature and vapor pressure characterizes any surface, in particular, any porous structure [22]. From a theoretical point of view, the sorption–desorption characteristics of a body were investigated using a simpler apparatus. The proposed measurement procedure used a closed impermeable system in which only the temperature was controlled while the total liquid water vapor content remained constant. The three-dimensional structure of the void space formed during the placement of active carbon grains was found to have a greater effect on the filter efficiency due to the change in the transport properties within the layer [23]. Image analysis algorithms allowing for the determination of the total void fraction, the void size distribution and the radial void fraction profiles were developed.

To study adsorption properties, it is necessary to know the shape and size of pores and their combination with each other to study their strength properties—the shape and size of particles and their packing density in a granule [24]. Therefore, it is important to know both the properties of the solid substance forming the granules and the pores’ structure. Any porous body can be described by one of these models; the second is obtained as a spatial addition to the first. This means that for a globular model, for example, it is sufficient to determine its parameters—the size of globules and their packing density—to determine the parameters of interglobular pores with the same accuracy. In [25], a mathematical expression is given for the circulation intensity in relation to the fraction of the volume occupied by pores (the porosity ε) and by a solid (the degree of the filling η).

The effect of the surface mass transfer on the flow caused by buoyancy in a medium with variable porosity adjacent to a heated vertical plate was studied for large Rayleigh numbers [26]. Their analysis included an expression linking the porosity and permeability and an expression linking the porosity and effective thermal diffusivity. A mathematical model was developed [27] that describes transport phenomena in porous media at the macroscopic level. The model consists of a balance equation for each transported extensive quantity, defining the relations describing the properties of individual involved phases, the initial functions of the extensive quantities and the initial and boundary conditions, all of which were set at the macroscopic level. The authors of [28] describe a methodology for developing a complete description of transport phenomena in a multiphase deformable porous medium and demonstrate their methodology by applying it to the transfer of vast quantities, such as volume, mass, phase components, momentum and heat. The systematic development of a continuous model of a porous medium and the transport processes occurring in it are presented in [29]. The concept of a representative elementary volume (REV), in contrast to any arbitrary volume of averaging quantities at the micro
level, was quantitatively defined. The universal criterion for the choice of the REV value was developed depending on the measured characteristics of the porous medium and the selected levels of the estimation error tolerance. The spatial averaging rules were extended to include the effects of both the configuration of the solid matrix and the phenomena of interphase transfer within one turn. Article [30] considers a continual approach to modeling the transfer of mass, momentum and energy of the liquid phase or its component in the region of a porous medium. Their review begins by defining a porous medium, using the notion of a representative elementary volume as a tool to overcome the effect of microscopic inhomogeneity resulting from the presence of a solid matrix and void space. It was shown in [31] that the averaging method leads to a better understanding of the concept of effective stress used in solving transport phenomena in deformable porous media. A one-dimensional finite-volume modeling of mass transfer phenomena in partially saturated open porous media has been developed [32]. The finite volume model was based on a stepwise solution strategy that solves equations sequentially. This appropriate partitioning thus reduces the size of the system to be solved at each time step. Therefore, to solve the discretization problem, two iterative algorithms were proposed. Article [33] describes the ANTHYC numerical code developed in G.3S for modeling transport phenomena in porous media. Using the method derived from the finite volume method, the code forces local carryover and mechanical processes to be retained, and the results showed a very good accuracy. The relationship between the effective coefficient of volumetric diffusion in macroporous media and the coefficient of diffusion in the absence of a porous medium was analyzed in terms of porosity, tortuosity and compressibility [34]. The need to separate these three parameters was confirmed via the description of diffusion in partially saturated homogeneous isotropic monodisperse spherical packing. The results obtained were generalized to volumetric diffusion in all homogeneous isotropic porous media in the porosity range of 0–50%. Knowledge about the influence of the porosity and thermal conductivity coefficient on double-diffusion transport is extremely necessary for the optimal design and analysis of vertical and horizontal adsorbers [35]. Mass transfer assumes a binary mixture with a solute characterized by its mass fraction. This paper investigates two situations related to the influence of porosity. In the first, the porosity changes with the permeability. In the second, the permeability is fixed, but the porosity takes on different values. The results show that decreasing both the porosity and permeability induces flow recirculation and increases the overall heat and mass transfer, resulting in higher levels of turbulent kinetic energy. Such effects are less pronounced when the permeability is kept constant as the porosity changes. An analytical model of permeability for incompressible fluid flow in porous media was proposed in [36]. Based on the general nonequilibrium thermodynamic theory of stability, the model was derived from maximizing the entropy production rate to achieve a stable system. The resulting formula has a form similar to that of the previous empirical equations but with calculated coefficients.

An analysis of the theoretical and experimental data on the structure of adsorption layers taking into account porous layers with a clearly ordered and chaotic structure shows that during adsorption purification, it is necessary to take into account the structural characteristics of the adsorption layer and porosity. In this regard, the aim of this work is to develop an adsorber with a fixed bed of adsorbent and the mathematical model of the adsorption bed based on fractal theory.

2. Material and Methods

To study the influence of the structure of the adsorption layer on the process of adsorption water purification, the installation shown in Figure 1 was used.

The water to be purified from water tank 2 is supplied by pump 4 into adsorber 1. The water intake can be controlled by means of water supply valve 6, and its flow rate can be measured using flow meter 5. The temperature of the entering water is controlled by a thermocouple that is connected to the indicating secondary device. The purified water then enters clean water tank 7.
The disadvantages of the known adsorption devices are the low efficiency of the equipment. The existing adsorbers do not fully utilize the capacity of the adsorbent, the low utilization rate of the useful volume of the apparatus and the degree of processing of the adsorption capacity of the adsorbent in the layer. In this regard, the task of the study was to develop the design of an adsorber [37] that would improve the efficiency of the apparatus and increase the utilization rate of the useful volume of the apparatus and the degree of processing of the adsorption capacity of the adsorbent in the layer, the stability of the quality of the purified stream and the compactness of the apparatus.

To study the adsorptive water treatment and determine the effect of the layer porosity and the structure of the adsorption layer, an adsorber was developed; it is presented in Figures 2 and 3. This problem is solved by the fact that the adsorber contains a housing, a chamber for putting the adsorption layer in contact with the stream to be cleaned; fittings for supplying and removing the flow for supplying and removing the regenerating agent; the branch pipe combining the branch pipes for removing the flow and supplying the regenerating agent; and hatches for loading and unloading the adsorbent, according to the description of the invention. It is additionally equipped with a vertical chamber for keeping the adsorbent in contact with the flow installed along the axis of the apparatus and a circular cross section connected to the branch pipe for diverting the flow and supplying the regenerating agent, while the lower part of the walls of the inner chamber are kept whole.

The essence of the work of the adsorber is illustrated in the following drawings. Figure 2 shows a section of the adsorber in the cross section and Figure 3 shows a section of the adsorber in section A-A. The adsorber contains a housing (1); external (2) and internal (3) chambers of contact for the adsorption layer with the stream to be cleaned; fittings for the supply (4) and discharge (5) of flow; fittings for supplying (6) and withdrawing (7) the regenerating agent during regeneration; a branch pipe (8) combining fittings for withdrawing the flow and supplying the regenerating agent; and hatches for loading (9) and unloading (10) the adsorbent. The adsorber works as follows: The stream to be cleaned enters through nozzle 4 into the inner part of adsorber body 1 and passes horizontally through the annular activated carbon layer located in outer chamber 2 of the contact of the adsorption layer with the stream to be cleaned. Furthermore, the stream to be cleaned is supplied to the upper part of inner chamber 3 at which the adsorption layer is in contact with the stream to be cleaned, where the stream is additionally filtered through the adsor-
bent layer and removed from the apparatus through branch pipe 8 and fittings 5. When the degree of stream cleaning by the adsorption layer decreases, as evidenced by an increase in the concentration of the absorbed substance in the purified stream, the filtering charge (adsorbent layer) is subjected to regeneration. To do this, using the valves of nozzles 4 and 5, the supply of the initial flow is turned off; a regenerating agent is introduced through nozzle 6 and supplied to contact chambers 3 and 2. The absorbed substance separated from the adsorbent in a mixture with the regenerating agent is discharged through nozzle 7. The adsorbent is loaded through hatch 9 and unloaded through hatch 10. Due to the installation of an additional internal chamber in which the adsorbent is in contact with the stream to be cleaned, the efficiency of the apparatus increases, the utilization rate of the useful volume of the apparatus and the degree of processing of the adsorption capacity of the adsorbent in the layer increase, and the stability of the quality of the purified stream is ensured with maximal compactness of the apparatus, reducing the total stagnant and unused areas.

Figure 2. Sectional view of the adsorber. 1: framework; 2 and 3: external and internal chambers for contact of the adsorption layer with the stream to be cleaned; 4 and 5: fittings for supply and discharge of the flow; 6 and 7: fittings for supply and discharge of the regenerating agent during regeneration; 8: branch pipe that unites the fittings to divert the flow and supply the regenerating agent; and 9 and 10: hatches for loading and unloading the adsorbent.

The characteristics of such systems are closely related to the mechanism of their formation. In the most general form, this mechanism can be represented as the formation of a single cluster by means of the coagulation of the constituent elements. To describe such a limited aggregation, a mathematical model of fractal theory can be used [38]. According to the fractal model, the adsorption layer is represented as a single cluster. The growth of this cluster occurs when particles arriving at the cluster surface attach. In this case, the dynamics of the cluster are expressed in the movement of the core, i.e., the area in which new particles join the cluster.

Particle trajectories start outside the region occupied by the cluster and end the moment the particle hits the cluster. This process can also be described using the Smoluchowski equation with the following form [39,40]:

\[
\frac{dn_k(t)}{dt} = \frac{1}{2} \sum_{i+j=k} K_{ij} n_i(t) n_j(t) - n_k(t) \sum_{j=1}^{\infty} K_{jk} n_j(t)
\]

where \( n_k(t) \) is the density of \( k \)-particle clusters, 1/m³.

The core \( K_{ij} \) of Equation (14) takes into account the dependence of the collision cross section on the size and mobility of clusters, and the following assumption can be made for the equation: the number of particles must be so large that it can be considered a continuous parameter, assuming there are no collisions between particles in the initial stage.

This equation can be modified to the Becker-Dering form [41], provided that the main contribution to the clustering process is made not by the sludge cohesion factor but by the process of limited aggregation:

\[
\frac{dn_i}{dt} = J_{i-1}(n) - J_i(n),
\]

\[
\frac{dn_i}{dt} = -J_1(n) - \sum_{i=1}^{\infty} J_i(n),
\]

where the vector \( n = (n_i) \).

Taking into account the phenomena of aggregation and fragmentation, the flow components in the Becker-Dering equations for all \( i \geq 2 \) can be reduced to the following form:

\[
J_i(n) = a_i n_i - b_i + 1n_i + 1,
\]

\[
\frac{dn_i}{dt} = \frac{1}{2} \sum_{s=1}^{i-1} a_{i,s} n_s n_{i-s} - n_i \sum_{s=1}^{\infty} a_{i,s} n_s + \sum_{s=i+1}^{\infty} b_{i,s} n_s - \frac{n_i}{i} \sum_{s=1}^{i-1} s b_{i,s},
\]
where the first term is the increase in the number of clusters due to the aggregation (merging) of clusters of lower order, that is, those with fewer particles; the second term is a decrease in the number of clusters of a given order (with a given number of particles) as a result of their merging with other clusters; the third term is the appearance of clusters of a given order as a result of the fragmentation (destruction) of clusters of a higher order; and the fourth term is a decrease in clusters of a given order as a result of their fragmentation.

As can be seen from the equilibrium and kinetics [38] as well as the coefficients [41] of the Becker–Dering equations, the most likely mechanism is the binary aggregation–fragmentation of clusters:

\[ a_i = a_{i,1} = a, \]
\[ 2a_1 = a_{1,1}, \]
\[ b_{i+1} = b_{i+1,1}, \]
\[ 2b_2 = b_{2,1}. \]

The rest of the coefficients \( a_{i,s} \) and \( b_{i,s} \) are taken to be equal to zero.

It was shown in [38,41] that the coefficients of Equations (4) and (5) are density functions:

\[ \rho = \sum_{i=1}^{\infty} \delta C_i(t), \]

Hence, it follows that in the fields of a constant local density value, the coefficients of the Becker–Dering equation system can be considered constant, and in the fields with sources of mass, these coefficients are determined by the intensity of chemical reactions or phase transitions.

The use of the Becker–Dering equations opens up possibilities for numerical studies of the processes of coagulation, fragmentation and sediment formation.

Since the surface of a cluster in a zone of limited aggregation has an extremely complex shape, there is practically zero probability that a particle will join a cluster within a fully developed field. The highest probability of particle attachment to the “protrusions” of the clusters \( P_m \) = max. The probability of attachment of a particle that has reached the cluster in the core can then be estimated as \( 1 - P_m \). As a result, the following kinetic equation exists for the cluster growth with a large number of particles \( N \):

\[ \frac{d\tau_N}{dN} = P_m(N)a \]

where \( a \) is the characteristic size of the attached particle (adsorbent grain), m.

The cluster simulating the adsorption layer is characterized by two parameters: the average cluster radius \( \tau_N \) and the core width \( \psi \). For large numbers of particles \( N \), fractal theory implies the following relation:

\[ \tau_N \sim N^{\delta} = N^{1/D_F} \]

where \( D_F \) is the fractal dimension of the cluster structure, and \( \delta \) is an indicator that depends on the characteristic length.

The corresponding expression for the core width is also given by fractal theory as the average distance between the branches of a cluster as follows:

\[ \psi \sim \tau_N^{(3-D_F+\chi)/2} \]

where \( \chi \) is the anisotropy index of the adsorbent layer.
The full thickness of the layer can be used as the characteristic length in the area of limited aggregation. To estimate the porosity of the layer, the following expression can be proposed:

\[ \epsilon_0 = \frac{r^3 - D_f + \chi}{r^3} \]  

(14)

Hence, it can be seen that the most important characteristic of cluster-type adsorption layers is the fractal dimension, for which it is necessary to develop a technique for its experimental determination. However, in this case, well-known methods for the experimental determination of porosity based on hydrodynamic studies of the flow of a neutral (not adsorbed in the layer) liquid can be used. A further determination of the fractal dimension of the layer is carried out according to the formulas indicated in this article.

This approach to modeling the structure of a layer to the greatest extent reflects its complex structure and allows for an adequate description of its main characteristics. In this case, it is necessary to develop a mathematical model that considers the features of adsorption in a fixed bed of adsorbent. This requires a systematic analysis of this complex process and the selection of the basic concepts of the mathematical model, taking into account its main features. To solve this problem, it should be noted that even in the case of the complete isotropy of the structure of the granular layer at each of its points, it is possible to distinguish the axis of its transfer characteristics that has the same direction as the vector of the average adsorption rate. Then, in the direction perpendicular to this axis, the process of convective transfer is determined by the pulsation components of the hydrodynamic characteristics of the flow.

To describe this feature, the approach proposed in [42] is used, extending it to the case of adsorption in the adsorption layer. According to this model, it is possible to propose the use of two proportionality coefficients, depending on the structure of the granular layer, i.e., the downstream and transverse directions.

The calculation of the characteristic size of the adsorption channel is performed using a formula that takes into account the grain size of the layer and its porosity \( \epsilon \):

\[ d_{ef} = \frac{2\epsilon d}{3(1 - \epsilon)} \]  

(15)

The estimation of the proportionality coefficients \( k_{\parallel} \) and \( k_\perp \) is performed based on their tetrahedral packing of grains in the layer (Figure 4). In this case:

\[ k_{\parallel} = \frac{V_{\parallel}}{V_0} \approx \frac{3 \sin(\pi/6)}{3(1 - \epsilon)} = \frac{1}{2(1 - \epsilon)} \]  

(16)

\[ k_\perp = \frac{V_\perp}{V_0} \approx \frac{(1 - \cos(\pi/6))V}{2V_0} \approx \frac{1}{4\sqrt{3}(1 - \epsilon)} \]  

(17)

\[ \text{Figure 4. Tetrahedral packing of grains in the adsorbent layer.} \]
In the process of moving the carrier through the adsorption layer, the layer is deformed, and its hydrodynamic characteristics can change. In this regard, it is necessary to supplement the mathematical model with an equation describing the change in the porosity of the granular layer when the filtering mixture moves through it.

The corresponding equation takes the following form:

$$\frac{\partial}{\partial x} \left( k_{\parallel} \frac{\epsilon^3 d^2 \partial \rho}{\rho V_0 (1 - \epsilon^2)} \right) + \frac{\partial}{\partial y} \left( k_{\perp} \frac{\epsilon^3 d^2 \partial \rho}{\rho V_0 (1 - \epsilon^2)} \right) = 0, \quad (18)$$

where $\rho$ is the carrier pressure in the granular layer, Pa.

The calculation of the matching rate and shear strain caused by the effect of the fluid flow allows us to calculate the change in the porosity of the layer in comparison to the porosity of the stationary stack $\epsilon_0$ as follows:

$$\epsilon = \epsilon_0 + \frac{2 \mu (1 - \epsilon_0)}{\gamma}, \quad (19)$$

where $\mu$ is the coefficient of the dynamic viscosity of the carrier flow, Pa·s; and $\gamma$ is the parameter of the shear stress, Pa·s.

The expression for $\gamma$ according to [43] can be written as follows:

$$\gamma = k \Delta \rho = k \xi \rho v^2 / 2, \quad (20)$$

where $\xi$ is the coefficient of resistance of the granular layer and $k$ is an empirical coefficient.

Figure 5 shows the dependence of the ratio of the characteristic size of the adsorption channel to the grain diameter on the porosity of the granular layer. Figure 6 shows a graph illustrating the dependence of the proportionality coefficients on the porosity of the layer. The figure shows that at the maximum porosity value, the values of the proportionality coefficients can differ by a factor of three. Figure 7 shows the dependence of the porosity of the deformed layer on the porosity of the fixed layer at different values of the shear stress parameter $\gamma$.
Figure 5. Dependence of the ratio of the characteristic size of the adsorption channel to the grain diameter on the porosity of the granular layer.

Figure 6. Dependence of the proportionality coefficients on the porosity of the granular layer where 1: $\vec{k}$; and 2: $\vec{k}_\perp$.

Figure 7. Dependence of the deformed layer porosity on the fixed layer porosity where $\gamma$ is the shear stress, 1: $\gamma = 2 \times 10^4$ Pa, 2: $\gamma = 5 \times 10^4$ Pa, 3: $\gamma = 1.5 \times 10^5$ Pa, and 4: $\gamma = 2.5 \times 10^5$ Pa.

The proposed mathematical model accurately and reliably describes the experimental data. This makes it possible to recommend it for transfer calculations in granular adsorption layers.

According to the hypothetical prerequisites, the granular layer must have a leveling effect on a stream. Indeed, as pilot studies show, at small speeds, in streams with granular layers of adsorbents possessing a uniformity of layering, essential heterogeneity does not occur, and the field of speeds also remains rather uniform. However, the assumption of saving the hydrodynamic characteristics of a layer in time and space is fair only in the narrow range of loadings on the filtered phase [44]. It is explained by a number of features of granular layers in the adsorptive devices.

The adsorptive layers, compared to, for example, layers of packing nozzles in mass transfer apparatuses, have a higher layer density. In addition, the grains of the materials used as adsorbents have shapes that are not as regular as those of nozzle elements. These circumstances lead to the fact that the role of the wall is influential [45], and the effects caused by the spatial reorientation of grains during a change in loadings in a continuous phase [46] increase.

The mathematical model of the dynamics of a granular layer of adsorbent that takes into account the influence of the mode of a current of a continuous phase through a layer on its hydrodynamic characteristics is given in this work.

The cornerstone of the model submitted here is the approach offered in [47]. As was already noted, the adsorbent grains of which the bulk layers in the adsorptive devices are formed often take a shape that is not spherical. At the same time, the structure of the gas flow can be essentially different in devices with various designs.

If we designate \( P(h) \) as the pressure of the overlying layers of grains upon an underly- ing layer, then the equation describing the distribution of the pressure \( P(h) \) on the height of all the layers of adsorbent can be written down as follows [47]:

\[
P(h) = P_0 + \gamma h - W^2 \int_0^h \xi(P(z); W) \, dz \tag{21}
\]

where \( \gamma \) is the bulk density of non-perturbed by the gas flow packing layer in a static state; and \( \xi \) is the coefficient of the hydrodynamic resistance of the grains, which changes under the influence of the flow of the continuous phase with the rate \( W \) from \( \xi_0 \) for a static layer and \( \xi_d \) for a layer in a dynamic state.

To simplify our further analyses, we consider the grains of the adsorbent to have a rotated ellipsoid appearance with half shafts: (A) big and (B) small (see Figure 8).

Figure 8. (A) big. (B) small. The scheme of a possible arrangement of grains of adsorbent in a layer.
We estimate the characteristic distance \( r_g \) between the grains in a layer by means of a share of the minimum section through passage \( \phi \). For this purpose, we accept the following ratio [47,48]:

\[
\phi = \frac{\varepsilon}{\delta}
\]

(22)

where \( \varepsilon \) is the porosity of a layer; and \( \delta \) is the coefficient of the bend in the microchannels of a layer.

The approach most convenient for practical calculations is that which uses the provided characteristics for the unit of mass of the bulk material of a layer. Then, by finding the specific average surface of the adsorptive layer \( S_{cp} \) per adsorbent unit of mass (measured in \( \text{m}^2/\text{kg} \) and unaffected by dynamic changes in the ratio of (22)), it is possible to obtain the following formula for parameter \( r_g \):

\[
r = \frac{2\varepsilon}{(1 - \varepsilon)p_m S_{cp}}
\]

(23)

where \( p_m \) is the true density of the material of the grains, which is also the invariable characteristic.

Based on the methods and results of transfer work in inhomogeneous media [46] and the hydrodynamic characteristics of a boiling nozzle with elements of a complex configuration [47], in Figure 9, the schedules of the change in the coefficients of hydrodynamic resistance of a layer of adsorbent taking into account the dynamic loads of a layer using only easily determined empirical characteristics,

To simplify the results of our calculations, we express the geometrical characteristics of ellipsoidal grains through the coefficient of their shape \( \phi \).

The coefficient of a shape is determined by the following formula [46]:

\[
\phi = \frac{\pi \left( \frac{3V}{4\pi} \right)^2}{F}
\]

(24)

where \( V \) is the volume of the grains of the adsorbent, in \( \text{m}^3 \); and \( F \) is its surface, in \( \text{m}^2 \).

Taking the shape of the grains as close to spherical, the volume and surface of the grain can be calculated with the help of the following formulas for a revolving ellipsoid with a small amount of eccentricity \( \delta \approx 0 \) [46]:

\[
V = \frac{4}{3} \pi ab^2
\]

(25)
\[ F = 2\pi b^2 + 2\pi ab \frac{\arcsin \delta}{\delta} \approx 2\pi b^2 + 2\pi ab \]  

(26)

Let us consider the known coefficient of a form and the compound radius of the grains as follows:

\[ \overline{R} = \sqrt{ab} \]  

(27)

Then, we obtain the ratio connecting the compound and minimum radius of the grain with the coefficient of its shape:

\[ \frac{2\left(3b^2 / \overline{R}^2\right)}{1 + b^2 / \overline{R}^2} = \phi \]  

(28)

By means of ratios (22)–(24) and (28), it is possible to make a practical calculation of the change in coefficients of hydrodynamic resistance of a layer of adsorbent taking into account the dynamic loads of a layer using only easily defined empirical characteristics, namely: a specific average surface of the adsorptive layer \( S_{cp} \) per adsorbent unit of mass, the true density of the material of the grains \( \rho_m \), and the compound radius of the grains \( \overline{R} \) and coefficient of their form \( \phi \).

The graph of dependence (28) presented in Figure 10 can be used for calculating the characteristic grain radius, and then the hydrodynamic resistance coefficient of the layer can be also calculated.

![Figure 10. Dependence of coefficient of the shape of grains of adsorbent on the geometrical ratio.](image)

For calculating the change in the layer resistance coefficient with increasing loads on the continuous phase, we propose the usage of the model equation in [47]:

\[ \xi = \frac{\xi_{\text{min}}(S + \xi_{\text{min}}) - S \exp(-k\xi_{\text{min}}W^3 / 3)}{S + \xi_{\text{min}}} \]  

(29)

In Figure 11, the characteristic schedules of dependence of the coefficient of resistance of a layer of adsorbent with regard to an increase in flow rate are shown.
Figure 10. Dependence of coefficient of the shape of grains of adsorbent on the geometrical ratio. For calculating the change in the layer resistance coefficient with increasing loads on the continuous phase, we propose the usage of the model equation in [47]:

\[ \xi = \xi_{\text{min}} + \beta + \gamma \exp(-\delta) \]

In Figure 11, the characteristic schedules of dependence of the coefficient of resistance of a layer of adsorbent with regard to an increase in flow rate are shown.

Figure 11. Characteristic schedules of dependence of coefficient of resistance of the adsorptive layer during an increase in loading on the continuous phase. Designations of curves: \( \xi_{\text{st}} - \xi_{\text{min}} = S \): 1—\( S = 1.4 \times 10^2 \); 2—\( S = 1.1 \times 10^2 \); 3—\( S = 0.8 \times 10^2 \); and 4—\( S = 0.5 \times 10^2 \).

Thus, it is possible to offer the submitted approach for use in engineering calculations of the hydrodynamic characteristics of adsorptive layers.

3.3. Modeling of Diffusive Processes in a Layer of Porous Adsorbent

The most effective use of adsorbents can be reached when translating them to a highly dispersed state with a high specific surface of adsorbent per unit of volume of the device. In addition, a high adsorptive activity is also reached via a high specific surface area. It is necessary to take into account the kinetics of physical adsorption [48], diffusion coefficients [49], the dynamics of adsorption processes [50], interphase boundaries between the adsorbent and adsorbate [51] and the fractal characteristics of materials [52]. Analyses of the processes happening on granules of adsorbent and in their layers play an extremely important role in engineering calculations of adsorptive devices. Empirical research can provide answers to many questions for each case, but the development of an evidence-based calculation procedure and the optimum design of adsorbers require theoretical research and the creation of a rather general mathematical model. The problem of adequately describing the heterogeneous environment in an adsorber represents a complex and basic problem, as the modeling of the processes of transfer in heterogeneous environments significantly differs from the modeling of homogeneous environments. When modeling, the adsorptive device’s approach, in which the environment of the reacting substances is described as quasi-homogeneous, is widespread. However, the area of applicability of the quasi-homogeneous model is limited mainly to isothermal systems and catalysts with a small adsorptive resistance.

The scope of applicability of the quasi-homogeneous model is limited to cases of small drops in the temperature and concentration of the adsorbed substance along the surface of the adsorbent grains. The specific values of these characteristics are determined at given physical and chemical parameters of the interacting media. In this work, a general theoretical description of heat and mass transfer processes in a porous adsorbent granule in a layer is provided, subject to the applicability of a quasi-homogeneous model.

The mathematical model of the internal diffusion in the adsorbent layer consisting of porous grains reads as follows:
We write down the equation of a mass transfer taking into account a possible chemical source of weight $I(c, t)$ [51]:

$$\frac{\partial c}{\partial t} = D_{\text{eff}} \Delta c + I(c, t)$$

(30)

where $c$: the concentration of the substance, in kg/m^3; $D_{\text{eff}}$: the effective coefficient of diffusion, in m^2/cm; and $t$: the time of the process, in s.

The equation of the transfer of heat in grain is as follows [50]:

$$C_p \frac{\partial T}{\partial t} = \lambda_{\text{eff}} \Delta T - q_r I(c, t)$$

(31)

where $T$: the temperature, in K; $C_p$: the adsorbent thermal capacity; $q_r$: the thermal effect in case of adsorption; and $\lambda_{\text{eff}}$: the effective coefficient of heat conductivity.

We determine the chemical source of the weight in the form of Arrhenius as follows [48,50]:

$$I(c, t) = -kc \exp\left(-\frac{E}{RT}\right)$$

(32)

where $E$: the energy of activation; and $k$: a constant.

Let us consider the particle form coefficient $\varphi$. Then the operating equations of the process can be written down as follows:

$$\frac{\partial c}{\partial t} = D_{\text{eff}} \left(\frac{\partial^2 c}{\partial r^2} + \frac{\varphi}{r} \frac{\partial c}{\partial r}\right) - kc \exp\left(-\frac{E}{RT}\right)$$

(33)

$$C_p \frac{\partial T}{\partial t} = \lambda_{\text{eff}} \left(\frac{\partial^2 T}{\partial r^2} + \frac{\varphi}{r} \frac{\partial T}{\partial r}\right) - q_r kc \exp\left(-\frac{E}{RT}\right)$$

(34)

where $r$ is the direction along the grain radius.

The boundary conditions for the process of the transfer of heat and weight on a surface of a granule are relevant (here $r$: the characteristic radius of a granule):

$$\beta (c_S - c) = D_{\text{eff}} \frac{\partial c}{\partial r}, \quad a(T_S - T) = \lambda_{\text{eff}} \frac{\partial T}{\partial r}$$

(35)

$$r = 0: \quad \frac{\partial c}{\partial r} = \frac{\partial T}{\partial r} = 0$$

(36)

where $\beta$: the coefficient of a mass transfer, in m/s; $a$: the heat emission coefficient; and $c_S$ and $T_S$: the concentration and temperature on a granule surface, respectively. Let us use the dimensionless variables and criteria offered in [52] as follows:

$$z = r/R, \quad y = c_S/c, \quad \gamma = \frac{E}{RT_S}, \quad \theta = \frac{T - T_S}{T_S}, \quad \delta = \frac{q_r c_S D_{\text{eff}}}{\lambda_{\text{eff}} T_S}, \quad \phi = R \sqrt{\frac{k}{D_{\text{eff}}}}, \quad \tau = \frac{t \lambda_{\text{eff}}}{C_p R \tau}$$

(37)

$$Sh = \frac{\beta R}{D_{\text{eff}}}, \quad Nu = \frac{a R}{\lambda_{\text{eff}}}, \quad Le = \frac{\lambda_{\text{eff}}}{C_p D_{\text{eff}}}$$

(38)

The system of the equations of a mathematical model in a dimensionless form takes the following form:

$$Le \frac{\partial y}{\partial t} = \frac{\partial^2 y}{\partial z^2} + \phi \frac{\partial y}{z} - \phi^2 y \exp\left(\frac{\theta}{1 + \theta / \gamma}\right)$$

(39)

$$\frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial z^2} + \frac{\theta}{z} + \gamma \phi^2 y \exp\left(\frac{\theta}{1 + \theta / \gamma}\right)$$

(40)
The system of boundary conditions at the same time is transformed to the following:

\[ z = 1: \ 1 - y = \frac{1}{Sh} \frac{\partial y}{\partial z}, \ \theta = -\frac{1}{Nu} \frac{\partial \theta}{\partial z} \]  

\[ z = 0: \ \frac{\partial y}{\partial z} = \frac{\partial \theta}{\partial z} = 0 \]  

In the stationary mode of the course of the process between key parameters, the following connection is established:

\[ \theta = \gamma \delta (1 - y) \]  

Expression (43) is a dimensionless type using the formula of Prater [52].

For the completeness of the submitted mathematical model, an evaluation of the effective heat and mass transfer coefficients is given.

An assessment of the size of the coefficient of internal diffusion can be given in the form of [49,51] as follows:

\[ D_{\text{eff}} \approx \frac{R^2}{4t_c} \approx \frac{R \langle V \rangle}{4} \]  

where \( t_c \): the characteristic time of internal diffusion, in s; \( \langle V \rangle = \sqrt{\frac{8k_BT}{m}} \): the average speed of the thermal motion of the molecules; \( k_B \): Boltzmann’s constant; and \( m \): the molecular weight.

An assessment of the effective coefficient of heat conductivity can be given with the help of Lewis’s number \( Le \) [51] as follows:

\[ \lambda_{\text{eff}} = Le \cdot C_p \cdot D_{\text{eff}} \]  

As the characteristic time of internal diffusion, we use the relaxation time, i.e., the time to reach the state saturation of the internal surface of the adsorbent with the adsorbed component. It can be assumed that the achievement of such a state of saturation is completed when the characteristic distance between the vacant active centers of the surface of the adsorbent granule becomes of the order of the path length of the adsorbate molecules at the process temperature. At this moment, the degree of the coverage of the adsorption surface satisfies the following relation [51,52]:

\[ l \approx \frac{a}{K_m (1 - \omega)^2} \]  

where \( a \): the average distance between the active centers of a surface of the catalyst; and \( K_m \): an empirical constant.

Communication between the entered parameters characterizing the microscopic structure of a granule and the macroscopic characteristics determined empirically can be received by means of an assessment of the Knudsen number using the following formula:

\[ \text{Kn} \approx \frac{1}{K_m (1 - \omega)^2} \]  

Thus, we obtain a closed mathematical model of the process of mass and heat transfer in a porous granule of adsorbent that connects all the main managing process parameters and considers the real structure of a granule.

Upon the transition to all the layers of the adsorbent in the tubular-type device, the system for solving equations takes the following form:

\[ D_{\text{eff}} \Delta C - (V, \nabla C) = \beta S_{cp} (C - C_s) \]  

where

- \( D_{\text{eff}} \): effective diffusion coefficient;
- \( V \): velocity;
- \( \nabla C \): gradient of concentration;
- \( S_{cp} \): surface area per unit mass; and
- \( C, C_s \): concentration in the adsorbent and in the adsorbed state, respectively.
\[ a \Delta T - C_p(V, \nabla T) + hS_{cp}(T_S - T) = \frac{4kT(T_W - T)}{D} \]  

(49)

where \( S_{cp} \): the specific surface of adsorbent in unit of volume, in \( \text{m}^2 \); \( C \): the concentration of the main component, in \( \text{kg/m}^3 \); \( D_e \): the effective coefficient of diffusion, in \( \text{m}^2/\text{s} \); \( V \): the speed of mix, in \( \text{m/s} \); \( C_P \): the mix’s thermal capacity; \( h \): the specific enthalpy; \( \beta \): the coefficient of a mass transfer, in \( \text{m/s} \); and \( a \): the heat diffusivity coefficient.

The system of the equations for the balance of heat and weight on the surface of the adsorbent has the following form:

\[ aqS_{cp}(C_s - C) + k\exp\left(\frac{E}{RT_s}\right)C_s = 0 \]  

(50)

\[ hS_{cp}(T_s - T) + k\exp\left(\frac{E}{RT_s}\right)C_s\Delta H = 0 \]  

(51)

where \( E \): the Arrhenius constant; \( \Delta H \): the warmth of adsorption; and \( a \): the heat diffusivity coefficient.

For an adsorbent layer in a tubular-type device, the system for solving dimensionless equations has the following form:

\[ \frac{1}{Pe_1}\Delta X - \nabla X + Q_1(X_S - X) = 0; \]  

(52)

\[ \frac{1}{Pe_2}\Delta \tau - \nabla \tau + Q_2(\tau_S - \tau) - \beta(\tau - \tau_W) = 0; \]  

(53)

\[ Q_1(X_S - X) - Da(1 - X_S)\exp\left(\frac{\tau_S}{1 + \tau_S \gamma}\right) = 0; \]  

(54)

\[ Q_2(\tau_S - \tau) - \Delta \tau_{ad}Da(1 - X_S)\exp\left(\frac{\tau_S}{1 + \tau_S \gamma}\right) = 0 \]  

(55)

The generalized operating parameter of the model is a Damkeler number [51]:

\[ Da = \frac{Le_{cat}}{V} \exp\left(-\frac{E}{RT}\right) \]  

(56)

where \( L \): the characteristic size of the adsorptive layer; and \( \epsilon_{cat} \): the specific surface of the porous adsorbent.

For the short circuit, the model has to be added to the equations for the condition of a surface of granules of adsorbent.

According to Polyani’s theory [50], for practically any mechanism of adsorption, it is possible to write the following ratio:

\[ \frac{X}{m} = V_a(\rho_a - \rho_g) = \sigma h(\rho_a - \rho_g) = \sigma V \]  

(57)

where \( X/m \): the mass of the adsorbed substance in grams on one gram of adsorbent; \( V_a \): the volume of the area which is in an area of coverage of superficial forces, in \( \text{m}^3 \); \( \rho_a \): the average volume density of an adsorbate, in \( \text{kg/m}^3 \); \( \rho_g \): the density of a continuous phase, in \( \text{kg/m}^3 \); and \( \sigma \): the specific active surface of the adsorptive layer, in \( \text{m}^2 \).

The chemical potentials of the adsorbent granule surfaces in the approximation of equilibrium thermodynamics can be written as follows:

\[ \mu_S - \mu = \int_{\infty}^{s} \left( V \frac{dP}{dz} + \frac{dG}{dz} \right) = 0 \]  

(58)

where \( G \): the potential of superficial forces.
As a result, we obtain the mathematical expression of the generalized mechanism of adsorption according to Polyani’s theory in the following form:

\[
\frac{X}{m} = V_a (\bar{\rho}_a - \rho_g) = V_a \left[ \int_0^\infty \rho_a f(G) dG - \rho_g \right]
\]  

(59)

where \( f(G) \): the corresponding function of the distribution of the superficial potential.

In Figure 12, the calculation of the coefficient of the internal diffusion is presented.

![Figure 12](image)

**Figure 12.** Dependence of coefficient of internal diffusion on grain radius. Designations of curves: \( \varphi \): coefficient forms (1: \( \varphi = 0.168 \); 2: \( \varphi = 0.318 \); 3: \( \varphi = 0.450 \); and 4: \( \varphi = 0.6 \)).

Figure 13 depicts the results of calculating the mass transfer coefficients in the solid phase. The Sherwood numbers, which are included as parameters in the model for the boundary conditions, are also presented.

In Figure 14, the dependence of the coefficient of a mass transfer in the liquid phase on the porosity calculated through the boundary condition (35) by definition \( \frac{dC}{dr} \) using the equations model (38) is shown.

The obtained system represents the complete mathematical model of a non-adiabatic absorber. It can be used in the practice of engineering calculations after the specification of the main control parameters. Unlike other known models, it requires minimal empirical information for its application, which makes the submitted equations especially useful when designing technological schemes and devices for new engineering procedures. Using the proposed mathematical model, it is possible to simulate adsorption with a fixed layer of adsorbent in the liquid phase. Adsorbents in the form of granules, for example, activated carbon, can be used.
Figure 12. Dependence of coefficient of internal diffusion on grain radius. Designations of curves: \( \phi = 0.168 \); \( \phi = 0.318 \); \( \phi = 0.450 \); and \( \phi = 0.6 \).

Figure 13. Dependence of coefficients of a mass transfer in a firm phase on the coefficient of internal diffusion. Designations of curves: diameter of particles of adsorbent of 1: 1 mm; 2: 1.5 mm; and 3: 2 mm. Dotted line: calculation via Sherwood number.

Figure 14. Dependence of coefficient of a mass transfer in the liquid phase on the porosity. Designations of curves: 1: diameter of particles of adsorbent 1 of mm; 2: 1.5 mm; 3: 2 mm; and 4: 2.5 mm.
4. Conclusions

The design of an adsorber with a fixed layer of adsorbent was developed and makes it possible to increase the efficiency of the apparatus, increase the utilization rate of the useful volume of the apparatus and the degree of processing of the adsorption capacity of the adsorbent in the layer, increase the stability of the purified stream quality with the maximum compactness of the apparatus, and reduce the formation of stagnant and unused zones.

An equation is proposed that describes the change in the porosity of a granular layer when water flows through it.

An equation is proposed for estimating the porosity of the layer, taking into account the average radius of the cluster, the fractal dimension of the cluster structure and the anisotropy index of the adsorbent layer. An equation that makes it possible to calculate the change in the porosity of the layer in comparison to the porosity of the stationary stacking was obtained. Based on the revealed adsorption mechanism in the adsorption layer, expressions for the proportionality coefficients were obtained, depending on the structure of the granular layer, proceeding from the tetrahedral packing of the grains in the layer.

An equation for the calculation of the characteristic distance between grains laying in a layer by means of a share of the minimum section through the passage and the influence of the mode of a current of a continuous phase through a layer regarding its obtained hydrodynamic characteristics is proposed.

The ratio connecting the compound and minimum radius of grain with the coefficient of its form was obtained. By means of this equation, it is possible to conduct practical calculations of the change in the coefficients of the hydrodynamic resistance of a layer of adsorbent, taking into account the dynamic loads of a layer, using only easily defined empirical characteristics, namely, the specific average surface of the adsorptive layer per adsorbent unit of mass, the true firmness of the grain material and the compound radius of the grains and coefficient of the form.

The steering equations, taking into account the coefficient of the shape of a particle of adsorbent, the coefficients of mass transfer and internal diffusion, the influencing characteristic parameters of the process and the granules reflecting its real structure are shown.

A communication assessment between the entered parameters characterizing the microscopic structure of a granule and the macroscopic characteristics determined empirically via an analysis of the Knudsen number is given.

Using the proposed model, the main characteristics of the adsorption process were calculated, on the basis of which the design parameters of the adsorber were calculated. The results of this work were involved in the production of InnovTechProduct LLP.

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Abbreviations

\( a \) thermal diffusivity coefficient, \( \text{m}^2/\text{s} \);
\( a_g \) the characteristic size of the attached particle (adsorbent grain), \( \text{m} \);
\( c_{\infty} \) impurity concentration in the flow core, \( \text{mol/m}^3 \);
\( C \) concentration of the substance, \( \text{kg/m}^3 \);
\( C_p \) the heat capacity of the adsorbent material, \( \text{J/C} \);
\( c_s \) concentration on the surface of the granule, \( \text{kg/m}^2 \);
\( D_f \) fractal dimension of the cluster structure;
\( D_l \) diffusion coefficient for the liquid phase, \( \text{m}^2/\text{s} \);
\( D_T \) diffusion coefficient for the solid phase, \( \text{m}^2/\text{s} \);
\( D_n \) grain diameter, \( \text{m} \);
\( D_{\text{eff}} \) effective diffusion coefficient, \( \text{m}^2/\text{s} \);
\( d \) grain diameter, \( \text{m} \);
\( d_{ef} \) the characteristic size of the filtration channel, \( \text{m} \);
\( E \) Arrhenius constant;
\( F \) surface, \( \text{m}^2 \);
\( G'/y \) amount of residue on the sieve, \( \text{kg} \);
\( G_y \) amount of coal weighed, \( \text{kg} \);
\( q \) coefficient of curvature of the microchannels of the layer;
\( q_r \) thermal effect of the reaction, \( \text{J/kg K} \);
\( h \) specific enthalpy;
\( K_{ij} \) cluster mobility, \( \text{m}^3/\text{s} \);
\( k_{\text{\textcircled{\textit{\textdegree}g}}} \) and \( k_{\text{\textcircled{\textit{\textdegree}L}}} \) coefficients of proportionality depending on the structure of the granular layer;
\( k_e \) empirical coefficient;
\( k_B \) Boltzmann constant;
\( k \) constant;
\( k_m \) empirical constant;
\( M \) the molecular weight of the solvent;
\( m \) molecular weight, \( \text{kg} \);
\( L \) characteristic size of the adsorption layer, \( \text{m} \);
\( N \) the number of particles;
\( N^\gamma \) the number of particles depending on the characteristic length;
\( N^{1/D_f} \) the number of particles in the cluster;
\( n(t) \) density of \( k \) particle clusters, \( 1/\text{m}^3 \);
\( P_m \) the probability of a particle attaching to the cluster "protrusion";
\( P \) carrier pressure in the granular layer, \( \text{Pa} \);
\( \bar{r}_N \) average cluster radius, \( \text{m} \);
\( r_g \) characteristic distance between grains, \( \text{m} \);
\( R \) cluster radius, \( \text{m} \);
\( r \) grain radius, \( \text{m} \);
\( S_{cp} \) specific surface area of the adsorbent per unit volume, \( \text{m}^2 \);
\( S \) cross-sectional area of the apparatus, \( \text{m}^2 \);
\( T \) temperature, \( \text{K} \);
\( t \) process time, \( \text{s} \);
\( T_s \) the temperature on the surface of the granule, \( \text{K} \);
\( V_0 \) reduced velocity of the main flow of the carrier, \( \text{m/s} \);
\( v \) flow rate, \( \text{m/s} \);
\( W \) flow velocity, \( \text{m/s} \);
\( X \) parameter that takes into account the association of molecules in the solvent;
\( \gamma' \) mass of adsorbed substance, \( \text{kg/kg} \);
\( \Delta H \) heat of adsorption, \( \text{J/mol} \);
\( \beta_e \) external mass transfer coefficient, \( \text{m/s} \);
\( \beta_i \) internal mass transfer coefficient \( \text{m/s} \);
\( \gamma \) shear stress, \( \text{Pa} \);
\( \gamma \) bulk density of the undisturbed packing in a static state, \( \text{kg/m}^3 \);
\( \sigma \) specific active surface of the adsorption layer, \( \text{m}^2 \);
\( \delta \) an indicator that depends on the characteristic length;
\( \varepsilon \) porosity; 
\( \varepsilon_0 \) fixed stacking porosity; 
\( \zeta \) coefficient of hydrodynamic resistance; 
\( \zeta_g \) coefficient of resistance of the granular layer; 
\( c \) concentration, mol/m³; 
\( \lambda \) thermal conductivity coefficient, J·m/K·m²·s⁻¹; 
\( \lambda_{\text{eff}} \) effective thermal conductivity coefficient, J·m/K·m²·s⁻¹; 
\( \mu \) coefficient of dynamic viscosity of the carrier flow, Pa·s⁻¹; 
\( \mu_l \) viscosity for the liquid phase, Pa·s⁻¹; 
\( \rho_l \) density for the liquid phase, kg/m³; 
\( \rho_m \) true density of the grain material, kg/m³; 
\( \rho_a \) average volume density of adsorbate, kg/m³; 
\( \nu_k \) kinematic viscosity, m²/s; 
\( \rho \) carrier pressure in the granular layer, Pa; 
\( \psi \) core width, m; 
\( \chi \) anisotropy index of the adsorbent layer;

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