

On the Influence of the Energy Field of the Pores in Solid on Its Filling with Gases and Peculiarities in the Condensation Process

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Abstract In the work is investigated the totality of processes when gas filling the pore in solids taking into account the availability of energy fields, which have a decisive influence on the ingress of gas molecules inside the pores. Dependence of filling the pores of the parameters characterizing the energy field is obtained, and shows the presence on it of the extremes, that makes more understandable ways of selecting porous bodies with the desired adsorption capacity in relation to this gas. It is shown that the density of the gas in the pore can be, depending on its radius, smaller and significantly exceeds the density of the gas in the outer scope. Where obtained the isotherms of filling the single pore with gas, taking into account the possibility of condensation in the internal volume, and therefore, having all of the elements, often observed in experimental dependencies. Is studied the influence of the energy field of the pores on the form isotherms filling and parameters of the condensation transition, and shown that it can both facilitate and impede the process of condensation in the pore, i.e. to shift its beginning as in the area of lower and higher external pressures.

Keyword Pore, Energy Field, Gas Filling, Condensation In Pore

1. Introduction

Heterogeneous system porous body – gas is a crucial element in a wide range of industrially significant processes, resulting in a constant quest for understanding of its operation. One of the major tasks carried out in the process of understanding this system, is the determination of the number of gas molecules located in the internal volume the pore of solid. The solution to this problem today is formulated on the basis of the work carried out by M.M. Dubinin and L. W. Raduškevič in 30-40 years of the last

century. The isotherm hat the name of the authors. On the Internet under address [1] is its conclusion and final appearance in the form of

$$W = W_0 \exp[-k(RT \ln(P/P_0))^2] \quad (1)$$

where: W_0 -total volume of micro pores, W - the volume, filled under pressure of P , P_0 - is the saturated pressure of gas, k - a constant, depending on the nature of adsorbats and adsorbents. Some modification of this dependence, the introduction in it of more constants, the authors conducted in [2].

If you apply an expression (1) to determine the degree of gas filling (W/W_0) a single pore, it is clear that it must be a constant, not dependent on geometry described by the pores and not changing as you move from one to the other with her unequal. Characteristics of pores per se are not in the equation that defines the W/W_0 . It is clear that such a claim may not be a general law, because its adoption would be inexplicable to many experimental facts, obtained for the system of gas-porous solid. However, for the task of this work more interesting is another moment of equation (1). In the papers [3]-[4] was shown that the pores of the solid body have energy and force fields and applies the technique of their descriptions. Based on the results of this work it was evident that described in these fields will have some impact on filling the pores with gases and the peculiarities of the process of condensation. Equation (1) and its subsequent modifications (for example, see [2]) do not take into account the availability of energy and force fields by pores of solid. The latter allows us to put before this work of the task of determining the number of gas molecules in the pore, taking into account the availability of energy field that influences both the filling of the internal volume with the gas, and especially its condensation in this volume.

2. Methodology Field

3.4 angstrom, i.e. $d_L = 0.34$ nm. Within each plane carbon atoms arranged at the vertices of regular hexagons such that the distance between the nearest atoms is 0.145 nm. With this information can be shown that the density of carbon atoms at the atomic line, modeling this plane, is equal to $4.6 \cdot 10^9 \text{ m}^{-1}$. Assume that when introducing the cylindrical pores with set of atomic rings, the density of the atoms is equal to the value obtained above, i.e. ρ in equation (5) is $4.6 \cdot 10^9 \text{ m}^{-1}$. Pore radius R_p will equal to 0.85 nm, i.e., its diameter will be five times greater than the distance between atomic planes of graphite.

The value of ε , defines the interaction between the carbon and oxygen atoms (C-O), is given in the Internet under the address [6] and it is equal 0.173 kcal/mol. We assume that our system coincides with this, and we will use this data. Transfer calories in Joules and dividing the result by the number of particles in one mole, we obtain that for one pair of interacting particles ε is equal to $1.20698 \cdot 10^{-21}$ J. Magnitude of parameter r_0 , also needed to determine interactions between the carbon and oxygen atoms, in [6] is not given, but shows the value of the minimum distance to the potential energy curve, and it is equal to 3.6 angstrom or 0.36 nm. Can be shown, that by dividing this value of the 1.12246, we get the desired value, i.e. r_0 for a system C-O is equal 0.320724 nm.

With this information, you can go to the calculation of the energy of interaction in a system using equation (5). This energy being defined by the equation, as noted above, is a function of two variables, x and R_0 . Having the dependence between E and x with R_0 , you can connect the dots with the same energy, by so-called equipotential lines, receiving thus the vivid picture of the energy field of the pores. To perform this data treatment, we used the "Maple" and "Mathematica" software. The coordinates of the points for the original definition of energy on the equipotential lines are selected in such a way that they are relatively evenly distributed between the walls of the pores. The values of these coordinates and the corresponding energy are given in the table below. Built with its help the picture lines are presented in Figure 2. From close to the outer form of the picture received in [4], it is different in that each line represents a specific value of the energy, while in [4] when building the picture is taken from the absolute value of the logarithm E , which naturally increased the possible interpretations of individual elements of the painting.

Table 1. Coordinates of the selected points in the cross section of the pores and the corresponding energy

x, nm	y, nm	E, J	x, nm	y, nm	E, J
0	0	$-6.74 \cdot 10^{-22}$	0	0.7	$2.55 \cdot 10^{-17}$
0	0.1	$-7.41 \cdot 10^{-22}$	0	0.75	$2.16 \cdot 10^{-15}$
0	0.2	$-9.84 \cdot 10^{-22}$	0	0.8	$4.29 \cdot 10^{-12}$
0	0.3	$-1.58 \cdot 10^{-21}$	0	0.82	$1.17 \cdot 10^{-9}$
0	0.4	$-3.03 \cdot 10^{-21}$	0	0.83	$1 \cdot 10^{-7}$
0	0.5	$-5.9 \cdot 10^{-21}$	0.4	0	$-2.8 \cdot 10^{-22}$
0	0.6	$6.43 \cdot 10^{-20}$	0.8	0	$-7.55 \cdot 10^{-23}$
0	0.65	$1.03 \cdot 10^{-18}$	-4	0	$-1 \cdot 10^{-21}$

Point 0 to the horizontal axis correspond to the beginning of pore, and point - 6.8 nm — its end. Through the zero on the vertical axis is the central axis of the pores, the radius of which, as noted above, is equal to 0.85 nm, i.e. presented in figure painting includes a cross section of internal volume of the pores with forming its atomic rings, and some of the adjoining external spaces. The situation of atomic rings is represented in Figure visually bright circles in a dark Halo while lines. You can see that equipotential lines, perpendicular to the walls of the pores, available only at the input and at the output from it. Virtually all internal volume is covered by its parallels to the walls. Last, obviously, means that in the space of only changes the energy along the coordinates of R_0 , remaining constant over the length of the pores, i.e. on x . Changing the energy status of the probe gas molecules moving in a straight line passing through the parallel port and the x axis will only take place at the beginning of pore and its end.

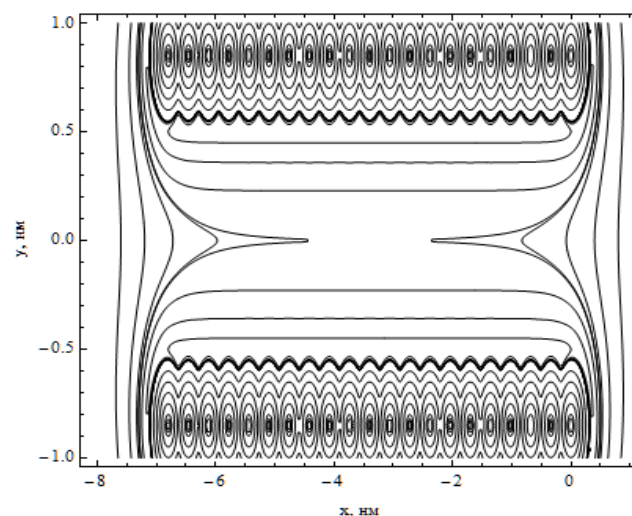


Figure 2. Equipotential lines in the axial section of the pores. Calculated using equation (5) in case of: $\rho = 4.6 \cdot 10^9 \text{ m}^{-1}$, $\varepsilon = 1.2 \cdot 10^{-21}$ J, $N_L = 21$, $r_0 = 0.33$ nm, $d_L = 0.34$ nm, $R_p = 0.85$ nm.

An interesting element of Figure 2 is a dark stripe that limits the space adjacent to the walls of the pores, from central region. This band exists and in the figures cited in the paper [4] with equipotential lines from the log of the absolute value of the energy for cylindrical pores. When it was discussed in [4] shows that in this band is changing the sign energy E at positive to negative value, from the walls of the pores, resulting in her is line with E equal zero. It can be shown that this is true including for paintings, presented in Figure 2, when each equipotential line corresponds to a specific value of energy. Coordinates of dark stripes is regulated by the parameter r_0 . Visually, it will bet occur only if its value is less than the radius measured pore R_p . With very small values of r_0 it practically coincides with the wall and the field of pores around the internal volume becomes negative value. If r_0 is slightly larger of radius pores, the band worked out of its internal volume, and it all turns out to be overridden field with positive values.

4. Methodology Filling

Having a method of approach to the description of the energy field of the pores in solid and some idea of its configuration, you can proceed to the analysis of the influence of the energy field to fill the pores of gas. For this, as a first step we will confine ourselves to a single at pores, that it represents a small amount of V_p , located in the outer volume V that contains gas under pressure P . With these assumptions, it is easy to find the number of molecules of gas in pore N_p . For that we write equation of State for gas in the pore

$$P_p (V_p - N_p V_m) = N_p k_B T \quad (6)$$

where k_B is the Boltzmann constant, T is the temperature, V_m - volume of gas molecules, P_p is the pressure in the volume of pores also proposed to take into account. In [3] the relationship between pore pressure P_p and external pressure P is given in form

$$P_p = P \cdot \text{Exp}\left(-\frac{E}{k_B T}\right) \quad (7)$$

where E is the potential energy of the gas molecules in pores. On the basis of (6) and (7) to determine N_p the following dependence

$$N_p = \frac{P \cdot \text{Exp}\left(-\frac{E}{k_B T}\right) \cdot V_p}{k_B T + P \cdot \text{Exp}\left(-\frac{E}{k_B T}\right) \cdot V_m} \quad (8)$$

that would be correct if E is in a value of the pores the constant. If $E = 0$, the equation (8) will constitute another form of State equation of gas in pore (6), assuming equal pressure in pore P_p and in an external volume P . Difference expression describing the gas filling the pores of expression applicable for small volume, would be that E in (8) as shown above, is not equal to zero, i.e. the N_p for the pores must take into account the interactions between gas molecules and atoms, forming a solid body.

Based on the earlier said it is clear that E not just is not zero, it changes in the volume of the pores until it sign. To address this problem, you must bind to port reference system that is most simply done by returning to the scheme presented in Figure 1. We mentally select inside the pores on distance x from the beginning the rectangular ring with internal radius R_0 , thick dR_0 and height dx . We assume that E inside of the ring is constant and equal to $E(x, R_0)$. Then for gas molecules inside this ring, you can use the equation (8) and it will have the form

$$dN_p = \frac{P \cdot \text{Exp}\left(-\frac{E}{k_B T}\right) 2\pi \cdot R_0 dx dR_0}{k_B T + P \cdot \text{Exp}\left(-\frac{E}{k_B T}\right) \cdot V_m} \quad (9)$$

To find the total number of molecules in a pore it is necessary to integrate equation (9) in the R_0 from 0 to pore radius R_p and in x from zero to the length of pore L_p . Finally we have

$$N_p = \int_0^{L_p} \int_0^{R_p} \frac{P \cdot \text{Exp}\left(-\frac{E}{k_B T}\right) 2\pi \cdot R_0}{k_B T + P \cdot \text{Exp}\left(-\frac{E}{k_B T}\right) \cdot V_m} dx dR_0 \quad (10)$$

Equation (10) is an isotherm of filling the pore with gas. If the molecules do not interact with the atoms forming a solid pore ($E = 0$), then it takes the view

$$N_p = \frac{P}{k_B T + P V_m} \int_0^{L_p} \int_0^{R_p} 2\pi R_0 dx dR_0 \quad (11)$$

which, when you consider that the double integral on the right-hand side is equal to the volume of the pores, coincides with the State gas equation (6). Last, obviously means that equation (10) are comes off from the generally accepted methods of physics solving such problems and, by all accounts, this interconnectedness must exist for any attempt to determine the amount of gas in the pore volume in solid.

5. Results and Discussion Filling

In the general case E in (10) is non-zero and should be calculated on (5). Interesting to see how changing the settings for the interaction energy of gas molecules with solid atoms forming a pore (ε and r_0) affect their filling with gas. The number of molecules in a pore is defined by equation (10). In analytical form last addition, after the insert into the function $E(x, R_0)$ is analytical not integrated, so the calculation was carried out with numerical method. Posed by persistent included in the integral functions of the equation (10) including r_0 , then conducted numerical integration and turned out the corresponding r_0 value N_p , i.e. one point on the graph. Then change the value of r_0 , and the procedure repeated. Received N_p under parameters, used in the calculation of the results presented in Figure 2, because of the smallness of its volumes, are less than one. To avoid this, all received values multiplied by 100, which is equivalent to a corresponding increase in the length of the pores.

Four curves are constructed in this way are given in Figure 3. You can see that at low ε filling pores are practically does not depend on r_0 , slope of the curve (1) for x is small, and it becomes zero if take that $\varepsilon = 0$. With the growth of ε this slope is increased, and the point of intersection with the x -axis of the settlement curve is shifted to the value of the radius of the pores (curve 2). When large enough of ε to stabilize the position on the value that is slightly larger R_p (curve 3). Further increase of ε leads to the formation and growth of the maximum fill the pores of the gas, which

coordinate is somewhat smaller as pores radius (curve 4). Clearly, that such a development based on the number of molecules of gas in the pore from its interaction energy parameters with atoms, forming a solid body, can have practical significance. An understanding of the reasons for selective absorption of certain porous solids of gases, and as a result, the possibility of purposeful formation of such bodies.

To understand the dependence of filling the pores of gas from r_0 and ϵ can be, if we consider the main features of the Lennard-Jones potential, the underlying output equation (5). With increasing r_0 all large part of the pores, adjacent to the walls will be covered of area with positive energies (Fig. 2), and, as a result, is difficult for the gas molecules. This will decrease the number of gas molecules absorbed in this pore. In the area of small r_0 this decrease has been observed in all the curves in figure 3. When r_0 few more R_p and sufficiently large value of ϵ area of positive energy will be cut off all the cross-section of the pores, making it practically inaccessible for a given gas, i.e. filling becomes zero (curve 3 and 4). When greater value of ϵ on the analyzed dependencies before exiting to zero, there is maximum (curve 4). It is connected with the presence of mechanisms, neutralizing the effect of the marked reduction of the effective volume of pores with the growth of r_0 . In the permitted space, adjacent to the central axis of the pores, the value of E is negative. With increasing ϵ (r_0) these values rise, which will increase the N_p in this part of the internal volume of pores. The interaction of these two opposite tendencies generates a maximum on the curve of filling the pores of the gas on the parameters of his interaction energy with atoms of the corresponding solid body (curve 4). Clearly, if the task is to increase the absorption capacity of the porous body with respect to this gas, its material should be collected so as to parameters of the energy interaction corresponded to the points that lying in the region of the maximum on the curve 4.

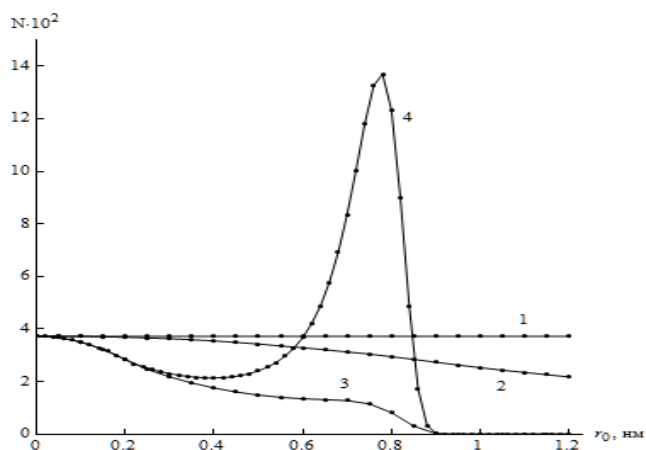


Figure 3. The dependence of the number of molecules of gas in the pore of parameters defining their energetic interaction with atoms of the solid. All curves are designed to (10): $k_B = 1.38 \cdot 10^{-23}$ J/grad, $T = 300$ K, $R_p = 0.85$ nm, $P = 10000$ Pa, $V_m = 1 \cdot 10^{-29}$ m³, $d_L = 0.34$ nm, $L_p = 6.8$ nm, $\rho = 4.6 \cdot 10^9$ m⁻¹; 1- $\epsilon = 0$; 2- $\epsilon = 1 \cdot 10^{-30}$ J; 3- $\epsilon = 1 \cdot 10^{-22}$ J; 4- $\epsilon = 2.3 \cdot 10^{-22}$ J.

Isotherm fill the pores of the gas in the form (10), together

with equation (5), which determines the E , lead to a new problem for the system and allow to solve this problem. If a solid body has pores of different radius, then, proceeding from the foregoing, it can be expected that the density of the gas in them will be different. Under certain conditions in the pores with radius is not much different from r_0 to in this system, the density of gas must be higher its density in the surrounding space. Define the density of the gas ρ in pores with different radius. The corresponding equation has the following form

$$\rho = \frac{N_p}{V_p} = \frac{N_p}{\pi R_p^2 L_p} \quad (12)$$

where N_p shall be determined by equation (10). It is clear that R_p is present in the equation (12), not only in the denominator of a fraction, but is also in the integral expression that sets the value of a function N_p in its numerator. The last has a determining impact on the nature of addition.

The calculation was made by the numerical method. Posed by persistent included in the integral functions of the equation (12) including the R_p , then conducted numerical integration and turned out the corresponding value of R_p and ρ , i.e. one point on the graph. After that changed the value of the R_p and the procedure was repeated. This yielded one curve on the graph of the dependence of ρ from R_p at the accepted values of r_0 and ϵ . Changing the past and repeats all steps, received a new curve, corresponding to the new values of these parameters. Figure 4 shows the three curves, which value r_0 the same and equal to 5 nm, ϵ values increase with increasing numbers of the curve. You can see that at low ϵ (curve 1) density of the gas in the pore volume is independent of its radius, while remaining constant when you change its value. It seems obvious that such a character ρ from R_p for an absences interactions between gas molecules and atoms, forming a solid body ($\epsilon \rightarrow 0$) is how existing notions and, apparently, objective reality. At low or zero ϵ , in this model, there is no natural cause which could lead to a change in pore gas density when its radius changed.

With only a slight increase ϵ , i.e. presence, but fairly weak interaction between gas molecules and the atoms of a solid body, the density of the gas in the pores with a radius smaller than r_0 is equal to zero (curve 2), and only for the pores with $R_p > r_0$ it is different from zero and increases with their radius, approaching as to asymptote from the bottom of the curve 1, i.e. the density of the gas in the outer scope. With greater ϵ on the investigated dependence, there is maximum (curve 3), i.e. the density of the gas is the most significant in the pores with R_p few more r_0 . With further increase of R_p density decreases asymptotically approaching a curve 1 and is already on the top side, i.e. it is always more than the density in the outer scope.

With large radiuses of all options changes ρ the density value in the pores when there are no interactions between gas molecules and atoms in a solid. It is clear that such a limit transition is physically justified, since, according to (5), E

with the increase of R_p will decrease.

If the external volume of the surrounding porous body has two gas with different values of r_0 and ε , their density in the pores, under certain conditions, will be submitted to the two curves of type 3 curve in Figure 4, but with different positions on the axis of high R_p (Fig. 5). From Figure 5, the gas composition in the pores of varying radius will vary, and, naturally, it will be different from the composition of the gas into the surrounding porous body. It can be seen that, in the absence of this porous body pore with radius large 0.6 nm, it will adsorb from the environment just gas 1 (fig. 5) and not noticing the presence of gas 2 in it. Clearly, given this picture understanding of the mechanism of purification of gas mixtures from one of the component allows a more conscientious approach to solving practical problems.

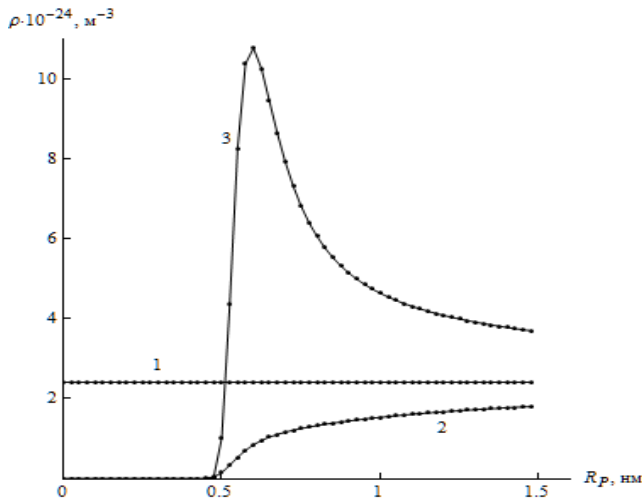


Figure 4. The dependence of the density of the gas in the pore of its radius. The curves are calculated according to (12); $k_B = 1.38 \cdot 10^{-23}$ J/grad., $T = 300$ K, $r_0 = 0.5$ nm and $P = 10000$ Pa, $V_m = 1 \cdot 10^{-29}$ m³, $L_p = 6.8$ nm, $d_L = 0.34$ nm, $\rho = 4.6 \cdot 10^9$ m⁻³; 1- $\varepsilon = 0$; 2- $\varepsilon = 2 \cdot 10^{-22}$ J; 3- $\varepsilon = 5.3 \cdot 10^{-22}$ J.

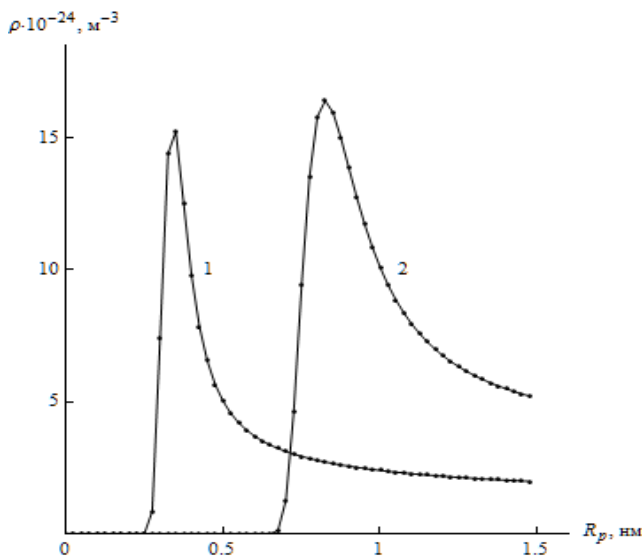


Figure 5. Influence parameter r_0 for gases filling of pore with different radius. Curves calculated to (12); $k_B = 1.38 \cdot 10^{-23}$ j/grad, $T = 300$ K, $V_m = 1 \cdot 10^{-29}$ m³, $L_p = 6.8$ nm, $d_L = 0.34$ nm, $\rho = 4.6 \cdot 10^9$ m⁻³; 1- $\varepsilon = 17 \cdot 10^{-22}$ J, $r_0 = 0.3$ nm and $P = 5000$ Pa; 2- $\varepsilon = 3 \cdot 10^{-22}$ J, $r_0 = 0.7$ nm and $P = 10000$ Pa.

6. Methodology Condensation

Having some idea of energy related fields since their features filling gases move to the analysis of the influence of these fields on the process of condensation in the pore. The easiest way to do it, by uses the method of reasoning and results shown in [7]. The proposed equation describing the change in the number of molecules in the gas phase of a closed volume when compressing

$$\frac{k_{a1} N_g^2}{V - NV_m} + \frac{k_{a2} (N - N_g) N_g}{V - NV_m} = N - N_g \quad (13)$$

(where k_{a1} and k_{a2} – a constants, N - is the total number of molecules in a closed volume V , N_g - is the number of molecules in the gas phase of this volume, V_m - volume of gas molecules) and it is shown that it physically meaningful solution of this square relatively N_g equation can be represented as

$$N_{g0} = \frac{k_{a2} N + (V - NV_m) - \sqrt{(k_{a2} N - (V - NV_m))^2 + 4k_{a1} N (V - NV_m)}}{2(k_{a2} - k_{a1})} \quad (14)$$

Then introduced the following function

$$N_{gf} = N_{g0} Hv(V - NV_m) + NHv(NV_m - V) - NHv(-V) \quad (15)$$

where $Hv(V - NV_m)$, $Hv(NV_m - V)$ and $Hv(-V)$ – Heaviside function (see e.g. [8]).

Using (15), the equation of State of gas in an enclosed volume to record in the form

$$P(V - NV_m) = N_{gf} kT \quad (16)$$

and analyzed the results.

This approach shall try to apply for the analysis of processes, occurring in the pore, i.e. a closed volume of work [7] will be in our case, the volume of pores. Equation (13) will keep its shape and only V it should be equal to the volume of pores of the V_p . The meaning of values of N , N_g also should be corrected for the volume of pores. With this in mind, equation (14) instead of V will stand V_p without additional of changes. The function (15) adjusted under the case in question will be of the form

$$N_{gf} = N_{g0} Hv(V_p - NV_m) + NHv(NV_m - V_p) - NHv(-V_p) \quad (17)$$

In view of the above equation of State of gas in the pore can be written in the form

$$P_p(V_p - NV_m) = N_{gf} kT \quad (18)$$

where N_{gf} shall be determined by (17). Because the pressure

in the pore P_p is connected with the pressure in the surrounding volume P with dependence (7), we obtain

$$P \cdot \text{Exp}\left(-\frac{E}{k_B T}\right) \cdot (V_p - NV_m) = N_{gf} kT \quad (19)$$

To simplify a first step, we assume that E in the volume of pores has a single value, and from the above considerations it is clear that this value may be positive, negative or zero. If E is known, equation (19) will have two variables - the pressure in the surrounding pore volume of P and the total number of gas molecules in the pore N , i.e., it will allow us to build a functional dependence of N on P with possible the condensation process in the pore.

7. Results and Discussion Condensation

Figure 6 shows the four curves calculated according to (19). Immediately is evident, that all the isotherms have the main elements, often observed by experimentally obtained results. There is a site monotonous increase of filling up to the saturation pressure, site of his sudden increase in pressure of saturation and subsequent stability filling, despite the increase of external pressure. Stability is clearly associated with the fact that in this area it is pore to completely fill with gas, there is no free volume. For curve 1 E is zero, curve 2 E is negatively, and curve 3 - positive, i.e. energy field of pores can both facilitate the process of condensation in her, shifting his start in the region of lower external pressure, and hinder his.

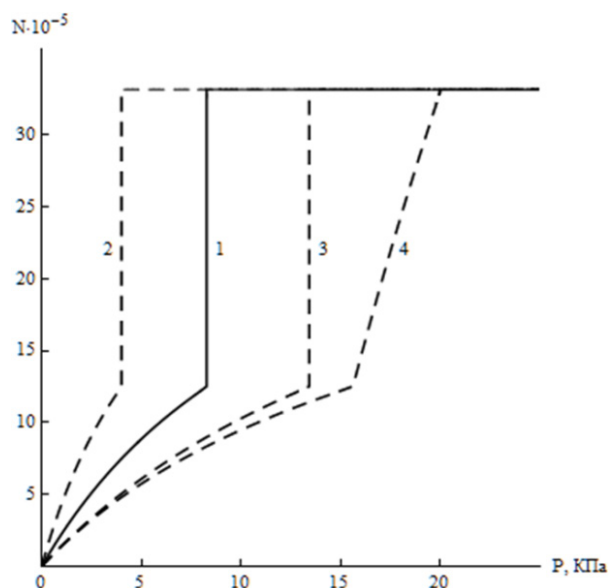


Figure 6. Isotherms to fill the pores of gas, taking into account the possibility of its condensation in the inner volume. Calculated according to (19) at: $k_B = 1.38 \cdot 10^{-23}$ J/grad, $T = 300$ K, $V_m = 3 \cdot 10^{-25}$ m³, $V_p = 1 \cdot 10^{-18}$ m³, $ka_1 = 1 \cdot 10^{-30}$ m³, $ka_2 = 5 \cdot 10^{-25}$ m³; 1- $E = 0$; 2- $E = -3 \cdot 10^{-21}$ J; 3- $E = 2 \cdot 10^{-21}$ J, 4- $E = 2 \cdot 10^{-21} + N \cdot 5 \cdot 10^{-28}$ J.

Interesting is curve 4. It is clear that starting the investigation, we strive to simplify put in its basis the model.

Molecules of gas, entering a pore, can only interact with the atoms of a solid body, forming pore, i.e. E does not depend on N (curves 1, 2 and 3). However, it is also clear that in a real system they can interact with the molecules of a gas already under the pore, i.e. E may be a function of N . Curve 4 obtained for the same values of all parameters included in the equation (19) as curve 3 and only for E is adopted the following simplest functional dependence on N

$$E = E_0 + k_0 N \quad (20)$$

E_0 taken to $2 \cdot 10^{-21}$ Joules, which is the same as the corresponding value for curve 3, and k_0 equal to $5 \cdot 10^{-28}$ J.

It is clear that the presence of a second positive element in the expression for the energy associated with the number of molecules of gas located in the pore, means that the latter will prevent the ingress in a pore of additional gas molecules from an external volume. The need to counteract this obstacle will lead to the slope of the plot condensation on the isotherm in the direction of increasing P (Fig. 6, curve 4), which naturally explains the numerous experimental dependencies with smooth, not stepwise increase of filling in the condensation (see for example [9]). It is interesting to note that if the second term in (20) is negative, then the slope of the terrain condensation reverse order, i.e. the isotherm will naturally explain the widely known phenomenon of adsorption hysteresis on porous bodies.

It is obvious that to obtain a clearer picture of the impact of the energy field of the pores on the condensation process it is necessary from arbitrary set its value to move to a current estimate of equation (5). We have to admit that in the internal volume of pores is the point at which condensation is most favourable and that the value E in these points determines condensation in the entire volume. This starting point will take centre pores, i.e., $R_0 = 0$ and $x = L_p/2$. When making this assumption E in equation (19) will not be specified arbitrarily, as it was made on receipt of the figure 6, and will be calculated according to equation (5) to point to the selected coordinates, i.e. the result of the calculation is dependent parameters pores that, accordingly, will analyse their impact on the process of condensation.

The first results obtained in this way are shown in Figure 7. Researched two pore radii respectively with equal $R_{p1} = 0.55$ nm and $R_{p2} = 0.61$ nm and their gas filling with $r_0 = 0.6$ nm. If all made assumptions still take that gas molecules do not interact with the atoms in a solid body, i.e. ϵ in equation (5) is zero, then we get curves 1 and 2 in Figure 7. This pictures show that the change in pore radius does not affect the process of condensation. Pressure saturation in both stages is the same. If you change the last allowing and take that gas molecules interact with the atoms of the solid state ($\epsilon = 6 \cdot 10^{-23}$ J), then the calculation under (19) leads to the curve (3) and (4) Figure 7. You can see that the inclusion in the energy field has increased pore pressure of saturation in the pores with a smaller radius (curve 3 compared to the curve 1) and to the reduction in the pores with large radius (curve 4 compared to the curve 2).

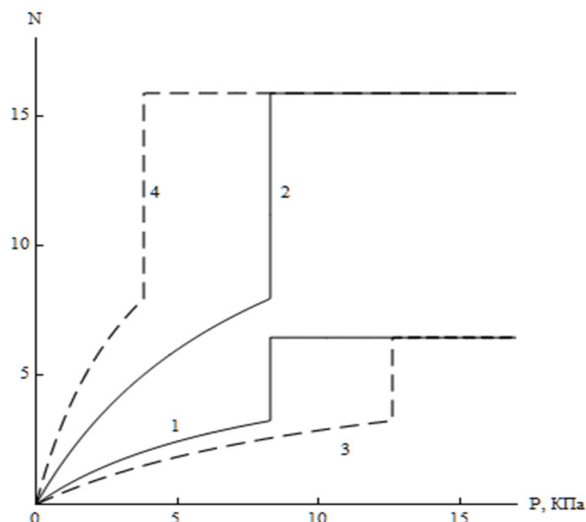


Figure 7. Isotherms of gas filling the pores with different radius. Calculated according to (19) in view of (5) and (17): $k_B = 1.38 \cdot 10^{-23}$ J/grad, $T = 300$ K, $V_m = 5 \cdot 10^{-25}$ m³, $V_p = \pi R^2 p L_p$, $x = -L_p/2$, $R_0 = 0$, $L_p = 68 \cdot 10^{-2}$ nm, $ka_1 = 1 \cdot 10^{-30}$ m³, $ka_2 = 5 \cdot 10^{-25}$ m³; 1- $R_p = 0.55$ nm, $\varepsilon = 0$;

2- $R_p = 0.61$ nm, $\varepsilon = 0$; 3 - $R_p = 0.55$ nm, $\varepsilon = 6 \cdot 10^{-23}$ J, $r_0 = 0.6$ nm;

4- $R_p = 0.61$ nm, $\varepsilon = 6 \cdot 10^{-23}$ J, $r_0 = 0.6$ nm. Estimated values for the curves 1 and 3 are reduced in two times.

Such a reaction of the condensation process in the pore of her energy field will take place only in the case when the pore radius lies on both sides of the values of r_0 . Two types of reaction can be observed by appropriate calculations according to (19), if we assume that both radius either less or more r_0 . Here it should be noted that the use in this paragraph turnover «changing the saturation pressure» is not fully competent. Indeed, from the point of view of the external observer, a sharp increase in filling the pores will occur-out at a lower external pressure (curve 4 in comparison with the curve 2). However, due to the energy field of pore pressure in the pore is not equal external and saturation pressure for observer measuring the P_p will not be change. Apparently, the possibility of such a mechanism for changing the saturation pressure for the external observer was not discussed in the literature. All known sources concerning this topic, assumes that the pressure in the pore is equal to the external pressure of, and then, naturally, there is a need to find a mechanism to changing the saturation pressure for the system.

8. Conclusion

The solution of this problem within the framework of the

given model, you can, apparently, put one task of future research in this area, in conclusion of this summarize its results. The proposed approach, taking into account the influence of the energy field of the pores on its filling with gas, has allowed to physically consistent picture of the process, in a natural form describing probably all experimentally known features of its flow. In particular, the factors underlying the selective absorption data porous body separate gases from their mixtures, which will undoubtedly help more conscious of the optimization of these processes in the industrial units. It seems that the obtained information about the features of the condensation of the gas in the energy field pores closer to reality than the existing ideas about this process. More natural and interconnected with the basic physical laws is obtained in the work of the isotherm, determines the number of gas molecules in the internal volume of pore.

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