

Basic thermodynamic description of adsorption of polar and nonpolar molecules on AOGW

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Abstract. In this article, the differential thermal adsorption, adsorption isotherm, integral entropy, and thermokinetics results and their analysis of the polar molecule H₂O vapor selected as adsorbate in the adsorbents obtained by the traditional method of thermal and water vapor activation of grape seed waste under the influence of temperature and their analysis, Q_d , ΔF , ΔS and isotherm, curves of differential heat, and kinetics of the experimental research results are presented, as a result of which the law of adsorption in active center's is determined.

1 Introduction

Today, it can be seen from the literature analysis that adsorbents are obtained from natural mineral compounds, mainly clay minerals, and other sources of raw materials. Adsorption of adsorbents and zeolites, including the adsorption of polar molecules on bentonites as well as the adsorption of organic and inorganic substances on synthetic zeolites, is known to us from the research works of the authors [1–2].

So far, in order to study the changes in the adsorption volume of adsorbents activated on the basis of tree trunks and their thermodynamic characteristics, research on the mechanisms of adsorption of adsorbates on adsorbents by the pyrolysis method or activation using water vapor at different temperatures has been studied [3–5].

To date, complete thermodynamic descriptions of adsorbents obtained on the basis of waste, taken precisely on the basis of grape compression, and data on the mechanisms of adsorbents Adsorbents with adsorbents have not been studied [6–10]. The results of Differential heat adsorption, H₂O vapor adsorption, integral entropy, thermokinetics, and their analysis were

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all studied in adsorbents that were made by activating water vapor with heat and water vapor under a certain pressure [11, 12]. By looking at these data on the adsorption of activated adsorbents in adsorbates and the adsorption of adsorbents forming a complex in coordination spheres, we can learn important basic information about where adsorbents can be used and how much adsorbate is adsorbed. [13-14].

Specific properties of adsorbent obtained from grape juice using water vapor (AOGW) type adsorbents, nature of hydrophobicity, thermodynamic processes taking place on the adsorbent surface with polar water vapor molecules-adsorbate, mainly surface chemistry and adsorption of solid phases with pore structure and active centers, provide important information for their use. Based on the determination of thermodynamic parameters of adsorbents of different natures in the calorimeter method as well as the analysis of the areas of absorption going into their active centers, it is possible to find out the complete data of the adsorbent and catalyst adsorption mechanisms [15–19]. Today, thermodynamic characteristics of adsorbents provide data on their adsorption capacity; it is known to have data on the capture of such important results as isotherm, differential heat, entropy, and thermal equilibrium time of water vapor adsorption [12, 20–31].

2 Research Methods

This article uses adsorption-microcalorimetric methods of analysis. In determining the thermodynamic parameters of adsorbents with high adsorption activity, the process of studying the adsorption mechanism used a universal high-vacuum adsorption device at a temperature of 303 K and a system of differential microcalorimeter-type differential temperature adsorption meters and a precision high-sensitivity high-vacuum microcalorimeter Tiana-Calve DAK-1-1 connected to it. Using the device, the values of the isotherm, differential heat content, entropy, and kinetics of water vapor adsorption on the adsorbent (thermal adsorbent derived from grape juice (TADG-6) and adsorbent obtained from grape juice using water vapor (AOGW-6)) were obtained.

3 Results and Discussion

The results of the study carried out on the adsorbents TADG-6 and AOGW-6, which were selected as the most optimal of the adsorbents that were activated using waste, are presented. The results of the experimental study showed that at a temperature of 303 K in a device with a microcalorimeter, when an H₂O molecule was selected as a polar molecule for adsorption in the adsorbent AOGW-6, a complete thermodynamic process was carried out. On the basis of the results of adsorption, entropy, and thermokinetics of H₂O vapor molecules in the adsorbent AOGW, activated with the participation of water vapor on the basis of grape seed waste, the law of adsorption in active centers was established on the basis of the differences in the adsorption mechanisms of these adsorbents. Figure 1 shows the results of the isotherm of adsorption of the polar molecule H₂O in the activated adsorbent AOGW-6 using water vapor.

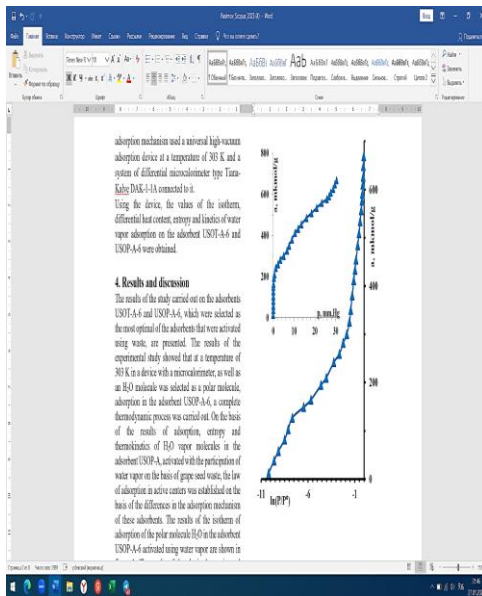


Fig. 1. Isotherm results of polar H₂O molecule adsorption in adsorbent AOGW-6

The results of the experimental study of the water vapor adsorption isotherm in the activated AOGW-6 adsorbent are shown to be able to be fully described by the two-member equation of the theory of volumetric filling of micropores (TVFM). Figure 1 shows the results of the isotherm of the adsorption of the molecule H₂O in the adsorbent AOGW-6. These results go along with the results of the differential heat of adsorption and help draw a clear conclusion about the full thermodynamic characteristic of the adsorbent, which is the adsorption mechanism.

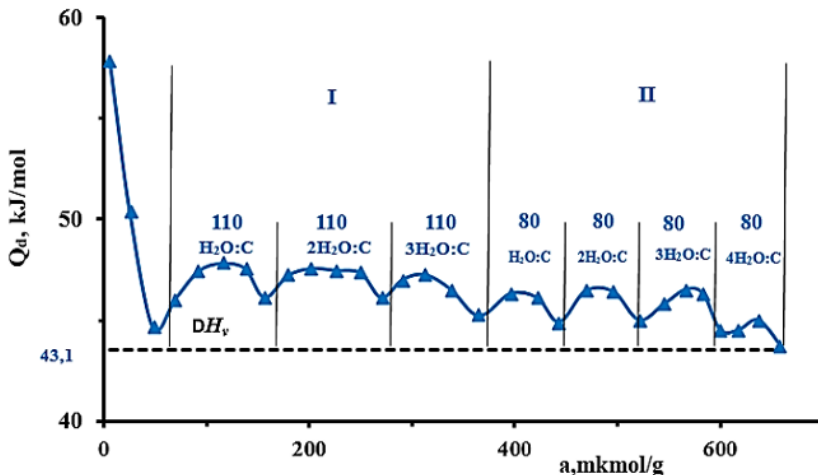


Fig. 2. Heat of adsorption of H₂O vapor molecules in activated AOGW-6 adsorbent

The adsorption heat curvature of the H₂O vapor molecules in the adsorbent AOGW-6 activated using water vapor is shown in Figure 2, where it can be observed that the adsorbent adsorption of a polar water molecule, selected as an adsorbate, is stepwise adsorbed in the adsorbent. On the graph, the amount of curvature (Q_d) is shown in kJ/mol, and the amount of adsorption (a) is shown in mkmol/g.

Initially, differential isocyclic adsorption Q_d was observed to adsorb at the highest value of 57.81 kJ/mol and an adsorption rate equal to $a=6.36$ mkmol/g, indicating that this higher value is adsorbed in existing adsorbent-containing additives. Later, the value of differential heat adsorption was characterized by the fact that adsorption isocyclic variation up to $Q_d=48.07$ kJ/mol was observed with adsorption up to $a=44.64$ mkmol/g.

The initial I-coordination sphere begins with the value of $Q_d=48.07$ kJ/mol of the differential adsorption heat and $a=44.64$ mkmol/g of the adsorption quantity, each of the three water molecules adsorbed uniformly from a quantity of 110 mkmol/g, a process that continues until the value of the adsorption heat $Q_d=45.20$ kJ/mol and the In this case, if each water molecule forms a $C_1:H_2O$ complex ($Q_d=48.07\div 46.10$ kJ/mol and $a=44.64\div 156.7$ mkmol/g) in the first adsorption in this coordination sphere, in the next step 2, 2si:adsorption of the H_2O complex ($Q_d=44.64\div 46.4$ kJ/mol and $a=156.7\div 270.64$ mkmol/g) based on the adsorbent-adsorbate mechanism, and in Step 3, with the same amount, the $3C_1:H_2O$ complex ($Q_d=46.4\div 45.20$ kJ/mol and $a=270.64\div 356.66$ mkmol/g) in the formation of differential heat there was a change in adsorption, varying around 4 kJ/mol. In the next adsorption, however, adsorption continues in the II coordination sphere, in which the adsorption of $C:H_2O$ by forming a complex ($Q_d=45.20\div 44.90$ kJ/mol and $a=356.66\div 443.67$ mkmol/g) continues. Further adsorption in the active center belonging to this coordination sphere ($Q_d=44.90\div 45.00$ kJ/mol and $a=443.67\div 521.35$ mkmol/g) leads to the complex formation of $2C:H_2O$.

It was observed that, based on the analysis of the results of the differential heat of water vapor adsorption of the AOGW-6 pargas activated adsorbent, the differential heat of adsorption of the H_2O molecule in the AOGW-6 adsorbent (Q_d) was observed to adsorb in the adsorbent in the proportion of 110 mkmol/gga and 80 mkmol/gga in active centers. The results of the differential adsorption entropy of water vapor molecules in the activated adsorbent AOGW-6 are shown in Figure 3. Based on the results of this study, it can be concluded that the fact that integral entropy is found around about 14 kJ/mol*K means that adsorption is close to the solid state. The molly differential entropy (ΔS_d) of H_2O adsorption in the AOGW-6 adsorbent was found, calculated from the isotherma and differential heat of adsorption based on the Gibbs-Helmhols equation.

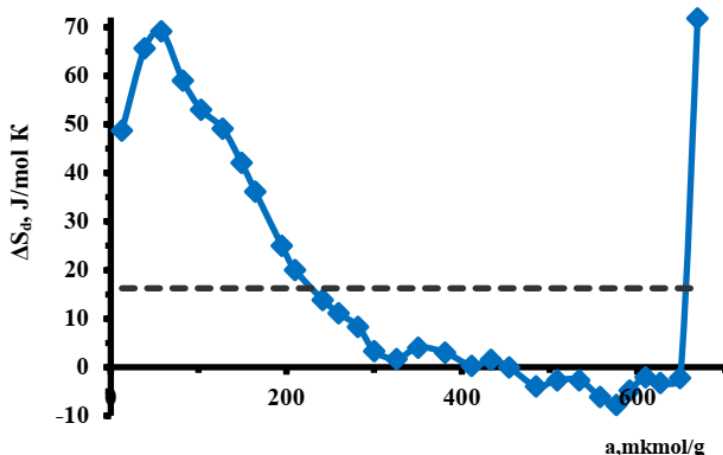


Fig. 3: Adsorption entropy of water vapor molecules in the adsorbent AOGW-6
 In the AOGW-6 adsorbent, the water entropy is the molly differential entropy of ΔS_d adsorption, which is different from its liquid state water entropy and has a waveform appearance. Starting from 38.46 J/mol*K, ΔS_d increases to ~30.7 mmol/g with small saturations, showing a relatively high saturation and crossing the maximum. The adsorbent-adsorbent interaction ensures this situation. At AOGW-6, the entropy of water ΔS_d passes

through the lowest minimum (-7.75 J/mol), which is different from the entropy of solid water, while towards saturation it rises sharply to the values of the Liquid Entropy of water. The integral mean moly entropy is equal to -16.24 J/mol \cdot K, which is much lower than that of Liquid Entropy. Thus, differential and integral entropy in the adsorbent AOGW-6 showed strong braking, in which the entropy of water is close to its entropy in its solid state. Analysis of the results of the adsorption thermokinetics of water vapor molecules in the adsorbent AOGW-6 (fig. Based on the data of adsorption Kinetics, it can be said that adsorption first went for 6 hours and 30 minutes and then went for around 2 hours in the last parts of adsorption, indicating the stability of the adsorbate in the adsorbent.

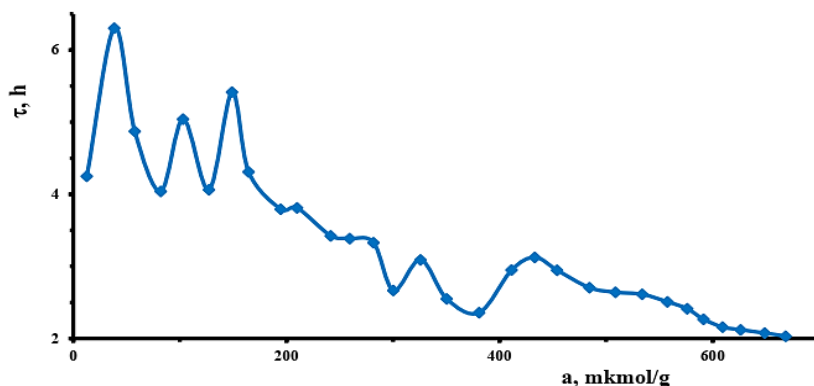


Fig. 4. Adsorption kinetics of water vapor molecules in the adsorbent AOGW-6

The results of the study, which are presented, are based on the results of the comparative differential heat of H_2O vapor adsorption in the carbon-based adsorbent AOGW-6, the adsorption heat of H_2O vapor molecules activated in the presence of water vapor based on isotherma, entropy, and thermokinetics, as well as the waste of Grape Grain. It was found that in studies using high-vacuum microcolorimetric research methods, the differential heat of adsorption of the H_2O molecule in the water vapor-activated AOGW-6 adsorbent (Q_d) results in an adsorbent of 110 mkmol/g in microgroups and an adsorbent-adsorbate interaction mechanism in mesagovaks as a result of adsorption in 80 mkmol/g carrally active centers. Based on the complete thermodynamic characteristics (Q_d , ΔF , ΔS) and isotherm of thermally and pargase-activated TADG-6 and USOP-A-6 adsorbents (Q_d , ΔF , ΔS), the correlation law of CO_2 adsorption was determined in the active centers of the adsorbent at a rate of 500 mkmol/g. According to the results of the differential heat of adsorption of the H_2O molecule (Q_d) in the USOP-A-6 adsorbent, the adsorbent-adsorbate interaction mechanism as a result of adsorption in adsorbent microgroups by 110 mkmol/g and in mesagovaks by 80 mkmol/g in multiples

In the course of the experiments, complete thermodynamic descriptions of the adsorbents TADG-6 and AOGW-6, which were activated using thermal and water vapor, i.e., based on Q_d , ΔF , ΔS and isotherma, from the results of an experimental study, are presented, as a result of which the

4 Conclusion

The results of the study were carried out on the basis of carbon-based AOGW-6 adsorbent H_2O vapor adsorption, isotherma, entropy, and thermokinetics of AOGW-6 adsorbent activated in the presence of water vapor based on Grape Grain waste, as well as the results of adsorption heat, isotherma, entropy, and thermokinetics of the information based on it.

According to the results of differential heat of adsorption of the H₂O molecule in the AOGW-6 adsorbent activated by water vapor (Q_d) in studies carried out using high-vacuum micrakolorimetric research methods, the mechanism of adsorbent-adsorbate interaction was determined by adsorbent interaction in adsorbent microgroups of 110 mkmol/g and in mesopores by adsorbent-adsorbent interaction in active centers of 80 mkmol/g.

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