To the adsorbent obtained on the basis of local Angren coal analysis of adsorption energy properties of benzene vapors

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Abstract. This article provides information on ensuring safety at coal mines by analyzing existing coal mining facilities. Information on the Angren coal mine is also given. It is shown that there are no accurate methods for determining the location of fires in order to increase the efficiency of spontaneous combustion prevention by supplying liquid compositions such as water and clay pulp flowing down the formation soil. Measures have been proposed to suppress spontaneous combustion centers, nitrogen is being increasingly used, the supply of which ensures volumetric processing of the collapsed mass and allows reducing the oxygen concentration in the mined-out space.

1 Introduction

At present, activated carbon adsorbents are widely used in the world for purification of various organic compounds, heavy metal ions and life-threatening radioactive metals. Today, hydrophobic carbon adsorbents are mainly modified on the basis of lignite, coal, coke and stems and barks of various plants. Activated carbon adsorbents obtained on the basis of coal and oil coke are important in cleaning of organic, aromatic compounds and heavy metal ions in oil refining waste water [1].

At present, scientific and research work is being carried out in the world on obtaining activated carbon adsorbents using local coal and oil waste products from mines. In this regard, studying the composition of industrial waste; to determine optimal conditions for obtaining carbon adsorbents based on them; absorbing organic substances into the obtained carbon adsorbents, determining the number and location of their micro-, meso-, and macropores, the complete molecular mechanisms of sorption processes occurring in adsorbents; Special attention is being paid to the creation of industrial wastewater treatment technology using carbon adsorbents [2].

Today, preventing the accumulation of coal dust and residues in our Republic and directing it to targeted production is one of the urgent issues of today. By enriching coal residues with additional substances, obtaining adsorbents and fully determining the adsorption properties of porous coal adsorbents, we will have the opportunity to determine the full thermodynamic properties of the obtained porous coal adsorbents using capillary and volumetric methods in a high-vacuum adsorption device, high-sensitivity DAK 1-1 calorimetric apparatus.

By determining the adsorption isotherm, differential heat, entropy and equilibrium time of benzene on the obtained coal, the adsorption capacity of the new adsorbent, location of active centers, and pore sizes can be described in detail [3].

2 Experimental research

Carbon microporous adsorbents (activated carbons, active fibers, and fabrics) are a class of high molecular weight solid porous carbon materials that absorb substances of various chemical natures (in gaseous, vapor, and liquid media) onto certain surfaces [1]. According to the classification of M.M. Dubinin, based on the sorption mechanisms occurring in the adsorption pores and capillary phenomena, the pores of various adsorbents are divided into the following types: micropores, macropores (equivalent radius r greater than 100-200 nm), mesopores (1.5 -1, 6 <r <1.5-1.6 nm).

Carbon microporous adsorbents are significantly different from materials such as coke, pumice, graphite because they contain micropores and supermicropores. In the same way, they differ from coal, which have a relatively high surface area due to small particle size (up to 100 m2/g and above) and belong to non-porous carbon adsorbents. Micropores and supermicropores are actually adsorbed into their pores, as they are crucial for the adsorption of gases and vapors and, in many cases, for liquid phase adsorption. It depends on the structure and geometric surface of adsorbates.

Its value is ~400-1400 m2/g according to, i.e. 15-55% of the theoretically possible value of 2630 m2/g obtained for a hypothetical model of pure aromatic carbon of hexagonal form with a condensed flat band structure. The volume of micropores and supermicropores is usually in the range of 0.2 - 0.6 cm3/g For the best
samples of carbon adsorbents, it can reach 1.3 - 1.5 cm³/g [1].

A formula for calculating the geometric volume of micropores from the value of adsorption energy of standard benzene vapor was proposed. The possibility of redescribing adsorption isotherms for several substances (benzene, ethyl chloride, carbon tetrachloride, etc.) using the equations of the theory of volume saturation of micropores (MHTN) was shown.

Thus, according to the MHTN equations and the parameters of the porous structure of activated carbon calculated from the adsorption isotherms of standard benzene vapor, it is possible to evaluate their adsorption properties with respect to vapors of a wide class of substances. However, it should be noted that in some cases there is a discrepancy between the parameters determined by the adsorption of benzene and other substances.

At the Institute of General and Inorganic Chemistry of the Russian Academy of Sciences, they are conducting quantitative research on the adsorption of polar and non-polar molecules on surfaces, microporous adsorbents, in a high-vacuum adsorption device using a microcalorimeter [4].

3 Research results

The adsorption isotherm of benzene on the resulting adsorbent was determined in the pressure determination section of the high-vacuum adsorption device. The differential heat of adsorption is measured by theoretical calculation of the pressure values, and the energy output from the DAK 1-1 calorimeter in the Tian-Calve model. Volumetric and capillary (liquid) methods were used to determine the adsorption isotherm. The adsorption isotherm has an accuracy of 0.1% and a heat of 1% [5].

The benzene obtained as an adsorbate was purified in a mixture of zeolites and under vacuum before use in sorption. Additional gases are expelled until the vapor pressure of the absorbing material is the same as the vapor pressure data given in the tables for absolute benzene.

Adsorption of benzene was carried out at 303 K on a sample of activated carbon adsorbent by activating local anthracite coal.

**Results obtained and discussion.** Local coal was mixed with asphaltene, a solvent for residual (powder) and small particles. After the mixtures are thoroughly mixed, they are kept until they become thick and elastic. Then they are prepared for granulation. After granulation, it is heated at 600°C. As a result of heating, additional gases in the composition are released. After that, activated carbon is obtained by the pyrolysis method.

The theoretical study of the sorption properties of the obtained activated carbon is based on the results obtained from experiments conducted in a high vacuum adsorption device. Figure 1 shows the adsorption isotherm of benzene on activated carbon from local coal mines at 303 K. The adsorption isotherm initially shows \( \ln(P/P_0) = -11 \).

This means that coal is being adsorbed in the micropores. Considering that the size of the benzene molecule is 0.6 nm, it indicates the presence of micropores in our obtained adsorbent [6].

Adsorption of benzene at values, up to about 1 mmol/g is \( \ln(P/P_0) = -7 \).

This means that benzene molecules are adsorbed in the internal micropores of coal. When adsorption reaches 4.5 mmol/g, the pressure in the device is 119.38 mm.sim. above will be equal. This value is equal to the saturation vapor pressure of benzene at a temperature of 30°C, and coal is saturated with benzene.

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a = 0.64 \exp([A/13.64]^2) + 2.48 \exp([A/4.93]^2) + 0.99 \exp([A/0.97]^3),
\]

where \( a \) is the adsorption value in \( a \)-micropores, mmol/g; \( a \) - is the work of free energy, kJ/mol, \( A = RT \ln(P/P_0) \).
The differential heat of adsorption of benzene vapors on the coal adsorbent obtained for research work at a temperature of 303 K is presented in (Fig. 2).

At first, the heat of adsorption of benzene is equal to 105.05 kJ/mol when $\alpha=0.055$ mmol/g at the initial saturation, and it is observed that the heat value of adsorption of benzene molecules decreases slightly. $Q_d=85.16$ kJ/mol at $\alpha=0.52$ mmol/g [7].

One of the main reasons for the high heat of adsorption of benzene molecules at low saturations is explained by their adsorption into micropores. Metal cations located in the micropores of the coal sample form $\pi$-complexes of $(\text{Me}^n\text{S}_6\text{N}_6)_n$ type. It was further observed that the adsorption exhibits a single maximum heat at a differential heat value of $\alpha=1.0$ mmol/g and increases to $Q=87.66$ kJ/mol. In the subsequent stages of adsorption, the differential heat decreases. After $\alpha=4.2$ mmol/g, the heat of adsorption becomes equal to the heat of condensation [8].

This decrease in the adsorption differential heat values is absorbed into the micro- and mesopores of the coal, and the heats of adsorption decrease with increasing benzene saturation. The value of condensation heat of adsorption of benzene vapors on the coal obtained for research work is close to 33.8 kJ/mol, and a total of 4.6 mmol/g of benzene is adsorbed [9].

Adsorption entropy describes the state of motion of absorbed adsorbate molecules in the adsorbent. The entropy curve of the adsorbent obtained from local coal residues -benzene system had a wavy appearance according to the amount of adsorbent saturation (Fig. 3).

It is known from the entropy graph that at values - up to 2 mmol/g, benzene is strongly adsorbed, that is, it is located below the average integral entropy line. After 4.3 mmol/g, it is higher than the standard state benzene entropy value. Adsorption entropy in the process up to 4.3 mmol/g indicates strong localization in the pores of the adsorbent. In the initial stages of saturation, benzene molecules are strongly adsorbed in the micropores of coal, that is, benzene molecules are in an unexcited state, during the adsorption process up to -68.7 J/mol*K, benzene goes to the solid state entropy value. Then, benzene slowly changes to the entropy of the liquid state. The average integral entropy of benzene adsorption on coal obtained in the research work is -68.7 J/mol*K [10].

4 Conclusion
In our research work, an adsorbent activated from local coal residues was obtained and its adsorption properties were studied. The adsorption differential heat, isotherm, molar entropy and thermokinetics of benzene molecules were calculated and it was determined that 4.5 mmol/g of benzene and 3.5 mmol/g of toluene are adsorbed on the activated carbon adsorbent. It was observed that benzene adsorption on the obtained activated carbon adsorbent starts with 104 kJ/mol and toluene with 90 kJ/mol, and the differential heat gradually decreases.

Based on the adsorption isotherm values of benzene and toluene on the activated carbon adsorbent, recalculated using the volume saturation theory equation of micropores, 84.5% of benzene and 94.2% of toluene were adsorbed on the micropores of the adsorbent.

The main features of the obtained adsorbent are that the raw materials necessary for the production industry are obtained by effectively using the residual products of coal.
References


