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HYDROGEN STORAGE IN POROUS CARBON MATERIALS OBTAINED BASED ON KAZAKHSTAN COALS

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The study is devoted to the investigation of hydrogen sorption properties of activated carbon adsorbents made of coals from the Kazakhstan deposits ”Shubarkol” and ”Shoptykol”. To activate the samples, KOH treatment in a ratio of 1:0.5 was used, followed by thermal activation at a temperature of 900 °C. The specific surface area of the samples was determined using the BET method, and their ability to absorb hydrogen at different temperature conditions was assessed. The study showed that the largest specific surface area (926.67 m^2/g) and maximum hydrogen sorption capacity (1.48 wt.%) at a temperature of 77 K are demonstrated by the powdered adsorbent ”Shoptykol;KOH” (ratio 1:0.5, treatment temperature 900 °C). Adsorption-desorption isotherms of these materials classify them as type I and type II, which indicates the mesoporous structure of extruded adsorbents and the more developed microporous texture of powder analogs. Temperature studies have revealed that lowering the temperature increases both the specific surface area and the adsorption capacity for hydrogen, reaching a peak of sorption at cryogenic temperatures. In this regard, powdered ”Shoptykol:KOH” (1:0.5, 900°C) is recognized as the optimal material for storing hydrogen due to its high specific surface area, developed microporous structure and exceptional ability to absorb hydrogen.

Key words: coal, adsorbent, porosity, carbonization, adsorption, hydrogen.

ҚАЗАҚСТАН КӨМІРЛЕРІНЕН АЛЫНҒАН КЕУЕКТІ КӨМІРТЕКТІ МАТЕРИАЛДАРДА СУТЕКТІ САҚТАУ

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Зерттеу Қазақстанның «Шұбаркөл» және «Шоптыкөл» кен орындарының көмірлерінен алынған белсендірілген көмір адсорбенттерінің сутегіні сорбциялау қасиеттерін зерттеуге арналған. Үлгілерді белсендіру үшін 1:0,5 қатынасында KOH-мен өңдеу, содан кейін 900 °C температурада термиялық белсендіру қолданылды. Үлгілердің меншікті бетінің ауданы БЭТ әдісімен анықталды және олардың сутегін сіңіру қабілеті әртүрлі температура жағдайында бағаланды. Зерттеу көрсеткендей, ең үлкен меншікті бетінің ауданы (926,67 $м^2/г$) және сутегінің максималды сорбциялық қабілеті (1,48 мас.%) 77 К температурада «Шоптыкөл:KOH» ұнтақ адсорбентімен (қатынасы 1:0,5, өңдеу температурасы 900 °C) көрсетілген. Бұл материалдардың адсорбциялық-десорбциялық изотермалары экструдталған адсорбенттердің мезокеуекті құрылымын және ұнтақ аналогтарының неғұрлым дамыған микрокеуекті құрылымын көрсете отырып, оларды I және II типке жатқызылды. Температуралық зерттеулер температураны төмендету меншікті бетінің ауданын да, сутегінің адсорбциялық қабілетін де арттырып, криогендік температурада сорбциялық шыңға жететінін анықтады. Осыған байланысты «Шоптыкөл:KOH» ұнтағы (1:0,5, 900°C) жоғары меншікті бетінің ауданына, дамыған

микрокеуекті құрылымына және сутекті сіңіру қабілетіне байланысты сутегін сақтау үшін оңтайлы материал болып танылды.

Түйін сөздер: көмір, адсорбент, кеуектілік, карбонизация, адсорбция, сутегі.

ХРАНЕНИЕ ВОДОРОДА В ПОРИСТЫХ УГЛЕРОДНЫХ МАТЕРИАЛАХ ПОЛУЧЕННЫХ НА ОСНОВЕ УГЛЕЙ КАЗАХСТАНА

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Исследование посвящено изучению водородосорбционных свойств активированных углеродных адсорбентов, изготовленных из углей Казахстанских месторождений «Шубарколь» и «Шоптыколь». Для активирования образцов использовалась обработка КОН в соотношении 1:0,5, а затем термическая активация при температуре 900 °С. Определены удельная поверхность образцов с помощью метода БЭТ, а также проведена оценка их способности поглощать водород при разных температурных режимах. Исследование показало, что наибольшую удельную поверхность (926,67 м^2/г) и максимальную водородосорбционную емкость (1,48 мас.%) при температуре 77 К демонстрирует порошкообразный адсорбент ”Шоптыколь;КОН” (соотношение 1:0,5, температура обработки 900 °С). Изотермы адсорбции-десорбции этих материалов классифицируют их как тип I и тип II, что свидетельствует о мезопористой структуре экструдированных адсорбентов и более развитой микропористой текстуре порошкообразных аналогов. Температурные исследования выявили, что понижение температуры повышает как удельную поверхность, так и адсорбционную способность к водороду, достигая пика сорбции при криогенных температурах. В связи с этим, оптимальным материалом для хранения водорода признан порошкообразный ”Шоптыкол:КОН” (1:0,5, 900°С) благодаря его высокой удельной поверхности, развитой микропористой структуре и исключительной способности поглощать водород.

Ключевые слова: уголь, адсорбент, пористость, карбонизация, адсорбция, водород.

Introduction. Future energy security is under threat due to the depletion of fossil fuel resources and the environmental impact associated with their use. To address these challenges, significant efforts have been made to develop efficient renewable energy systems, including geothermal, wind, solar, biomass, and hydrogen energy. Among these alternatives, hydrogen has garnered considerable attention as a potential replacement for fossil fuels, offering both high energy efficiency and environmental sustainability. This is attributed to its high gravimetric energy density and the production of only environmentally benign byproducts [1].

Hydrogen (H_2) is the most abundant element in the universe and the lightest, with a high energy content of 142 MJ/kg (higher heating value), making it a sustainable and non-toxic energy carrier. The chemical energy of hydrogen is nearly three times higher than that of other chemical fuels on a gravimetric basis [2,3]. However, in terms of volumetric energy density, hydrogen is significantly lower compared to gasoline and other hydrocarbon fuels. For instance, the average energy density of liquid hydrocarbons is approximately 43 MJ/kg on a gravimetric basis. Specifically, gasoline has an energy density of 31.7 MJ/l, whereas compressed hydrogen (at 70 MPa) possesses only 4.7 MJ/l, which is nearly one-sixth of that of gasoline [4-6].

Although various methods for hydrogen storage exist, meeting the requirements related to efficiency, size, capacity, safety, and cost in transportation remains challenging. Generally, hydrogen is stored

using one of four primary methods: high-pressure compression, liquefaction in a cryogenic tank, solid-state storage in metal hydrides, and adsorption in porous materials [7,8]. While compression and liquefaction have traditionally been the most common approaches, the storage of hydrogen molecules in porous materials has been considered an attractive alternative due to its rapid reaction kinetics, high adsorption capacity, and enhanced safety compared to compressed gas storage.

Moreover, hydrogen liquefaction presents several challenges, including high energy consumption and explosion risks, as it requires extremely low temperatures. In the case of chemical storage using metal hydrides, practical application is hindered by several factors, such as hysteresis effects between adsorption and desorption reactions, high reaction enthalpy, and the low thermal conductivity of metal hydrides, all of which negatively impact overall efficiency [9].

Among various hydrogen storage materials, carbon-based porous materials, particularly porous carbon adsorbents, have attracted significant attention as promising candidates due to their large pore volume, high surface area, tunable textural properties, low gas-solid interaction, and excellent chemical and thermal stability [10]. Hydrogen storage via physisorption on carbon materials does not require high pressures but necessitates cryogenic temperatures. This method exhibits rapid kinetics with a fully reversible adsorption-desorption process, offering relatively higher hydrogen storage capacities.

Porous carbon materials are of great importance due to their wide-ranging applications, including industrial adsorption in air and water purification, pollutant removal, gas separation, templating components, electrode materials, catalyst supports, chromatographic columns, and gas capture and storage. Activated carbon adsorbents have been widely utilized for centuries in various applications due to their low cost and high adsorption capacity. Variants of activated carbon with enhanced properties can be synthesized through chemical activation [11]. Structurally, activated carbon primarily consists of curved aromatic sheets with a locally variable slit-shaped microporous structure, which is formed as a result of activation processes [12].

Materials and methods. There are various methods for producing carbon materials, including preparation and modification of the initial carbon, carbonization and subsequent activation with a gas or chemical reagent. One of the promising methods for producing porous carbon materials from carbon-containing raw materials is the use of alkaline activators in heat treatment processes. The increase in the KOH potential is due to the large ionic radius of potassium (0.267 nm) compared to sodium (0.190 nm).

The activation medium (N_2, CO_2 or H_2O) also affects the structural properties of activated carbon. Nitrogen has been found to be a good alternative as an activation medium compared to CO_2 and water vapor. When the mixture is heated, the alkali melts (the melting points of NaOH and KOH under standard conditions are 318°C and 360°C, respectively). Among a large number of accompanying reactions, the main reaction can be written as:

$$6MOH + 2C \rightarrow 2M + 2H_2 + 2M_2CO_3$$

Here M is Na or K.

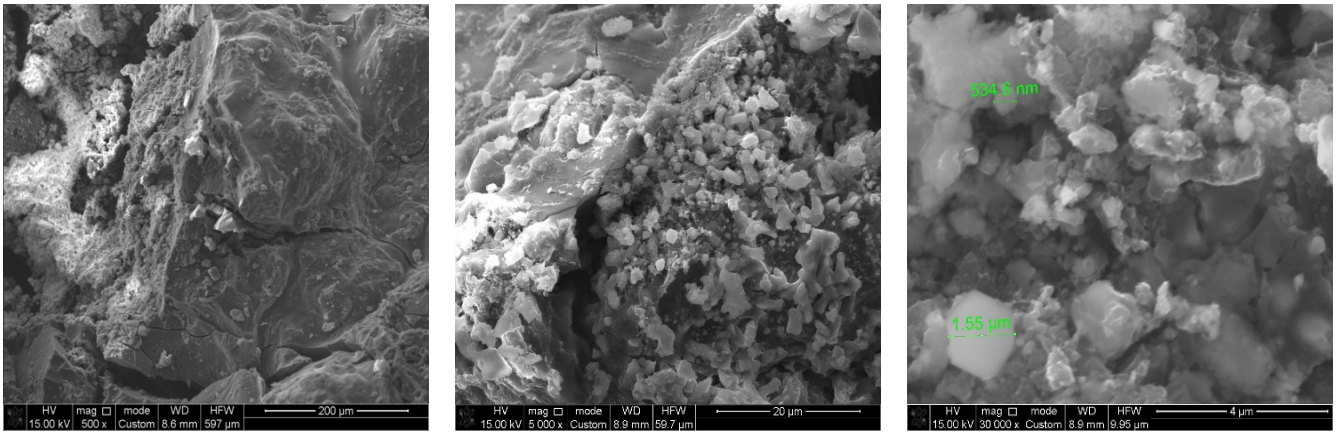
With increasing alkali-to-carbon mass ratio, heating temperature and holding time, the porosity of the carbon increases and the specific surface area of the resulting carbon increases. Potassium formed during activation with KOH is incorporated between the graphene layers of the carbon crystallite. This bond becomes more pronounced in the case of highly ordered carbon materials. The formation of alkali metal carbonates and their subsequent decomposition at high temperatures (> 800 °C) with the release of CO and CO_2 is a common feature of KOH activation.

It is known that as a result of atmospheric action in reservoir conditions, the organic mass of coal acquires a new set of various oxygen-containing groups, the presence of such functional groups determines the high reactivity of coal with respect

to the activator. (for example, KOH), which has a positive effect on the process of chemical activation in this process. The aim of the work is to study the method for obtaining carbon sorbents from oxidized coal ”Shoptykol” of the Maikoben basin and coal ”Shubarkol” with a developed structure and high adsorption characteristics, as well as the use of the obtained adsorbents for hydrogen storage.

Chemical analysis and surface morphology were studied by energy-dispersive X-ray spectroscopy using a SEM (Quanta 3D 200i) with an EDAX energy-dispersive analysis attachment. Specific surface area analysis was performed using a 3Flex 3500 high-performance adsorption analyzer (Micromeritics, USA) with a standard SmartVacprep programmable degasser.

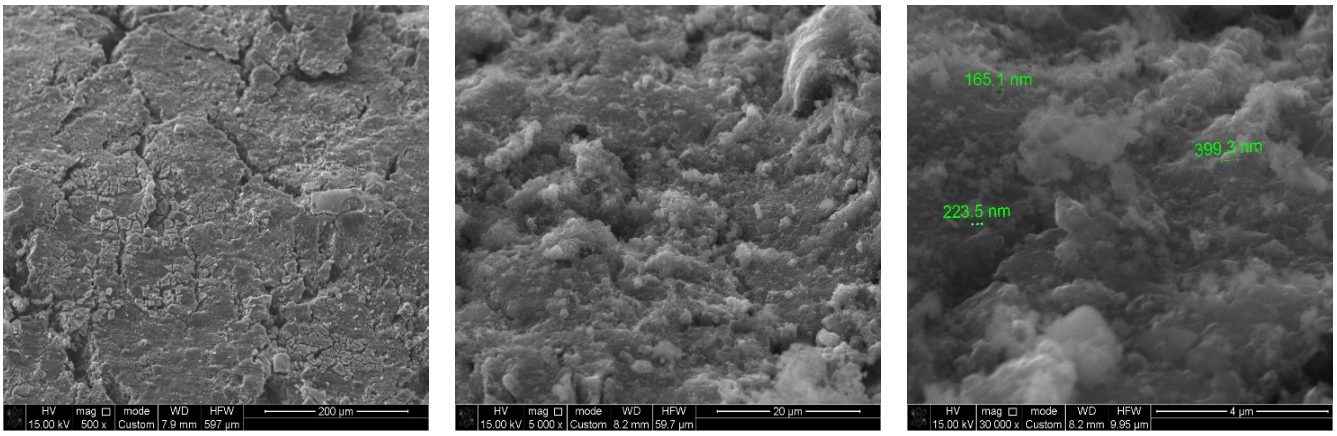
Results and discussion. The morphology of the obtained adsorbents was investigated at various scales using scanning electron microscopy (SEM). Figures 1 and 2 present the SEM analysis results for the powdered activated adsorbent ”Shubarkol-KOH” (1:0.5, 900°C) and the extruded activated adsorbent ”Shubarkol-KOH” (1:0.5, 900°C).



a **b** **c**

Fig.1 - SEM results for the powdered activated adsorbent ”Shubarkol-KOH” (1:0.5, 900°C):

a-x500; b-x5000; c-x30000



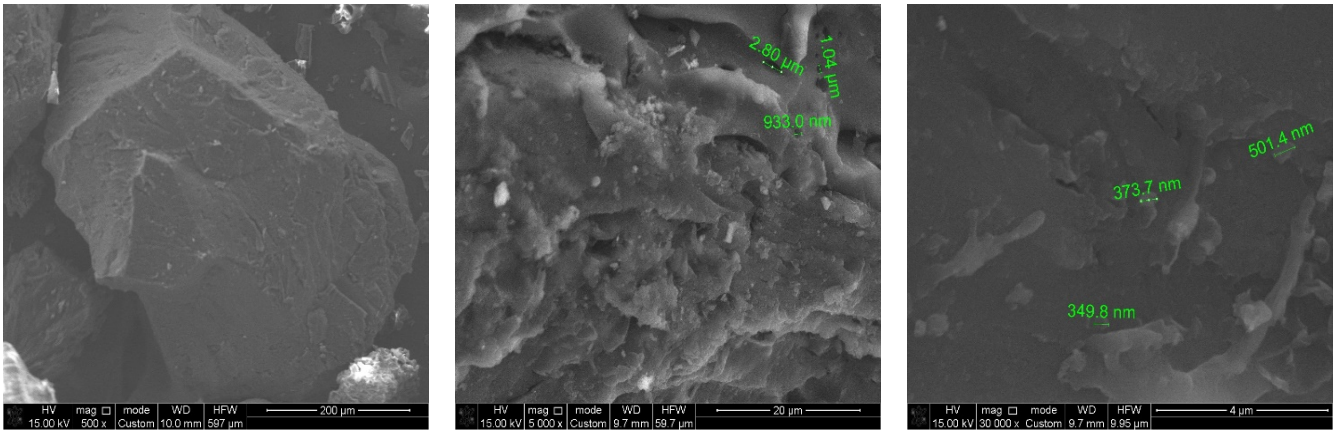
a **b** **c**

Fig.2 - SEM results for the extruded activated adsorbent ”Shubarkol-KOH” (1:0.5, 900°C):

a-x500; b-x5000; c-x30000

The morphological analysis of the obtained adsorbents revealed that the particle sizes of the surface of the adsorbents ranged from 534.6 nm to 1.55 μm for the powdered activated adsorbent ”Shubarkol-KOH” (1:0.5, 900°C), and from 165.1 nm to 399.3 nm for the extruded activated adsorbent ”Shubarkol-KOH” (1:0.5, 900°C), exhibiting a heterogeneous structure.

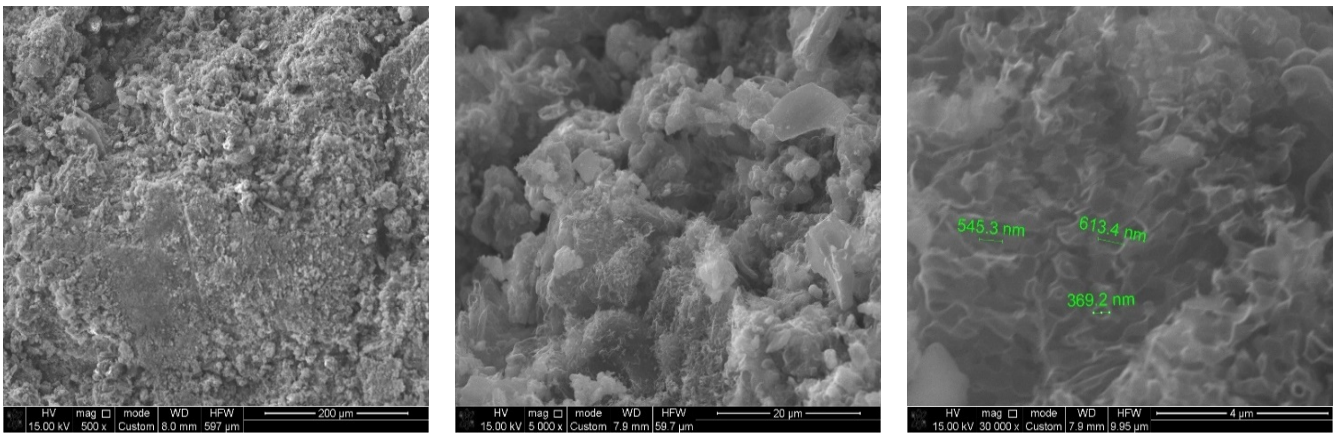
Figures 3 and 4 present the SEM analysis results for the powdered activated adsorbent ”Shoptykol-KOH” (1:0.5, 900°C) and the extruded activated adsorbent ”Shoptykol-KOH” (1:0.5, 900°C).



a **b** **c**

Fig.3 - SEM results for the powdered activated adsorbent ”Shoptykol-KOH” (1:0.5, 900°C):

a-x500; b-x5000; c-x30000



a **b** **c**

Fig.4 - SEM results for the extruded activated adsorbent ”Shoptykol-KOH” (1:0.5, 900°C):

a-x500; b-x5000; c-x30000

The morphological analysis of the obtained adsorbents revealed that the particle sizes of the surface of the adsorbents ranged from 349.8 nm to 501.4 nm for the powdered activated adsorbent ”Shoptykol-KOH” (1:0.5, 900°C), and from 369.2 nm to 613.4 nm for the extruded activated adsorbent ”Shoptykol-KOH” (1:0.5, 900°C), both exhibiting a heterogeneous structure.

The results of the elemental composition and physicochemical characteristics of the samples are presented in Tables 1 and 2.

Table 1 - Results of the elemental analysis of the samples

Name	Elemental content, mass %									
	C	O	Na	Mg	Al	Si	S	K	Ca	Fe
”Shubarkol-KOH” (1:0.5, 900°C) the powdered activated adsorbent	71.15	11.78	1.94	0.49	9.57	0.19	0.11	1.33	1.12	2.31
”Shubarkol-KOH” (1:0.5, 900°C) extruded activated adsorbent	89.61	8.11	0.08	0.04	0.44	0.96	0.01	0.48	0.10	0.17
”Shoptykol-KOH” (1:0.5, 900°C) the powdered activated adsorbent	88.19	7.60	0.15	0.40	0.11	0.15	0.24	0.73	1.65	0.77
”Shoptykol-KOH” (1:0.5, 900°C) extruded activated adsorbent	78.87	10.79	0.08	0.13	1.87	3.16	0.17	3.25	0.97	0.70

At elevated temperatures, potassium hydroxide reacts with carbon, leading to the formation of gaseous carbon oxides. This reaction promotes the development of a porous structure within the carbon material and increases its surface area. Additionally, the reduction of metal ions intercalated between carbon layers to their metallic state is observed. Subsequent treatment with water further contributes to the formation of pores. It is also important to note that during the activation process with potassium hydroxide, inorganic components, particularly silicon, form water-soluble potassium silicates. This results in a reduction of ash content following activation and washing.

Elemental analysis indicates that the relatively highest carbon content was observed in the extruded activated adsorbent ”Shubarkol-KOH” (1:0.5, 900°C) and the powdered activated adsorbent ”Shoptykol-KOH” (1:0.5, 900°C).

Table 2 - Characteristics of adsorbents obtained from coal from the ”Shubarkol” and ”Shoptykol” deposits

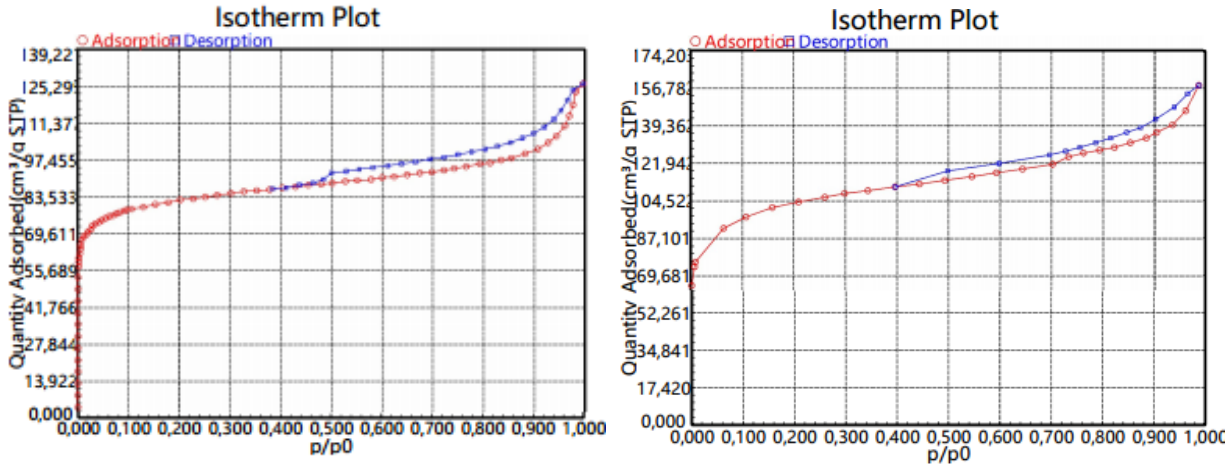
Name of activated adsorbent	W_t^r,%	A^r,%	V^d, %	$V_{\sum (water)}$, cm^3/g	ρ_{bulk}, g/cm^3	$pH_{aqueous\ extract}$	$A_{m.o.}$, mg/g	$A_{m.b.}$, mg/g	A_{iodine}, %
”Shubarkol-KOH” (1:0.5, 900°C) the powdered activated adsorbent	25.14	8.65	52.95	0.54	0.51	7.01	30.1	44.4	34.54
”Shubarkol-KOH” (1:0.5, 900°C) extruded activated adsorbent	10.83	21.44	62.61	0.56	0.62	7.37	52.0	89.8	31.42
”Shoptykol-KOH” (1:0.5, 900°C) the powdered activated adsorbent	8.66	20.45	54.09	0.61	0.48	7.52	24.2	45.4	38.72
”Shoptykol-KOH” (1:0.5, 900°C) extruded activated adsorbent	16.81	45.41	138.75	0.72	0.54	7.25	68.5	87.5	30.86

In terms of methyl orange adsorption, the Shoptykol-KOH extruded adsorbent demonstrated the highest capacity (68.5 mg/g). For methylene blue, the best performance was observed for the Shubarkol-KOH extruded adsorbent (89.8 mg/g), indicating its high sorption capacity for large

molecular weight dyes. Regarding iodine adsorption, the highest capacity was found in the Shoptykol-KOH powdered adsorbent (38.72 mg/g), suggesting a well-developed microporous structure.

Table 3- Specific surface area values of pores of adsorbents obtained from coal from the "Shubarkol" and "Shoptykol" deposits

Name of activated adsorbent	BET Surface Area, m^2/a	Cumulative adsorption surface area (BJH) for pores with a width from 17,000 Å to 3,000,000 Å, m^2/g	BJH adsorption cumulative pore volume for pores with a width from 17,000 Å to 3,000,000 Å, cm^3/g	BJH adsorption average pore width (4V/A), Å
"Shubarkol-KOH" (1:0.5, 900°C) the powdered activated adsorbent	507.2986	59.4994	0.12044	80.972
"Shubarkol-KOH" (1:0.5, 900°C) extruded activated adsorbent	316.8146	62.64589	0.09226	21.372
"Shoptykol-KOH" (1:0.5, 900°C) the powdered activated adsorbent	926.6728	130.0567	0.13067	40.191
"Shoptykol-KOH" (1:0.5, 900°C) extruded activated adsorbent	381.3587	123.41338	0.14172	21.459



a b

Fig.5 – BET isotherm of the specific surface area of the extruded activated adsorbent (a – "Shubarkol-KOH" 1:0.5, 900°C, b – "Shoptykol-KOH" 1:0.5, 900°C)

Extruded adsorbents generally exhibited higher efficiency in removing organic dyes, particularly methylene blue. Shoptykol-based adsorbents showed superior adsorption of iodine, indicating a more developed microporous structure. The choice of adsorbent should depend on the target application: Shubarkol-KOH (extruded) is more effective for dye removal, while Shoptykol-KOH (powdered) is better suited for the adsorption of small molecules such as iodine.

Figure 5 shows the BET isotherm of the specific surface area of the extruded activated adsorbents "Shubarkol-KOH" (1:0.5, 900°C) and "Shoptykol-KOH" (1:0.5, 900°C).

Figure 6 shows the types of adsorption-desorption isotherms.

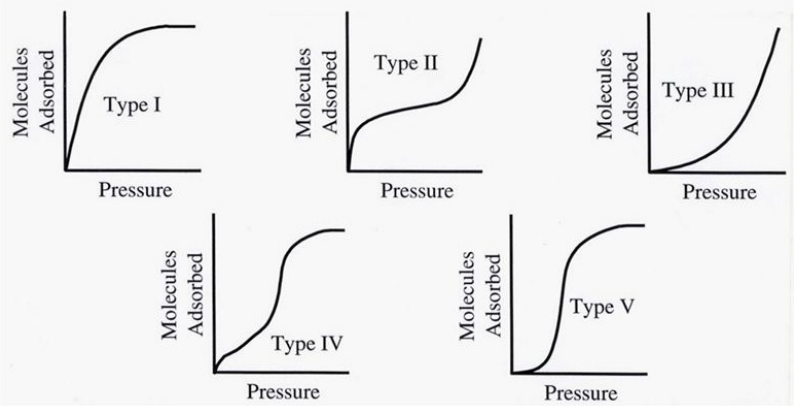


Fig.6 - Types of adsorption-desorption isotherms

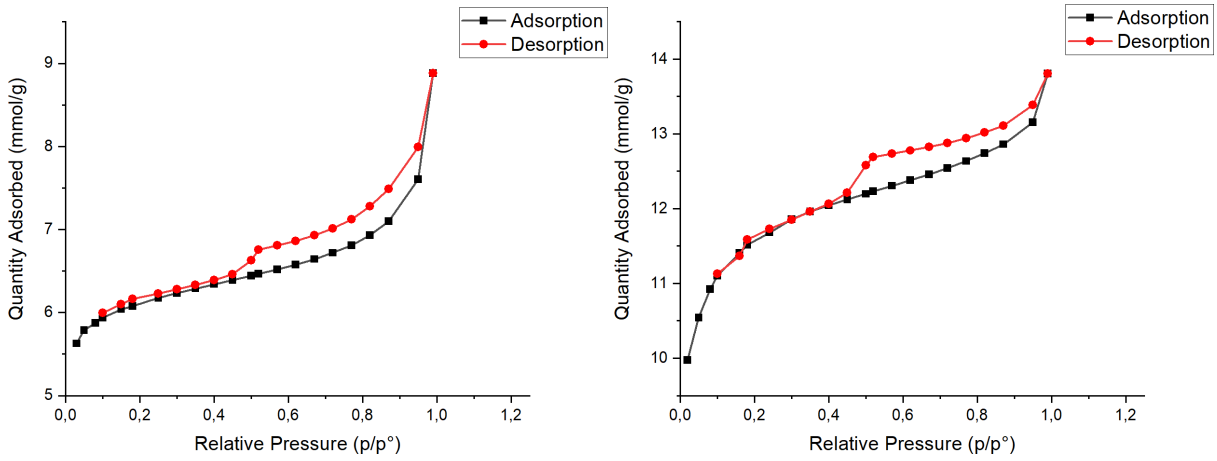


Fig.7 – BET isotherm of the specific surface area of the powdered activated adsorbent (a – "Shubarkol-KOH" 1:0.5, 900°C, b – "Shoptykol-KOH" 1:0.5, 900°C)

The types of adsorption-desorption isotherms of the obtained adsorbents were determined, and conclusions were drawn. The adsorption-desorption isotherms of the mesopores of the "Shubarkol-KOH" (1:0.5, 900°C) extruded activated adsorbent and the "Shoptykol-KOH" (1:0.5, 900°C) extruded activated adsorbent correspond to Type I and Type II isotherms.

Type I – "Langmuir-type" isotherm is characterized by the cessation of adsorption growth

at low and medium relative pressures. This type of isotherm occurs in two cases:

During monomolecular adsorption on macroporous adsorbents, where strong adsorbate-adsorbent interactions are observed.

During adsorption in microporous adsorbents. Unlike the first case, in the presence of micropores, a sharp increase is observed at low relative pressure values ($p/p_s < 0.1$), which is due to the high adsorption potential. Additionally, the specific surface area of microporous samples significantly exceeds that of macroporous or non-porous materials.

Type II – ”S-shaped” isotherm indicates the formation of polymolecular adsorption. Typically, this form of isotherm is characteristic of dispersed macroporous and non-porous materials.

The obtained isotherms of the samples belong to type I - a microporous material; there is also a type IV hysteresis loop, also characteristic of a microporous material with slot-like pores, characteristic of the layered structure of coals.

Among the powdered activated adsorbents, ”Shoptykol-KOH” (1:0.5, 900°C) exhibits the highest BET surface area (926.67 m^2/g), significantly higher than ”Shubarkol-KOH” (507.30 m^2/g). Among the extruded activated adsorbents, ”Shoptykol-KOH” (381.36 m^2/g) again outperforms ”Shubarkol-KOH” (316.81 m^2/g) in terms of specific surface area. In both cases, the powdered form of the adsorbents shows a higher surface area than the extruded form, indicating that pelletization may lead to some loss of porosity.

”Shoptykol-KOH” (1:0.5, 900°C) powdered activated adsorbent demonstrates the highest BET surface area (926.67 m^2/g), which is a critical factor for gas adsorption. The hydrogen storage capacity of this adsorbent is 77% with a K-value of 1.48, indicating strong potential for hydrogen adsorption. A higher surface area typically correlates with improved hydrogen uptake due to enhanced microporosity and available adsorption sites.

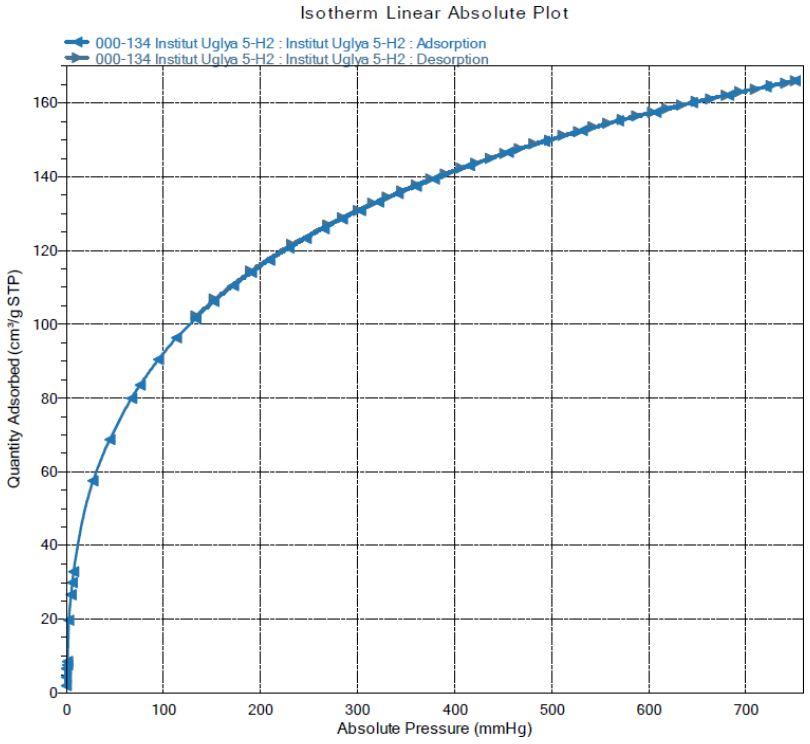


Fig.8 - Adsorption curve of the powdered activated adsorbent ”Shoptykol:KOH” 1:0.5, 900ºC (H_2)

Hydrogen sorption was carried out at 3 different temperatures.

Table 4 - Results of the study of hydrogen sorption with PCM

Name	S(DFT) specific, m^2/g	Mass H2, % 77 K	Mass H2, % 273 K	Mass H2, % 298 K	Heat of adsorption of H2, kJ/mol
Shoptykol: KOH = 1:0.5	1184,29	1,48	0.021	0.0084	17,31

For the case of 77 K, it is also possible to determine the specific surface area and pore distribution using DFT methods for carbon materials. Unfortunately, the method has not been developed for other temperatures and heterogeneous surfaces which these samples belong to. As logically follows, an increase in temperature significantly reduces the sorption of hydrogen. From the capacitance values obtained at 3 different temperatures, the heat of adsorption of hydrogen molecules can be determined.

A comparison table comparing the specific surface area $S_{(BET)}$ for N_2, CO_2 and H_2 is presented in Table 5.

Table 5 - Comparative table comparing the specific surface area $S_{(BET)}$ for N_2, CO_2 and H_2

Temperature, K	S(BET), m^2/g (based on N2)	Equivalent surface area (S), m^2/g (based on CO2)		Specific surface S(DFT), m^2/g (according to H2)	Amount of adsorbed H2 gas		Heat of adsorption of H2, kJ/mol
		Dubinin-Radushkevich	Dubinin-Astakhov		%	mg/g	
Powdered activated adsorbent Shoptykol:KOH (1:0.5) 900^0C							
77	926,6728	706,124	1605,444	1184,29	1,48	14,8203	17,31
273,15	-	-	-	-	0,021	0,21024	-
298	-	-	-	-	0,0083	0,08570	-

Due to the smaller radius and transverse radius of the hydrogen molecule, the specific surface area and porosity values will be higher compared to nitrogen sorption. Classical BET methods in the case of H_2 will be incorrect, since the saturation pressure value was used as a constant (760 Torr) to calculate the pore distribution, the theoretical model of hydrogen sorption DFT HS H_2 Carbon heterogeneous, taking into account the heterogeneity of the carbon surface. For most samples, this model showed good agreement; the nitrogen limitation to fill pores with a radius of less than 0.35 nm was also taken into account. To calculate the heat of adsorption in the case of hydrogen, the affinity coefficient parameter was considered equal to 0.165 according to [13], for nitrogen β=0.33.

The change in specific surface area using the (BET) method for hydrogen (%) and the amount of adsorbed hydrogen versus temperature for activated adsorbents are presented below in Figure 9,10.

The data indicate that low temperatures (-200°C) are optimal for maximizing both specific surface area and hydrogen adsorption capacity.

As the temperature increases, the surface area reduces, leading to a significant decline in hydrogen adsorption efficiency.

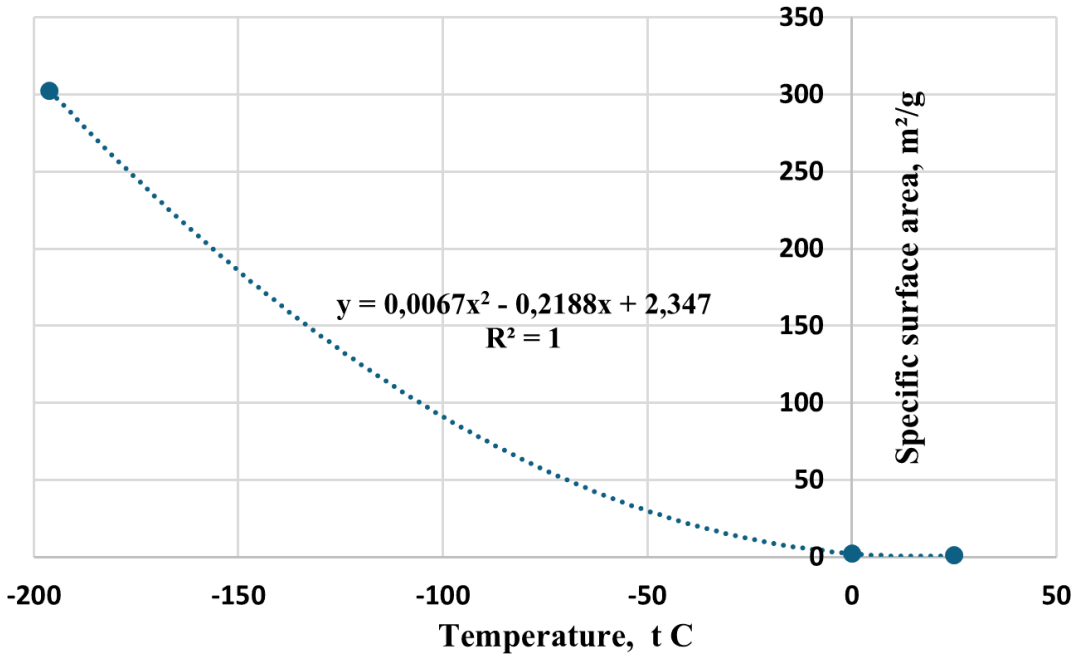


Fig.9 - Change in specific surface area using the (BET) method for hydrogen (%) from the temperature of the powdered activated adsorbent "Shoptykol: KOH" (1:0.5) at 900ºC

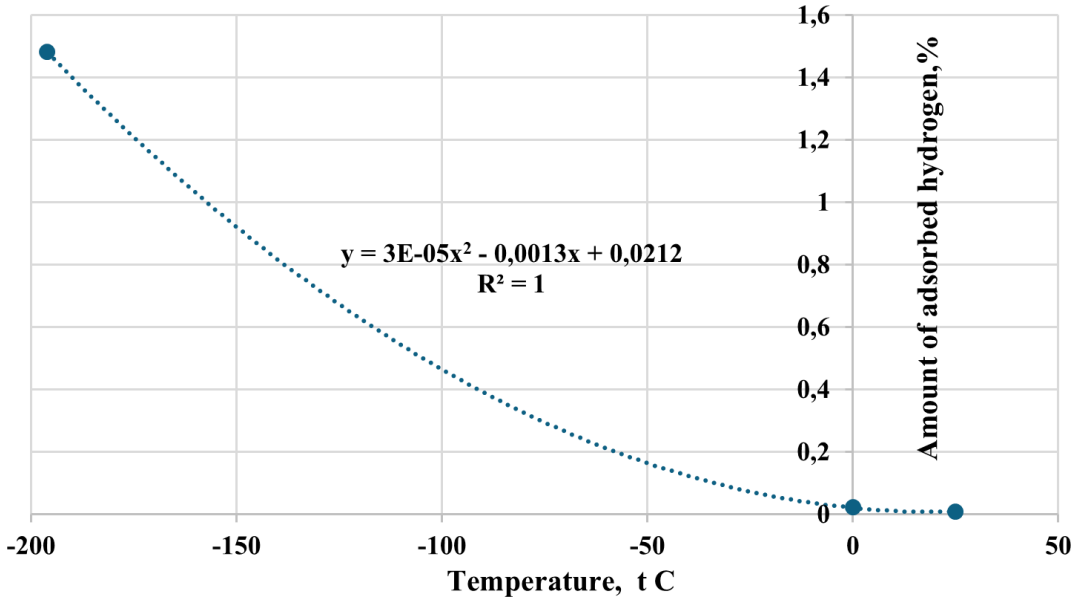


Fig.10 - Change in the amount of adsorbed hydrogen as a function of temperature for the powdered activated adsorbent "Shoptykol: KOH" (1:0.5) at 900ºC

Conclusion. This study comprehensively investigated the hydrogen sorption properties of activated carbon adsorbents derived from coals from the Kazakhstan deposits "Shubarkol" and "Shoptykol." The research focused on the effect of activation conditions, material structure, and surface

characteristics on hydrogen adsorption efficiency. The findings demonstrate that the activation process using KOH in a 1:0.5 ratio, followed by thermal treatment at 900°C, significantly enhances the porous structure of the resulting carbon materials, increasing their specific surface area and adsorption capacity.

Among the obtained adsorbents, the powdered ”Shoptykol-KOH” (1:0.5, 900°C) material exhibited the highest BET surface area (926.67 m^2/g) and the greatest hydrogen storage capacity (1.48 wt.% at 77 K). The results suggest that the porous carbon adsorbents prepared under these conditions possess a well-developed microporous structure, which is crucial for hydrogen adsorption through physisorption mechanisms. The adsorption-desorption isotherm analysis further classified the materials into Type I and Type II, indicating the presence of both microporous and mesoporous structures, making them suitable for various gas storage applications.

Temperature-dependent hydrogen sorption studies revealed a strong correlation between adsorption efficiency and operating temperature. Hydrogen uptake was maximized at cryogenic temperatures (77 K), confirming that low temperatures significantly enhance adsorption due to increased van der Waals interactions. However, at room temperature (298 K), the adsorption capacity dropped considerably, underscoring the challenge of efficient hydrogen storage under ambient conditions.

In summary, the powdered ”Shoptykol-KOH” (1:0.5, 900°C) adsorbent has been identified as the most promising material for hydrogen storage due to its high specific surface area, well-developed microporous structure, and superior hydrogen adsorption capacity at low temperatures. These findings contribute to the ongoing development of efficient and sustainable hydrogen storage technologies. Future studies should focus on optimizing activation conditions, exploring alternative activation agents, and functionalizing the adsorbent surface to enhance hydrogen uptake at ambient temperatures. Additionally, scaling up the production of these materials and evaluating their long-term stability in real-world hydrogen storage applications will be essential for their commercial implementation.

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References

1. Park J.H., Ramasamy P., Kim S., Kim Y.K., Ahilan V., Shanmugam S., Lee J.S. Hybrid metal—Cu2S nanostructures as efficient co-catalysts for photocatalytic hydrogen generation// Chem. Commun. -2017. - Vol.53 (22). - P.3277–3280. DOI 10.1039/C7CC00071E.

2. Moriarty, P.; Honnery, D. Hydrogen’s role in an uncertain energy future // Int. J. Hydrog. Energy. - 2009. Vol.34. -P.31 -39. DOI 10.1016/j.ijhydene.2008.10.060.

3. Schlapbach, L.; Züttel, A. Hydrogen-storage materials for mobile applications. Mater. Sustain //Energy. -2010. -P.265-270. DOI 10.1142/9789814317665_0038.

4. Dincer I. Environmental and sustainability aspects of hydrogen and fuel cell systems. Int J Energy Res. -2007. - Vol.31(1). - P.29-55. DOI 10.1002/er.1226.

5. Weinberger B, Lamari FD. High pressure cryo-storage of hydrogen by adsorption at 77K and up to 50MPa // International Journal of Hydrogen Energy. - 2009. - Vol.34(7). - P.3058-3064. DOI 10.1016/j.ijhydene.2009.01.093.

6. Hwang S.-H., Kim Y. K., Seo H.-J., Jeong S. M., Kim J., Lim S. K. The enhanced hydrogen storage capacity of carbon fibers: the effect of hollow porous structure and surface modification // Nanomaterials. - 2021. - Vol.11(7). - 1830. DOI 10.3390/nano11071830.

7. Xia Y., Yang Z., Zhu Y. Porous carbon-based materials for hydrogen storage: advancement and challenges // Journal of Materials Chemistry A. - 2013. -Vol.1 (33). - P.9365-9381. DOI 10.1039/c3ta10583k.

8. Bader N., Ouederni A. Optimization of biomass-based carbon materials for hydrogen storage // Journal of Energy Storage. - 2016. -Vol.5. - P.77-84. DOI 10.1109/IREC.2015.7110967.

9. Kopac T. Hydrogen storage characteristics of bio-based porous carbons of different origin: A comparative review // International Journal of Energy Research. - 2021. Vol.45(15). - P.20497-20523. DOI 10.1002/er.7130.

10. Minoda A., Oshima S., Iki H., Akiba E. Synthesis of KOH-activated porous carbon materials and study of hydrogen adsorption // Journal of Alloys and Compounds. - 2013. -Vol.580. - P. S301-S304. DOI 10.1016/j.jallcom.2013.02.085.

11. Zhang C., Geng Z, Cai M., et al. Microstructure regulation of super activated carbon from biomass source corncob with enhanced hydrogen uptake // International Journal of Hydrogen Energy. - 2013. - Vol.38(22). - P.9243-9250. DOI 10.1016/j.ijhydene.2013.04.163.

12. Dincer I, Acar C. Review and evaluation of hydrogen production methods for better sustainability // International Journal of Hydrogen Energy. - 2015. -Vol.40(34). - P.11094-11111. DOI 10.1016/j.ijhydene.2014.12.035.

13. Rzepka M., Lamp P., de la Casa-Lillo M. A. Physisorbption of hydrogen on Microporous Carbon and Carbon nanotubes // The Journal of Physical Chemistry. - 1998. - Vol.102 (52). - P.10894-10898. DOI 10.1021/jp9829602.

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