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Inverse gas chromatographic characterization of halloysite-carbon composites as adsorbents for skin disinfectants from water solutions

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Abstract: The influence of physicochemical parameters of halloysite-carbon composites on the adsorption of skin disinfectants was investigated. The dispersive surface free energy and acid-base properties of halloysite-carbon composites were determined using inverse gas chromatography. The free adsorption energy was higher for all halloysite-carbon composites compared to the unmodified halloysite, which acted as a less electron-donating adsorbent. In contrast, the composite obtained using halloysite nanotubes (HNT) and ground microcrystalline cellulose as the carbon precursor exhibited the highest free adsorption energy and the Kb/Ka ratio. These results suggest that the free adsorption energy can be an additional factor influencing the adsorption process. We demonstrated that the composite with the highest free adsorption energy is effective for removing triclosan, chloroxylenol and chlorophene from water. The acid-base properties of halloysite-carbon composites enhance the adsorption of these compounds due to their acidic character. The composite with the highest Kb/Ka ratio removes adsorbates from aqueous solutions with the greatest efficiency. Parameters such as free dispersion energy, electron-donating, or electron-accepting properties of the adsorbent help explain why these composites exhibit high adsorption capabilities.

Introduction

Inverse gas chromatography (IGC) is often used for characterizing surface properties of adsorbents, including surface energy heterogeneity, adsorption heat, specific adsorption interactions , free surface energy, and acid–base properties (Shi B et al. 2011). The surface energy of solid adsorbents consists of dispersive and specific components, with the dispersive surface free energy significantly affecting surface properties (Shi B et al. 2011). The Dorris–Gray method (Dorris G.M., Gray D.G. 1980) and the Schultz method (Schultz J. et al. 1987) are commonly used to calculate surface dispersive free energy. Numerous studies have used IGC to characterize the surface properties of silica, alumina, polymers, paper fillers, wood, minerals, carbon fibers, single-wall and multi-wall carbon nanotubes, carbon blacks and graphite, and activated carbons (Gholami F. et al 2023), Mezgebe M. et al. 2012), Nuriel S. et al. 2005), Barber A.H. et al. 2004), Singh G. S. et al. 2004) , Peng Y. et al. 2013).

Chlorophenols are used in the production of biocides, cosmetics, plant protection products, and disinfectants. Although the use of triclosan in cosmetics or pharmaceuticals that come into contact with the skin is prohibited, its concentrations in surface waters can reach up to 2,300 ng/L (Bilal, M. et al (2020). Triclosan, chloroxylenol, and chlorophene have toxic effects on organisms and are commonly found in both surface and underground waters. Since these waters serve as a source of drinking water for humans, monitoring their occurrence and effectively removing these compounds from the aquatic environment is a crucial and ongoing research challenge (Gogoi, A. et al. 2018).

In our previous works, we presented the synthesis of halloysite-carbon adsorbents using sucrose as the carbon precursor and demonstrated their use for removing ketoprofen, naproxen, and diclofenac from water. (Szczepanik B. et al. 2019, Szczepanik B. et al. 2020). In another study, we explored two methods for preparing halloysite-carbon composites with cellulose as the carbon precursor. These composites were characterized using the SEM/EDS analysis, low-temperature nitrogen adsorption/desorption methods, and infrared spectrometry (FT-IR). We evaluated their adsorption properties for removing triclosan, chloroxylenol and chlorophene from water (Frydel L. et al. 2023). While the adsorption properties of the halloysite-carbon adsorbents were described by their specific surface area and carbon content, this information alone may be insufficient to fully explain their adsorption behavior.

In this study, we characterized halloysite-carbon composites using IGC and investigated how the obtained physicochemical parameters influence the adsorption of triclosan, chloroxylenol, and chlorophene by these materials. Understanding the impact of these parameters on the adsorption process can help explain the adsorption abilities of halloysite-carbon composites.

Theoretical background

Inverse gas chromatography (IGC) is a fast and precise technique that modifies conventional gas chromatography. The main goal of IGC is to study the interaction between the adsorbent and the adsorbate by introducing test substances with known properties into a column containing the tested adsorbent. The retention times and peak profiles of these substances provide information on the physicochemical parameters of the adsorbent (Ocak H. et al. 2008, Voelkel A. et al. 2015, Słomkiewicz P. M. 2019). The most important factors influencing the adsorption process include temperature, pressure, and the flow rate of the carrier gas.

Surface energy includes dispersion interactions, van der Waals forces, and polar interactions, such as acid-base interactions, hydrogen bonds, and π-π interactions (Szczepanik B. et al. 2020). Two main types of interactions occur between the adsorbent and the test substances: London dispersion forces (temporary dipole-induced dipole interactions) and specific intermolecular interactions (resulting from the interactions between polar functional groups). These interactions are characterized using adsorption free energy (ΔG_a) and surface free energy (γ_s).

The adsorption free energy is the sum of the dispersive (ΔG_{ad}) and the specific (ΔG_{asp}) adsorption free energy, while the surface free energy is the sum of the dispersive (γ_{sd}) and the specific (γ_{ssp}) surface free energy (Voelkel A. et al. 2015.). In the Schultz method, the adsorption free energy is calculated only on the basis of the dispersion part:

$$\Delta G_a = \Delta G_a^d = -RT \cdot \ln\left(V'_{N,n}\right) + C \tag{1}$$

where: R is the gas constant (J/(mol K)), T is the column temperature (K), $V'_{N,n}$ is the corrected retention volume of n-alkane (cm^3), C is a constant.

Free adsorption energy of the methylene group ΔG_{CH_2} is also taken into account in order to describe the interactions between the adsorbent and the adsorbate:

$$-\Delta G^{CH_2} = 2N_A \cdot a_{CH_2} \cdot \sqrt{\gamma_s^d} \cdot \sqrt{\gamma_l^d} \tag{2}$$

where: $-\Delta G^{CH_2}$ is the free energy of adsorption of the methylene group (J/mol), N_A is the Avogadro's number, a_{CH_2} is the cross-sectional area of the methylene group (m^2), γ_s^d is the dispersion component of surface free energy (mJ/m^2), and γ_l^d is the dispersion energy of the tested molecule (mJ/m^2).

The cross-sectional area of the methylene group a_{CH_2} can be calculated from the following equation:

$$a_{CH_2} = 1{,}09 \cdot 10^{14} \cdot \left(\frac{M}{\rho \cdot N_A}\right)^{\frac{2}{3}} \tag{3}$$

where: M is the molar mass (g) and P is the pressure at the exit of the column (Pa).

The value of γ_s^d can be calculated from the linear form of the following equation:

$$RT \cdot ln(V'_{N,n}) = 2N_A \cdot a_{CH_2} \cdot \sqrt{\gamma_s^d} \cdot \sqrt{\gamma_l^d} + C \tag{5}$$

The dependency graph of RT·ln $(V'_{N,n}) = \mathrm{f}\left(a_{CH_2} \cdot \sqrt{\gamma_l^d}\right)$ is a straight line. The surface free energy value is determined based on the slope coefficient of the line. The vertical distance on the axis from the n-alkane line to the point corresponding to the polar substance represents the specific adsorption energy component (ΔG_{asp}). The Schultz method allows for determining both the dispersive component of surface free energy γ_s^d and the specific adsorption free energy component ΔG_{asp}.

Experimental

Materials and Reagents

The hexane, heptane, octane, nonane were all purchased from P.O.Ch. (Gliwice, Poland).
The acetone acetonitrile, ethyl acetate, dichloromethane were purchased from Aldrich.
All reagents were of analytical grade.

The characterization of materials by IGC method

Chromatographic tests were performed using the IGC SEA - Inverse Gas Chromatography & Surface Energy Analyzer, equipped with a flame ionization detector supplied with hydrogen at 40 cm^3/min. and air at 250 cm^3/min. Helium was used as the carrier gas , with a constant flow rate of 20 cm^3/min through the column. Retention measurements were performed at 140°C, with the detector and dispenser temperatures set at 180°C. Glass columns, 30 cm in length and 3 mm in internal diameter, were used for the chromatographic measurements. Each adsorbent was isolated on both sides with approximately 2 cm of glass wool . Unmodified halloysite nanotubes (HNT) were used as a comparative material for the carbon-halloysite composites. The mass of the adsorbents ranged from 18 to 45 mg. Test substances were divided into two groups: non-polar substances (hexane, heptane, octane, nonane) and polar substances (acetone, acetonitrile, ethyl acetate, dichloromethane). Methane served as the calibration substance. The test substances were introduced using an autosampler onto the column with the adsorbent, with adsorbent

Table 1. Properties of the polar solvents used (AN – acceptor number, DN – donor number).

Solvent	**AN (kJ/mol)**	**DN (kJ/mol)**
Ethyl acetate	6.3	71.6
Acetone	19.7	71.2
Acetonitrile	10.5	59.0

Table 2. Parameters of the porous structure and carbon content obtained for HNT, H-carbon and HNT-carbon composites [14].

Adsorbent	SBET (m^2/g)	Carbon content (%)
HNT	53.65	-
HZn5	118.88	15.92
Hm5	115.07	15.64
HZn8	129.50	23.24
Hm8	101.94	18.21
HNTZn5	192.69	30.00
HNTm5	123.08	14.2
HNTZn8	187.07	32.26
HNTm8	112.24	17.88

Table 3. Dispersive surface free energy of adsorbents determined by the Schultz method.

Adsorbent	γ_{sd} [kJ/mol]
HNT	- 42.78
HZn5	- 55.09
HZn8	- 35.63
Hm5	- 52.29
Hm8	- 86.98
HNTZn5	- 52.18
HNTZn8	- 86.61
HNTm5	- 64.01
HNTm8	- 113.8

Table 4. Specific component of adsorption free energy ΔG_a^{sp} (kJ/mol) for adsorbents.

Solvent / Adsorbent	Acetone	Acetonitrile	Ethyl acetate	Dichloro-metane
HNT	- 9.10	- 11.83	- 14.70	-
HZn5	- 6.09	- 5.20	- 5.64	- 5.47
HZn8	- 6.74	- 9.70	- 7.26	- 7.54
Hm5	-	-	-	-
Hm8	- 11.17	- 18.55	- 11.09	- 12.56
HNTZn5	- 8.01	- 9.92	- 7.47	- 6.79
HNTZn8	- 14.00	- 17.49	- 14.10	- 13.71
HNTm5	- 10.16	- 15.45	- 10.93	- 11.01
HNTm8	- 11.79	- 17.83	- 11.07	- 11.48

Table 5. Acid-base properties of adsorbents.

Adsorbent	K_a	K_b	K_b/K_a
HNT	0.2111	0.2202	1.04
HZn5	0.0581	0.4107	7.07
HZn8	0.061	0.3659	6.00
Hm5	0.1266	0.7725	6.10
Hm8	0.0842	0.6907	8.20
HNTZn5	0.0692	0.352	5.09
HNTZn8	0.1265	0.6583	5.20
HNTm5	0.0919	0.556	5.62
HNTm8	0.0911	0.6425	7.05

Table 6. Dispersive surface free energy of HNT and obtained halloysite-carbon composites.

Adsorbent	γ_{sd} [mJ/m^2]
HNT	- 42.78
HZn5	- 55.09
HZn8	- 35.63
Hm5	- 52.29
Hm8	- 86.98
HNTZn5	- 52.18
HNTZn8	- 86.61
HNTm5	- 64.01
HNTm8	- 113.8

Table 7. Removal efficiencies on triclosan, chloroxylenol, and chlorophene for the applied adsorbents (adsorbent mass 0.1 g, concentration of adsorbate solution 20 mg/dm^3, contact time 24 h, temperature 25°C).

Adsorbent	Removal efficiencies on adsorbate [%]		
	triclosan	chloroxylenol	chlorophene
HNT	4.3	3.5	6.6
HZn5	49.1	46.2	42.6
HZn8	67.2	60.0	54.5
Hm5	38.8	31.3	41.4
Hm8	72.2	61.0	59.8
HNTZn5	56.0	81.4	74.1
HNTZn8	64.7	57.9	77.9
HNTm5	55.2	57.6	56.5
HNTm8	95.6	92.3	78.8

surface coverage values ranging from 0.0063 to 0.7 mmol/g. Adsorption parameters of the adsorbents were determined using the Cirrus Plus operational program.

Among the polar solvents, acetone and ethyl acetate are amphoteric substances, acetonitrile is a basic substance, and dichloromethane is an acidic substance (Table 1) (Gutmann, V 1978, Riddle F.L., Fowkes F.M. 1990).

Adsorption measurements

The details of the batch adsorption measurements are described in Frydel L. et al. (2023). For the adsorption experiments, we used halloysite from the Dunino mine (H), halloysite nanotubes (HNT), and halloysite-carbon composites prepared by two methods. The first method involved dissolving microcrystalline cellulose in a solution of zinc chloride(II) dissolved in hydrochloric acid before adding it to the halloysite. The second method involved milling halloysite and microcrystalline cellulose, with temperatures set at 500 and 800^{o}C for both methods. The samples were labelled as follows: HZn5 (referred to as H-Zn 500 in Frydel . et al. 2023,), Hm5 (referred to as H-m 500 in Frydel . et al. 2023), HZn8 (in Ref . Frydel L. et al. 2023 H-m 800), HNTZn5 (in Ref . Frydel L. et al. 2023), HNTm5 (referred to as HNT-m 500 in Frydel et al. 2023), HNTZn8 (referred to as HNT-Zn 800 in Frydel et al. 2023), and HNTm8 (referred to as HNT-m 800 in Frydel et al. 2023).

The removal efficiency of adsorbates from the solution (%R) was calculated based on the equation (5):

$$R = \left(\frac{C_0 - C_e}{C_0}\right) \cdot 100\ [\%] \qquad (5)$$

where: C_0 and C_e are the initial and equilibrium concentrations of the solution (mg/dm^3), respectively.

Results and Discussion

Characteristics of adsorbents

Parameters of the porous structure and carbon content for HNT, H-carbon and HNT-carbon composites are presented in Table 2 (Frydel L. et al. 2023). The carbon content in halloysite-carbon composites ranges from 14.12% for HNTm5 to 32.26% (% wt.) for HNTZn8, following the order: HNTm5 < Hm5 < HZn5 < HNTm8 < Hm8 < HZn8 < HNTZn5 < HNTZn8. The HNTZn5 and HNTZn8 samples contain the highest carbon amounts (30.00 and 32.26%, respectively). In addition, the largest specific surface areas are observed for the HNTZn5 and HNTZn8 composites.

Characteristics of adsorbents by inverse gas chromatography

Tables 2-4 present the values of adsorption free energy (ΔG_a) determined by the Schultz method, the specific free energy of adsorption (ΔG_{asp}), and the acid-base constants for all tested adsorbents.

The values of free adsorption energy for the tested adsorbents are summarized in Table 2. The highest free adsorption energy (ΔG_a) is observed for the following adsorbents: HNTm8, Hm8 and HNTZn8, suggesting that these materials exhibit the best adsorption properties. Adsorption-free energy values above 100 mJ/m^2 indicate very high activity (Voelkel A. et al. 2015).

The specific free adsorption energy (ΔG_{asp}) and the ratio of carbon content to oxygen content (C/O) are influenced by the presence and concentration of surface functional groups. As shown in Table 3, ΔG_a^{sp} values increase together with a higher C/O ratio. The HNTm8 and HNTZn8 composites exhibit both a high C/O ratio and high ΔG_a^{sp} values. The HNTm8 and HNTZn8 adsorbents have the highest specific free energy of adsorption as determined by the Schultz method. The $\frac{K_b}{K_a}$ ratios for the tested adsorbents are summarized in Table 4.

The values are greater than 1 for all of the tested materials, indicating that the surfaces of all adsorbents are basic (they are electron donors) and have more basic sites and fewer acidic sites. These adsorbents will interact more strongly with acidic substances. Among the halloysite-carbon composites, the most basic (electron-donating) materials include Hm8, HZn5, and HNTm8. This is confirmed by the $\frac{K_b}{K_a}$ ratio and the high values of the specific component of the free adsorption energy (ΔG_a^{sp}) for basic acetonitrile. The most acidic (electron-acceptor) material is HNTZn8, as evidenced by the lowest the $\frac{K_b}{K_a}$ ratio and the highest ΔG_a^{sp} value for acidic dichloromethane in the case of this adsorbent. The highest concentration of acidic (electron-acceptor) functional groups on the surface of HNTZn8 results in a low value of the $\frac{K_b}{K_a}$ ratio and a high ΔG_a^{sp} value for acidic dichloromethane. Conversely, the high concentration of basic (electron-donating) functional groups on the surface of Hm8 and HNTm8 results in high $\frac{K_b}{K_a}$ ratios and ΔG_a^{sp} values for basic acetonitrile. (see Table 5)

The values of the dispersive surface free energy for the obtained adsorbents were compared with those obtained for carbon materials (see Table 6). The HNTm8 adsorbent exhibits higher values of the specific component of surface free energy than the carbon materials, with the exception of spherical activated carbon.

The free adsorption energy of halloysite-carbon composites and halloysite nanotubes increases in the following order: HZn8 < HNT < HNTZn5 < Hm5 < HZn5 < HNTm5 < HNTZn8 < Hm8 < HNTm8. Conversely, the K_b/K_a ratio increases in the order: HNT < HNTZn5 < HNTZn8 < HNTm5 < HZn8 < Hm5 < HNTm8 < HZn5 < Hm8.

Adsorption experiments in batch system

This paper also discusses the influence of the adsorbent type on the adsorption of triclosan, chloroxylenol and chlorophene from water. The removal efficiencies of these adsorbates for the adsorbents used are collected in Table 7. The detailed data on the adsorption process are presented in Frydel L. et al. (2023).

Triclosan adsorption measurements on halloysite-carbon composites and halloysite nanotubes (HNT) show that the removal efficiency is in the range of 4.3 – 95.6% and displays the following order: HNT < Hm5 < HZn5 < HNTm5 < HNTZn5 < HNTZn8 < HZn8 < Hm8 < HNTm8.

For chloroxylenol adsorption on halloysite-carbon composites and halloysite nanotubes (HNT), the removal efficiency ranges from 3.5 to 92.3% and increases in the following order: HNT < Hm5 < HZn5 < HNTm5 < HNTZn8 < HZn8 < Hm8 < HNTZn5 < HNTm8.

In the case of chlorophene adsorption on halloysite-carbon composites and halloysite nanotubes (HNT), the removal efficiency is in the range of 6.55 - 78.8% and increases

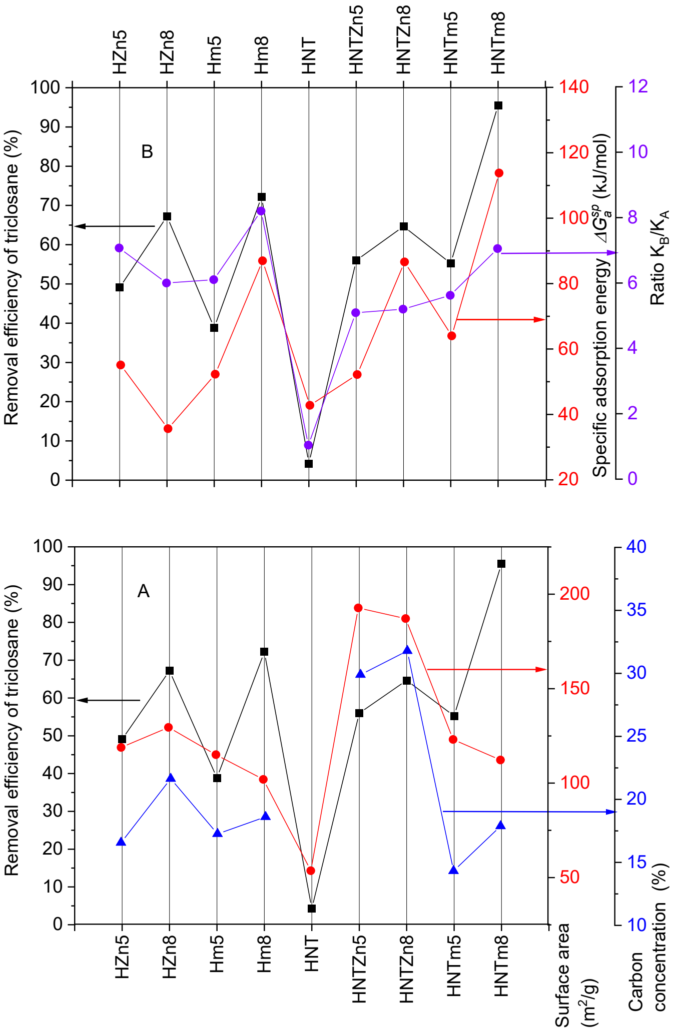

Figure 1. Dependence of the degree of triclosan removal by carbon-halloysite composites and halloysite nanotubes (HNT) on:
(A) - specific surface area and carbon content after pyrolysis,
(B) - $\frac{K_b}{K_a}$ ratio and specific adsorption energy.

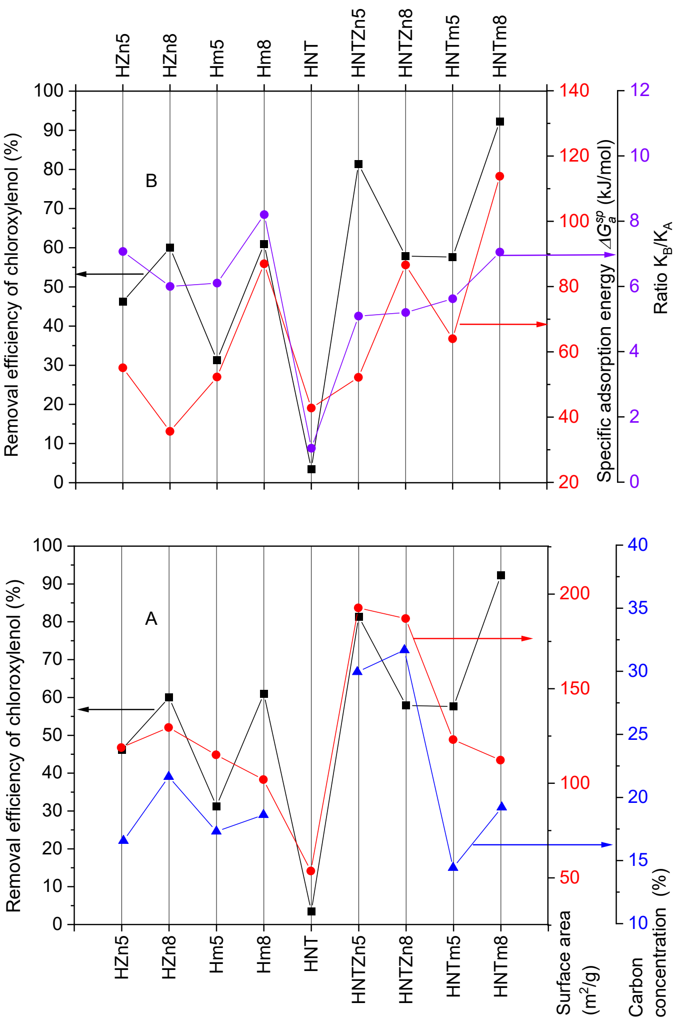

Figure 2. Dependence of the degree of removing chloroxylenol by carbon-halloysite composites and halloysite nanotubes (HNT) on:
(A) - specific surface area and carbon content after pyrolysis,
(B) - $\frac{K_b}{K_a}$ ratio and adsorption free energy.

sequentially: HNT < Hm5 < HZn5 < HZn8 < HNTm5 < Hm8 < HNTZn5 < HNTZn8 < HNTm8.

The HNTm8 composite proves to be the most effective adsorbent for removing all adsorbates from water. The removal efficiency of triclosan, chloroxylenol and chlorophene by HNTm8 is 95.55%, 92.26%, and 78.79%, respectively. In contrast, unmodified halloysite removed triclosan, chloroxylenol and chlorophene at significantly lower levels, specifically 4.26%, 3.5%, and 6.55%.

The influence of the selected physicochemical parameters of adsorbents on the adsorption of triclosan, chloroxylenol and chlorophene

The dependence of the specific surface area and carbon content in halloysite-carbon and HNT-carbon composites on the removal efficiency for triclosan, chloroxylenol, and chlorophene is presented in Figs. 1-3. However, it is chalenging to demonstrate a direct correlation between these physicochemical properties of individual adsorbents and the removal efficiency for all compounds.

The specific surface area of the HNTm8 adsorbent is 112.24 m²/g, with a carbon content of 17.88%. The removal rates for triclosan is 95.55%, for chloroxylenol 92.26%, and for chlorophene 78.79%. However, as shown in the graphs , the HZn8 adsorbent has a larger specific surface area and higher carbon content compared to the HNTm8 adsorbent. Despite this, the triclosan removal rate for HZn8 is only 67.21%, the chloroxylenol removal rate is 60%, and the chlorophene removal rate is 54.47%.

In order to explain this effect, the values of the $\frac{K_b}{K_a}$ ratio of halloysite-carbon composites and halloysite nanotubes (HNT) were additionally taken into account. These values range from 1.04 to 8.2, increasing in the following sequence: HNT < HNTZn5 < HNTZn8 < HNTm5 < HZn8 < Hm5 < HNTm8 < HZn5 < Hm8. Additionally, the free energy of adsorption of these composites and halloysite nanotubes (HNT), is in the range from -35, 63 to -113.8 kJ/mol, increasing in the sequence; HZn8 < HNT < HNTZn5 < Hm5 < HZn5 < HNTm5 < HNTZn8 < Hm8 < HNTm8.

The dependence of the $\frac{K_b}{K_a}$ ratio and the free adsorption energy of the halloysite-carbon composites and halloysite

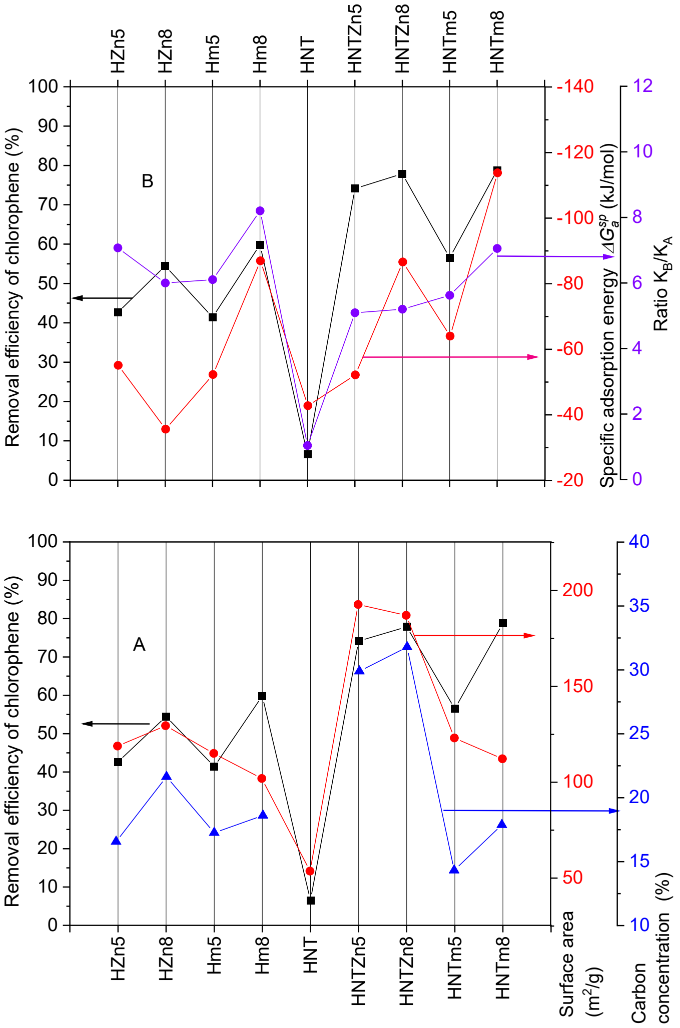

Figure 3. Dependence of the degree of removing chlorophene by carbon-halloysite composites and halloysite nanotubes (HNT) on:
(A) - specific surface area and carbon content after pyrolysis,
(B) - $\frac{K_b}{K_a}$ ratio and adsorption free energy.

nanotubes (HNT) on the degree of removing triclosan (Fig. 1), chloroxylenol (Fig. 2) and chlorophene (Fig. 3) is presented .

The $\frac{K_b}{K_a}$ ratio for the HNTm8 adsorbent is 7.05, with a free adsorption energy of -113.8 kJ/mol. In contrast, the HZn8 adsorbent has values, with a $\frac{K_b}{K_a}$ ratio = 6 and a free adsorption energy of -35.63 kJ/mol.

Conclusions

The physicochemical parameters, such as high specific surface area and carbon content of halloysite-carbon composites, do not fully explain the high removal efficiencies for triclosan, chloroxylenol and chlorophene from aqueous solutions when these materials are used as adsorbents. The most effective adsorbent for removing these compounds from water was HNTm8 composite, with the removal efficiencies of 95.55% for triclosan, 92.26% for chloroxylenol, and 78.79% for chlorophene. In contrast, unmodified halloysite exhibited low removal efficiencies, with triclosan, chloroxylenol and chlorophene removed by only 4.26%, 3.5%, and 6.55%, respectively.

We have demonstrated that surface energy and acid–base properties, as determined using the IGC method, can be additional factors influencing the adsorption process for halloysite-carbon composites.

We investigated the influence of free dispersion energy, acid-base properties, specific surface area, and carbon content of adsorbents on the removal efficiency of triclosan, chloroxylenol and chlorophene from water. The results indicated that an increase in free adsorption energy enhances the adsorption properties of the composites, leading to higher removal efficiencies of triclosan, chloroxylenol and chlorophene from water.

Considering the chemical nature of these adsorbates, the K_b/K_a ratio (which reflects acid-base properties) also influences the adsorption process. Since triclosan, chloroxylenol, and chlorophene are acidic, they tend to adsorb more efficiently onto adsorbents with a more basic character. HNTm8 adsorbent, with the highest K_b/K_a ratio, demonstrates that a higher K_b/K_a ratio correlates with greater removal efficiency for triclosan, chloroxylenol and chlorophene. Thus, HNTm8 is the most effective adsorbent for removing triclosan, chloroxylenol and chlorophene from water.

Comparing the removal efficiency of triclosan, chloroxylenol, and chlorophene with the specific surface area, carbon content, and especially the free dispersion energy and the electron-donating or electron-accepting properties of the adsorbent surface allows for a better assessment of the adsorbents' capacity to adsorb these compounds.

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Wyznaczanie właściwości kompozytów haloizyt-węgiel jako adsorbentów środków do dezynfekcji skóry z roztworów wodnych metodą inwersyjnej chromatografii gazowej

Streszczenie: Badano wpływ parametrów fizykochemicznych kompozytów haloizyt-węgiel na adsorpcję środków dezynfekcji skóry. Dyspersyjne właściwości swobodnej energii powierzchniowej i właściwości kwasowo-zasadowe kompozytów haloizyt-węgiel uzyskano za pomocą inwersyjnej chromatografii gazowej (IGC). Wartość swobodnej energii adsorpcji była wyższa dla wszystkich kompozytów haloizyt-węgiel w porównaniu do haloizytu niemodyfikowanego (z wyjątkiem H-Zn 8), kompozytu otrzymywanego z wykorzystaniem haloizytu z kopalni „Dunino" i rozpuszczonej celulozy mikrokrystalicznej jako prekursora węgla). Wykazaliśmy, że kompozyt HNT-m 8 charakteryzujący się najwyższą energią swobodnej adsorpcji jest najlepszym adsorbentem do usuwania triklosanu, chloroksylenolu i chlorofenu z wody. Właściwości kwasowo-zasadowe kompozytów haloizyt-węgiel (stosunek Kb/Ka sugerujący zasadowy charakter powierzchni kompozytu) sprzyjają adsorpcji triklosanu, chloroksylenolu i chlorofenu na powierzchni kompozytu ze względu na ich kwaśny charakter. HNT-m 8 posiada najwyższą wartość stosunku Kb/Ka i z największą skutecznością usuwa triklosan, chloroksylenol i chlorofen z roztworów wodnych. Takie parametry jak swobodna energia powierzchni, właściwości adsorbentu w zakresie oddawania i przyjmowania elektronów ułatwiają zrozumienie, dlaczego kompozyty te wykazują wysokie zdolności adsorpcyjne. Aspekt ten jest szczególnie przydatny przy określaniu właściwości kompozytów haloizytowo-węglowych, poza najczęściej stosowanymi parametrami, np. powierzchnią właściwą i zawartością węgla.