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## ADSORPTION PROPERTIES OF AMMONIA MOLECULES ON DIACETATECELLULOSE–SILICA HYBRID BIONANOCOMPOSITE

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### Abstract

In this study, the adsorption isotherm of ammonia molecules on diacetatecellulose (DAC)–silica hybrid bionanocomposite at 303 K was described from the initial stage to saturation using the three-term TVFM equation. The adsorption thermokinetics indicated that the equilibrium time for the initial adsorption of ammonia molecules was 6.5 hours, and the differential heat of adsorption was 38.7 kJ/mol. The differential molar entropy curve showed that up to an ammonia amount of 1 mmol/g, the mobility of molecules on the adsorbent surface was high, whereas beyond 1 mmol/g, the ammonia molecules were found to be firmly anchored to the adsorbent.

**Keywords:** adsorption, isotherm, diacetatecellulose, silica, ammonia, differential heat and entropy

### Introduction

Atmospheric air pollution by harmful gases is one of the pressing environmental problems of our time. Among them, ammonia (NH<sub>3</sub>) is of particular concern due to its large-scale emissions from industrial and agricultural sources. Even at low concentrations, ammonia has adverse effects on human health and the environment, which necessitates the development of new materials for its efficient adsorption (Amanda M. B. et al. 2013). In recent years, increasing attention has been paid to organic–inorganic hybrid bionanocomposites as environmentally friendly and highly efficient adsorbents (Musawenkosi G. Shange et al., 2024; Inês Portugal et al., 2010) In this

context, the combination of biodegradable and functionally rich diacetatecellulose with silica, which is characterized by high surface area and stability, is considered promising. The sol–gel method enables the synthesis of homogeneous DAC–silica hybrid materials with a porous structure at relatively low temperatures (Vitaly Kocherbitov et al., 2008; Ahmed Salama, 2016).

The investigation of the ammonia adsorption properties of DAC–silica hybrid bionanocomposites is scientifically and practically relevant from the standpoint of developing new functional materials for gas purification and sensor systems (Hua Zou et al., 2008; Sadanand Pandey et al., 2011).

**The aim of the study** is to analyze the adsorption isotherm, thermokinetics, differential heat, and entropy of ammonia molecules on the DAC–silica hybrid bionanocomposite at 303 K.

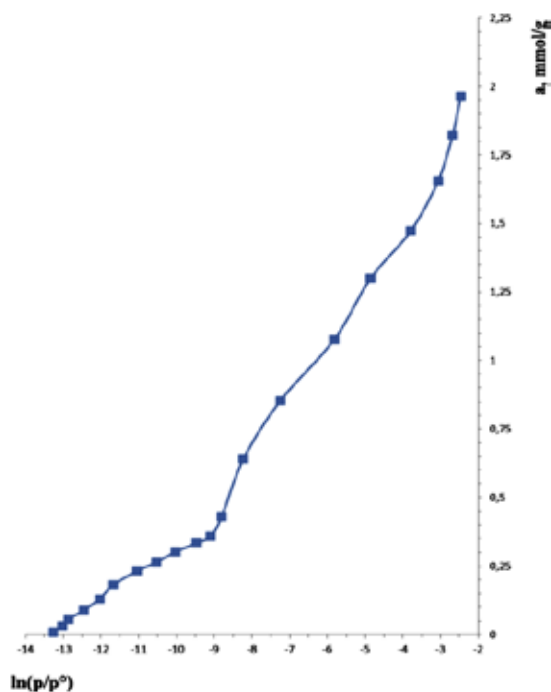
### Materials and Methods

Adsorption-calorimetric investigation were performed on a universal high-vacuum volumetric installation. The volumetric-liquid method and an isothermal differential automatic microcalorimeter of the Tian-Calvet were used to measure the values of adsorbed compounds on the bionanocomposite (Yarkulov A. et al., 2022).

### Theory of volumetric filling of micropores (TVFM) equation

The adsorption processes occurred on the microporous zeolites related to the bulk filling mechanism. The TVFM method was

**Figure 1.** Adsorption isotherm of ammonia on the DAC–silica hybrid bionanocomposite at 303 K



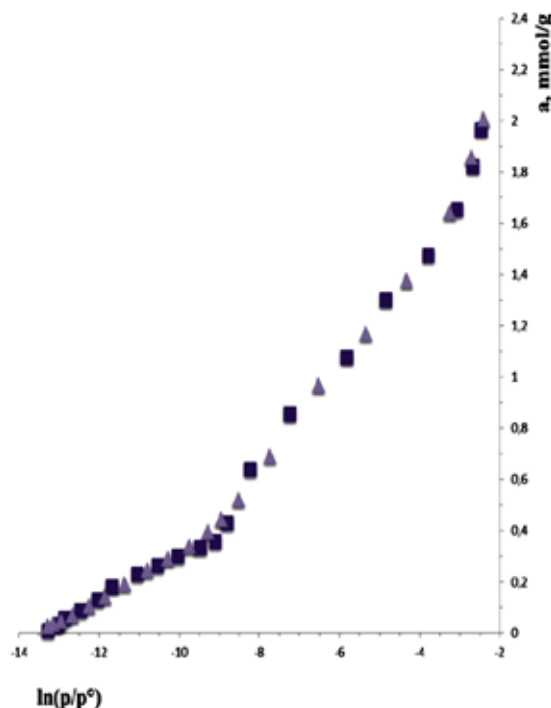
In Figure 2, the adsorption isotherm of ammonia on the DAC–silica hybrid bionanocomposite was analyzed using the TVFM equation (Yarkulov A. Yu., 2024). As can be seen from Figure 2, the calculated data ob-

performed to calculate the adsorption degree ( $\theta$ ) according to Equation.  $\theta = \exp[-(A/E)n]$  where  $n$  is independent parameter and  $E$  is adsorption energy. The  $n$  exponent depends on the structure of the adsorbent (Akhror Yarkulov et al., 2024).

### Results and Discussion

For the DAC–silica hybrid bionanocomposite, ammonia adsorption at low relative pressure ( $\ln(p/p_0) = -9.0$ ) increases linearly up to 0.36 mmol/g. With further increase in pressure, the isotherm rises monotonically and reaches saturation at approximately 2.0 mmol/g (Figure 1). The sharp initial increase of the isotherm indicates the presence of active adsorption sites in the bionanocomposite, where rapid adsorption occurs. It also suggests structural uniformity of the micropores and a high sorption capacity of the material.

**Figure 2.** Adsorption isotherm of ammonia on the DAC–silica hybrid bionanocomposite at 303 K calculated using the TVFM equation



tained using TVFM are in good agreement with the experimental results.

The ammonia adsorption isotherm on the DAC–silica hybrid bionanocomposite is well described by the three-term TVFM equation:

$$a = 0,358 \exp [-(A/30,10)]^9 + 0,953 \exp [-(A/19,35)]^5 + 5,014 \exp [-(A/1,43)]^3$$

The parameters of the equation are as follows:

for the first term,  $a_{01}=0,358$  mmol/g,  $E_{01}=30,10$  kJ/mol, ( $n_1 = 9$ );

for the second term,  $a_{02}=0,953$  mmol/g,  $E_{02}=19,35$  kJ/mol ( $n_2 = 5$ );

for the third term,  $a_{03}=5,014$  mmol/g,  $E_{03}=1,43$  kJ/mol,  $n_3=3$ .

The TVFM analysis indicates that ammonia adsorption on the DAC–silica hybrid bionanocomposite proceeds predominantly in three types of adsorption phases. Approx-

imately 5.7% of ammonia adsorption occurs in the first adsorption phase, about 15% in the second phase, and nearly 80% in the third phase.

To determine the number, strength, and localization of adsorption centers, as well as to clarify the structure of the nanocomposite material, the adsorption mechanism of polar molecules, the nature of intermolecular interactions, molecular conformations, and the state of adsorption clusters, a correlation between molecular structure and thermodynamic characteristics was established, and the adsorption thermokinetics were investigated (Yakubov Y. et al., 2016).

**Figure 3.** Dependence of the adsorption equilibrium time on the amount of ammonia adsorbed on the DAC–silica hybrid bionanocomposite

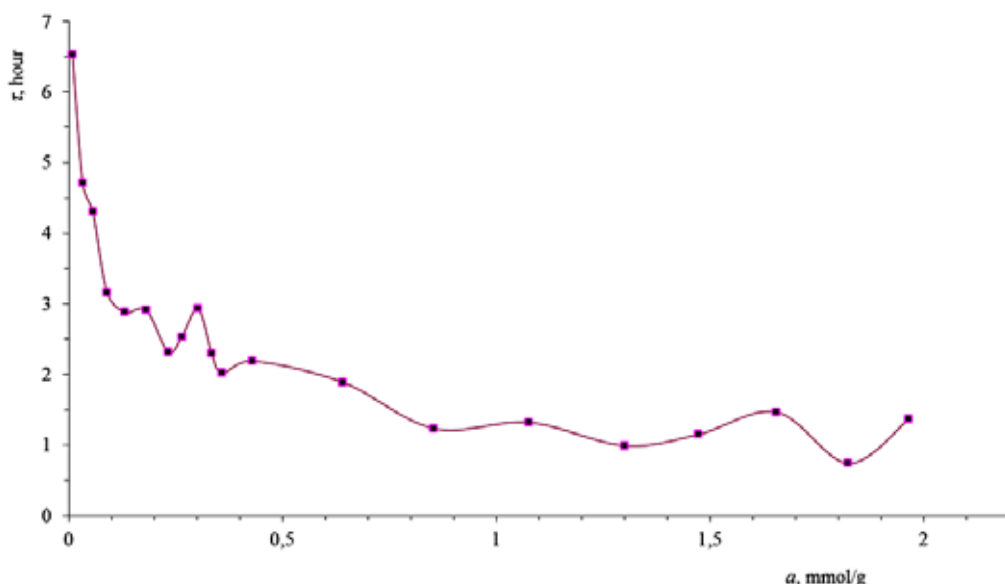


Figure 3 shows the dependence of the adsorption equilibrium time ( $\tau$ ) on the adsorption amount of ammonia on the DAC–silica hybrid bionanocomposite. The initial adsorption of ammonia molecules proceeds relatively slowly, with the equilibrium time reaching 6.5 h. When the adsorbed amount approaches 0.131 mmol/g, the equilibrium time decreases to 2.88 h. Subsequently, in the thermokinetics of ammonia adsorption on the DAC–silica hybrid bionanocomposite, the equilibrium time initially changed stepwise and later varied linearly, with the final adsorption equilibrium being reached in approximately 1.5 h.

A number of scientific studies have been carried out on the thermodynamics of ad-

sorption, and positive results have been achieved. In order to investigate adsorbate–adsorbent and adsorbate–adsorbate interactions during the uptake of adsorbate molecules with different structures within the pores of an adsorbent, it is important to study the heat and entropy of adsorption (Yakubov Y. et al., 2024).

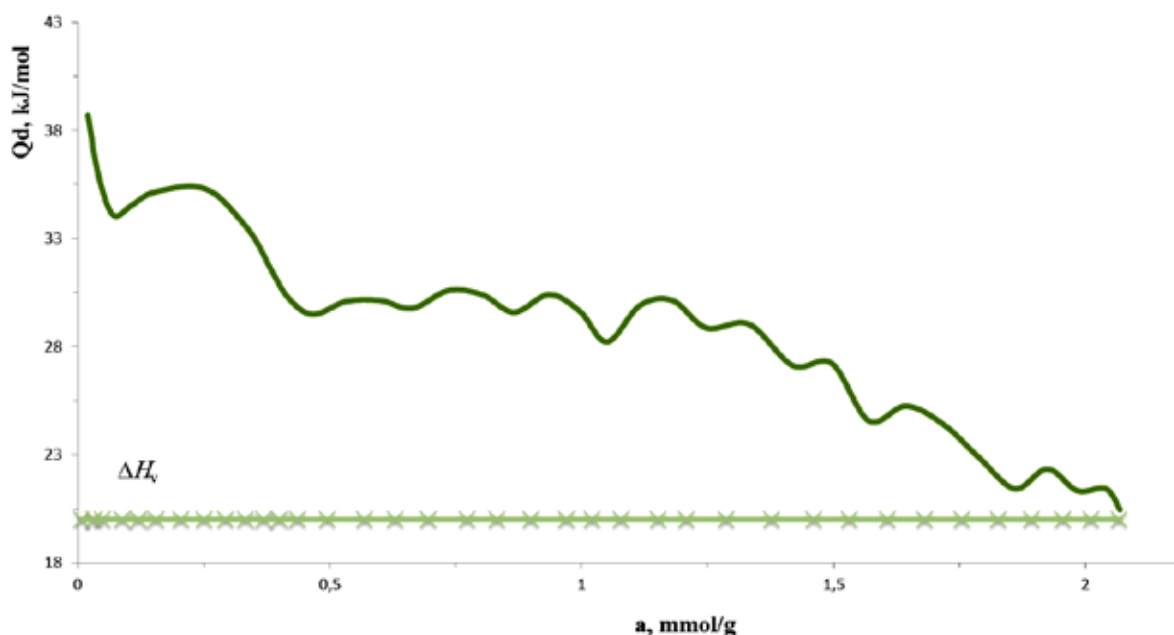
The application of the heat flow compensation method based on the Peltier effect made it possible to measure the heat of adsorption with higher accuracy. Adsorption measurements were performed using a universal high-vacuum apparatus, which enabled precise control of adsorption experiments and highly accurate dosing of the adsorbate (Yarkulov A. Yu., 2020).

The figure 4 shows the differential heat of adsorption of ammonia gas on the DAS–silica hybrid bionanocomposite.

The initial differential heat of ammonia adsorption on the DAC–silica hybrid bionanocomposite was found to be 38.7 kJ/mol. Subsequently, the heat of ammonia adsorption proceeded in a stepwise manner, which can conventionally be divided into two major hydrophilic centers.

In the first high-energy hydrophilic region, ammonia adsorption varies within the range of 0.07–0.467 mmol/g, and the differential heat of adsorption sharply decreases from 34.10 to 29.50 kJ/mol. The first region can be attributed to the functional groups present in the adsorbent structure, whereas the second hydrophilic region is likely formed due to interactions between ammonia molecules and the porous layers of the adsorbent.

**Figure 4.** Differential heat of adsorption of ammonia gas on the hybrid DAC–silica bionano-composite at 303 K. The dashed line represents the heat of condensation of ammonia at 303 K



According to the steps observed in the (Qd) curve, this region can be divided into nine sections, where the heat of adsorption changes from 29.5 kJ/mol down to the heat of condensation.

The complex nature of isotherms and the values of differential heats of adsorption reflect even the subtle details of the adsorption interactions between the adsorbate and the adsorbent, as well as the interactions among adsorbate molecules themselves.

In the second, relatively lower-energy hydrophilic region, ammonia adsorption varies from 0.467 mmol/g up to complete saturation. Each of the nine sections corresponds to approximately 0.2 mmol/g and is characterized by a gradual decrease in the heat of adsorption from 29.5 kJ/mol to approximately the condensation heat of ammonia (20 kJ/mol).

Thus, ammonia adsorption on the DAC–silica hybrid bionanocomposite occurs at two types of hydrophilic centers. The net heat of adsorption is approximately 10 kJ/mol. The stepwise character of the differential heat curve, together with the presence of active centers corresponding to 0.4 mmol/g and porous hydrophilic layers corresponding to 0.2 mmol/g for ammonia adsorption, indicates that adsorbent–adsorbate interactions occur with an initial heat of 38.7 kJ/mol and that a polymolecular adsorption process takes place.

In studying the adsorption of various molecules on adsorbents, it is important to investigate not only the heat of adsorption but also the entropy, in order to better understand adsorbent–adsorbate and adsorbate–adsorbate interactions.

The adsorption entropy ( $\Delta S_d$ ) of ammonia gas on the DAC–silica hybrid bionanocompos-

ite was calculated using the Gibbs–Helmholtz equation, based on the adsorption isotherm

and the differential heat of adsorption (Abdurakhmonov Eldor Baratovich et al., 2020).

**Figure 5.** *Differential entropy of adsorption of ammonia molecules on the DAC–silica hybrid bionanocomposite at 303 K. The dashed line represents the average molar integral entropy; the entropy of liquid ammonia was taken as zero*

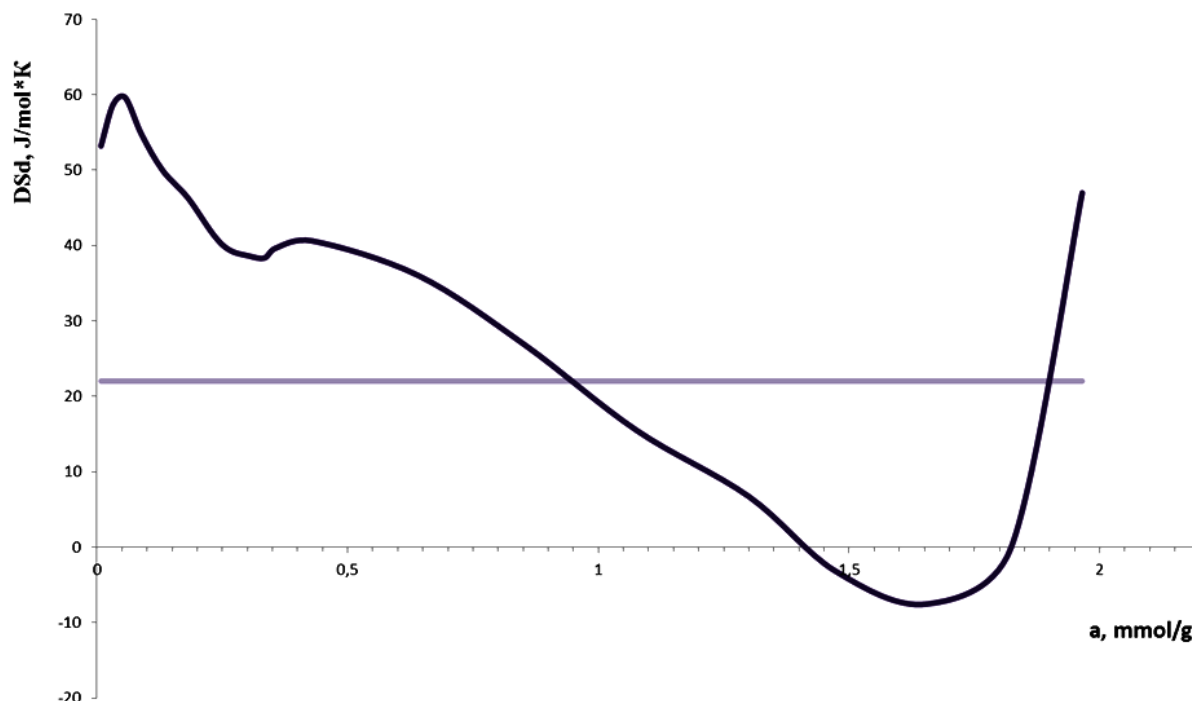


Figure 5 shows the dependence of the differential adsorption entropy of ammonia gas on its adsorption amount on the DAC–silica hybrid bionanocomposite.

The average molar integral entropy of ammonia adsorbed on the DAC–silica hybrid bionanocomposite is 22.04 J/mol·K. As can be seen from the figure, when the adsorbed amount is up to 1 mmol/g, the mobility of ammonia molecules on the adsorbent surface is relatively high. After 1 mmol/g, a more rigid fixation of ammonia molecules on the adsorbent surface is observed. With a further increase in the amount of adsorbed ammonia, beyond 1.97 mmol/g, the mobility of the adsorbate molecules increases again.

### Conclusions

1. Adsorption isotherms of ammonia molecules on the DAC–silica hybrid bionanocomposite were obtained using a precision adsorption–calorimetric method.

2. The obtained isotherms were analyzed based on the equations of the theory of volume filling of micropores. The adsorption isotherm of ammonia was well described by the three-term equation of the micropore volume filling theory for the hybrid bionanocomposite.

3. The thermokinetic study of ammonia adsorption on the DAC–silica hybrid bionanocomposite showed that the establishment of adsorption equilibrium proceeds slowly, with an equilibrium time of 6.5 hours.

4. The differential heat of ammonia adsorption on the DAC–silica hybrid bionanocomposite exhibits a stepwise character, with an initial heat value of 38.7 kJ/mol.

5. The differential molar entropy curve indicates that when the ammonia amount is up to 1 mmol/g, the mobility of molecules on the adsorbent surface is high, whereas beyond 1 mmol/g the ammonia molecules become more firmly fixed on the adsorbent surface.

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