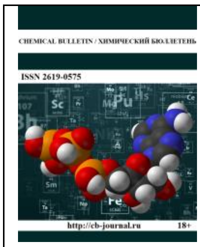

*Научно-исследовательский журнал «**Chemical Bulletin**»*
https://cb-journal.ru
2025, Том 8, № 2 / 2025, Vol. 8, Iss. 1 https://cb-journal.ru/archives/category/publications
Научная статья / Original article
УДК 544.723.212
DOI: 10.58224/2619-0575-2025-8-2-1

Adsorption of Acetone on HNO_3-Treated AG-3 Activated Carbon: Performance and Kinetic Study

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Abstract: *the study focuses on enhancing the adsorption of acetone, a prevalent oxygenated volatile organic compound (VOC), using HNO_3-modified AG-3 activated carbon (AC) to mitigate its environmental and health impacts. It aims to optimize HNO_3 modification of AG-3 AC, targeting enhanced acetone adsorption capacity and improved kinetics.*

Methods: *In this work, commercial AG-3 was treated with 2 M, 4, M and 6 M HNO_3 solutions through reflux heating at 100 °C, followed by washing and drying. Adsorption experiments were conducted using gravimetric analysis at 25 °C and 1 atm, with kinetic data fitted to pseudo-first-order, pseudo-second-order, Elovich, and Morris-Weber models. The modified ACs were evaluated for their specific adsorption capacities and time-dependent adsorption behaviors.*

Results: *Results showed that HNO_3 treatment enhanced acetone adsorption, with the 2 M HNO_3-treated AC (HAC-2) exhibited the highest capacity of 0.2951 g/g, a 15 % improvement over unmodified AG-3 (0.2570). Kinetic studies revealed that the pseudo-second-order kinetic model best described the adsorption process, indicating chemisorption as the primary mechanism. As concentration of HNO_3 increased (4 M and 6 M), it led to reduced adsorption capacity compared to HAC-2, suggesting excessive oxidation may damage the carbon structure.*

Conclusions: *The study concludes that the optimal HNO_3 concentration for enhancing acetone adsorption on G-3 AC lies around 2 M. This approach highlights the potential of HNO_3-modified AG-3 as an effective adsorbent for acetone remediation in adsorption application.*

Keywords*: Granular Activated Carbon, Acetone Adsorption, HNO_3 Modification, VOCs, Adsorption Kinetics*

For citation: Tkabo Tewelde Sahle Adsorption of Acetone on HNO_3-Treated AG-3 Activated Carbon: Performance and Kinetic Study. Chemical Bulletin. 2025. 8 (2). 1. DOI: 10.58224/2619-0575-2025-8-2-1

The article was submitted: January 9, 2024; Approved after reviewing: March 14, 2025; Accepted for publication: May 15, 2025.

Introduction

Volatile organic compounds (VOCs) are organic chemicals with an initial boiling point of 25 °C or lower at standard atmospheric pressure. They typically have high vapor pressure and low solubility in water at room temperature [1]. Due to their toxic and carcinogenic nature, VOCs pose health risks through both skin contact and inhalation. Additionally, they contribute to the formation of secondary air pollutants via photochemical reactions [2]. VOC emissions originate from both human activities and natural sources. Human-related (anthropogenic) sources include mobile sources like vehicles, stationary fuel-burning systems, and various industrial operations. A specific group—oxygenated VOCs—mainly arises from the oxidation of atmospheric hydrocarbons, solvent evaporation, and incomplete fuel combustion. These compounds can include alcohols, ethers, aldehydes, ketones, esters, and organic acids [3].

Acetone (C_3H_6O) is among the most prevalent oxygenated volatile organic compounds (VOCs) found in the atmosphere. It is also one of the most commonly detected hydrocarbon compounds in indoor environments such as laboratories and office spaces. Due to its excellent solvent properties and chemical reactivity, acetone is extensively utilized as a solvent or chemical intermediate across a range of industrial sectors, including pharmaceuticals, plastics production, printing, and electronics manufacturing [4]. Additionally, it promotes more efficient fuel burning as it contains high oxygen which helps to enhance thermal efficiency by ensuring better energy release during combustion and has also high vaporization rate leading to more complete combustion. Furthermore, its low viscosity improves atomization. This finer atomization, along with its rapid vaporization, ensures better fuel-air mixing, optimizing combustion performance in engines and other combustion systems [5]. However, exposure to acetone vapor poses significant risks to human health and environment. When inhaled, it can lead to a variety of acute symptoms such as headaches, throat irritation, coughing, and dizziness. Prolonged or high-level exposure may have more severe effects, potentially impairing the central nervous system and disrupting normal neurological function [6]. Due to these effects, effective removal of acetone vapors from industrial and laboratory emissions is crucial to mitigate environmental and health risks.

Various technologies have been employed for the abatement of VOC emissions like acetone, including condensation, catalytic oxidation, and biodegradation [7,8]. Among these methods, adsorption has emerged as a particularly advantageous method for VOC removal from polluted air streams. The efficacy of adsorption lies in its potential for high removal efficiency, operational simplicity, and relative cost-effectiveness [9,10]. Consequently, numerous studies have focused on identifying and developing cost-effective adsorbents for VOC treatment. Activated carbon (AC) stands out as a preferred adsorbent due to its established performance in gas separation and storage applications [11]. Its widespread use stems from its intrinsic properties, namely, a high specific surface area, resulting in a high adsorption capacity; a rapid adsorption rate, facilitating efficient pollutant capture; and the potential for regeneration, enabling repeated use and reduced waste generation. These characteristics collectively position AC as a prominent solution for VOC control [12, 13].

However, commercially available ACs often exhibit limitations in adsorption capacity and selectivity stemming from their inherent surface chemistry and pore structure [14]. To overcome these limitations, various modification strategies are implemented to tailor these properties, including physical methods, chemical treatments, surface oxidation, and impregnation with metal oxides or salts [15]. Chemical modification is often favored for directly influencing the adsorbent's surface chemistry to enhance the adsorption capacity of the AC [16]. A range of activating agents, such as H_3PO_4, H_2SO_4, KOH, NaOH, $CaCl_2$, and $ZnCl_2$, are utilized in chemical activation [17]. Surface modification of AC is a well-established strategy for enhancing adsorption performance. Introducing oxygen-containing functional groups, such as hydroxyl and carboxyl groups, onto the AC surface increases its overall polarity. This enhanced polarity, in turn, improves the adsorption capacity for polar molecules [18]. HNO_3 oxidation treatment results in an AC surface characterized by both a high concentration of oxygen-containing functional groups and increased acidity [19].

This study used HNO_3 impregnation to modify a commercial Russian brand activated granular carbon (AG-3) for acetone adsorption. The objective was to enhance its adsorption capacity for acetone. While AG-3 is commonly used in Russia for VOCs removal including acetone, its modification with HNO_3 to enhance adsorption capacity of acetone is not yet studied and need to be investigated. The research gaps include optimization of the acid concentration to modify AG-3 and understanding of its correlation with its adsorption performance. Addressing these gaps is crucial for developing effective and sustainable acetone removal strategies tailored to increased adsorption capacity of acetone and other polar VOCs.

Materials and methods

Chemicals used

Acetone, a colorless transparent liquid with 99.7% purity (GOST 2768-84) obtained from ХИММЕД (Russia) was used as an adsorbate. A commercial AG-3 grade activated carbon (GOST 20464-75) was used as an adsorbent. A solution of HNO_3 (65%, GOST 4461-77) also obtained from ХИММЕД (Russia) was used as a chemical modifier.

Preparation of Modified AG-3 Activated Carbons

In this experiment, AG-3 was modified via reflux heating with nitric acid (HNO_3) at 100 °C for 2 hours. AG-3 was treated with 2 M, 4 M, and 6 M HNO_3 solutions. Following the reflux process, the mixtures were cooled to room temperature and washed with distilled water until the filtrate reached a neutral pH. Th resulting solids were dried in an oven at 110 °C until a constant mass was achieved. The modified ACs were designated HAC-2, HAC-4, and HAC-6, corresponding to the 2 M, 4 M, and 6 M HNO_3 treatments, respectively.

Specific Adsorption Capacity, Kinetics and mechanisms of Adsorption Study

The adsorption processes of acetone onto both commercial and HNO_3-modified AG-3 were investigated using a gravimetric analysis method at room temperature and 1 atm pressure. The mass change of the ACs were recorded at predetermined time intervals (20, 40,60, 90, 120, 180 and 240 minutes) using the analytical balance to determine the mass of adsorbed solvent. The mass of acetone adsorbed per gram of AG-3 (g/g) was determined using the following formula:

$$q_t = \frac{m_t - m_o}{m_o}$$

where q_t is the amount of adsorbed acetone in one-gram activated carbon, g/g; m_0 and m_t are the mass of the AG-3 at the beginning of the experiment and at the current time, g.

The equilibrium adsorption (q_e) of each AC was determined by measuring until negligible mass change was observed on the AC under study. To investigate the kinetics, the time-dependent changes in adsorption capacity (q_t) at 25 °C give the progress of the adsorption process. The experimental data were then further analyzed using Lagergren equation of pseudo-first-order (PFO), Ho-Mackay pseudo-second-order (PSO), Elovich, and Morris-Weber intraparticle diffusion models to study the kinetics and mechanisms of adsorption of the ACs. The equations are given as follows [20].

$$Log(qe - qt) = Log(qe) - \frac{k1}{2.303} \times t \text{ ----------------------------- PFO equation}$$

Where q_e is the adsorption capacity of the AC at equilibrium ; q_t is the adsorption capacity of the AC at time t, min ; k_1 is the pseudo-first-order velocity constant, g/g.min.

$$\frac{1}{qt} = \frac{1}{k2 \times qe^2} + \frac{t}{qe} \text{ ------------------------------------- PSO equation}$$

Where q_e is the adsorption capacity of the AC at equilibrium ; q_t is the adsorption capacity of the AC at time t, min ; k_2 is the pseudo-second-order velocity constant, g/g.min.

$$qt = \frac{1}{\beta} \times \ln(\alpha \times \beta) + \frac{1}{\beta} \times lnt \text{ ------------------------------ Elovich equation}$$

where q_t is the adsorption capacity at time t, g/g; β is the desorption constant, g/g; α is the initial adsorption rate, g/g.min.

$$qt = k \times t^{1/2} + C \text{ --- Morris-Weber equation}$$

where q_t is the adsorption capacity at time t, g/g; t is time, min; k is the diffusion rate constant of the Morris-Weber equation, g/g×min$^{1/2}$. C is the mass transfer resistance constant in the boundary layer.

Results and Discussion

Adsorption Capacity of acetone by the Commercial and HNO_3-Modified AG-3

The data presented in Table 1 reveal the specific acetone adsorption capacities (q_e) of AG-3 AC following modification with varying concentrations of HNO_3.

Table 1

Specific Acetone Adsorption Capacities of Commercial and HNO3-modified AG-3.

Solvent	Specific Adsorption capacity (q_e), g/g			
	HAC-0	HAC-2	HAC-4	HAC-6
Acetone	0.2570	0.2951	0.2857	0.2782

The unmodified AG-3 (HAC-0) exhibits an adsorption capacity of 0.2570 g/g. Treatment of AG-3 with HNO_3 generally increases the acetone adsorption capacity, with HAC-2 demonstrating the highest capacity of 0.2951 g/g, representing an approximately 15% improvement over HAC-0. However, increasing the HNO_3 concentration beyond 2 M appears to have a diminishing effect on adsorption capacity. HAC-4 showed a slightly reduced adsorption capacity of 0.2857 g/g compared to HAC-2, and HAC-6 exhibited the lowest capacity among the modified ACs at 0.2782 g/g. These results suggest that the optimal HNO_3 concentration for enhancing acetone adsorption on AG-3 AC lies around 2 M under room temperature (25 °C ± 1) and 1 atmosphere. The initial increase in adsorption capacity with 2 M HNO_3 can be attributed to the introduction of oxygen-containing functional groups onto the AC surface. As an oxidizing agent, HNO_3 promotes the formation of surface functionalities such as carboxylic acids, hydroxyls, and carbonyl groups [19,21]. These polar functional groups enhance the interaction between the AC surface and the polar acetone molecules through mechanisms such as hydrogen bonding and dipole-dipole interactions, leading to increased adsorption. However, the subsequent decrease in adsorption capacity at higher HNO_3 concentrations (4 M and 6 M) suggests that excessive oxidation may have detrimental effects on the AC's structure and surface properties.

Kinetics of Adsorption

The kinetic profiles of acetone adsorption on commercial and HNO_3-modified AG-3 are presented in Fig. 1, illustrating the time-dependent adsorption capacity (q_t) at 25 °C and 1 atm.

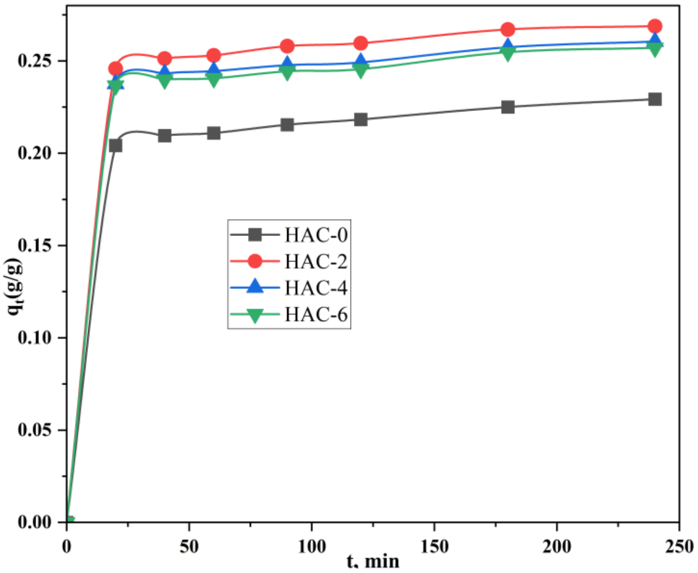

Fig. 1. Kinetics of adsorption of acetone by unmodified and HNO_3-Modified AG-3.

Within the first 20 minutes, all ACs exhibited rapid initial adsorption as indicated by a step increase in q_t. This fast adsorption is typical of physisorption, where acetone molecules readily interact with the AC surface due to the presence of vacant adsorption sites. HAC-2 showed the highest initial adsorption rate followed by HAC-4, HAC-6, and then HAC-0. This suggests that the 2 M HNO_3 modification significantly enhances the initial adsorption kinetics likely due to the increase in surface polarity and favorable surface functionalities, allowing for more efficient acetone molecule capture. In the intermediate time 20-120 minutes, the rate of adsorption decreases progressively for all ACs, and the slope flattens out, indicating that the adsorption process is slowing down as the available adsorption site became occupied. HAC-2 continues to exhibit the highest adsorption capacity across this time frame. Beyond 120 minutes, the adsorption curve of all begin to approach a plateau, indicating that the system is approaching equilibrium, at a point where the rate of adsorption is equal to the rate of desorption. Overall, the HNO_3 modification of AG-3 AC significantly improved the adsorption rate of acetone.

The adsorption kinetics and mechanisms of adsorption of acetone was further investigated by fitting the experimental data to PFO, PSO, Elovich and Morris-Weber intraparticle diffusion models. The kinetic parameters and correlation coefficients (R^2) obtained are summarized in Table 2. These results insights into the adsorption kinetics and mechanisms of acetone onto HAC-0, HAC-2, HAC-4 and HAC-6.

Table 2

Kinetic Parameters for acetone Adsorption on Unmodified and HNO3-Modified AG-3.

Kinetic Parameter	Activated Carbons			
	HAC-0	HAC-2	HAC-4	HAC-6
Pseudo-first order equation				
K_1, min^{-1}	0.0060	0.0064	0.0062	0.0067
q_e, g/g	0.0880	0.0864	0.0850	0.0788
R^2	0.5010	0.4683	0.4723	0.4871

Continuation of Table 2

Pseudo-second order equation				
k_2, g/g*min	0.8179	0.9574	0.9109	0.9149
q_e, g/g	0.2323	0.2721	0.2633	0.2600
R^2	0.9994	0.9997	0.9996	0.9995
Elovich equation				
α, g/g*min	361827	71909147	1.12E+08	716019054
β, g/g	101.0101	105.2632	111.1111	120.48193
R^2	0.9538	0.9693	0.9373	0.8834
Morris-Weber equation				
K	0.0023	0.0021	0.0020	0.0019
C	0.1942	0.2371	0.2288	0.2268
R^2	0.9949	0.9855	0.9805	0.9598

The most striking observation is the significantly higher correlation coefficients (R^2) for the PSO model across all the AC sample, indicating a perfect fit to the experimental data. This implies that the rate-limiting step in these adsorption processes is chemisorption, which involves the exchange of electrons between acetone and the commercial and HNO_3-modified AG-3 AC. In addition, the equilibrium adsorption capacity (q_e) values predicted by the PSO model align with the experimental results. The PSO model rate constants (K_2) of the modified ACs showed a higher value compared to HAC-0, indicating that the rate of chemisorption is slightly enhanced by HNO_3 modification.

In the data, the high R^2 values suggest that he Morris-Weber intraparticle diffusion model play a significant role in the adsorption kinetics. The plot of q_t versus $t^{1/2}$ is linear and don’t pass through the origin (Fig. 2), it indicates that intraparticle diffusion is still rate-limiting but not the only rate-limiting step and other mechanisms (chemisorption) also control the adsorption rate. The C values, representing the intercept, are not equal to zero, indicating that boundary layer diffusion may also contribute to the adsorption process.

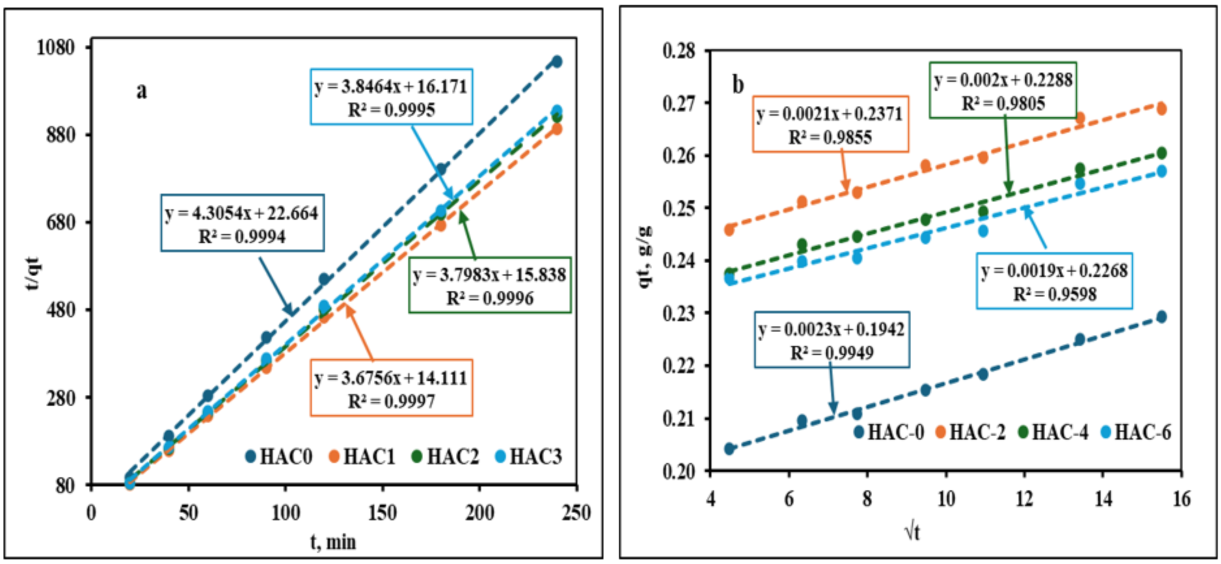

Fig. 2. Kinetics of Adsorptions of n-hexane vapors in the coordinates of the pseudo-second-Order (a) and Morris-Weber intraparticle diffusion (b) models.

Generally, the kinetic study of acetone adsorption on both commercial and HNO3-modified AG-3 revealed that the process is best described by the PSO kinetic model. HNO3 modification, with the highest at 2 M, enhanced the rate of adsorption. While intraparticle diffusion also plays a role, surface chemisorption dominates the kinetics.

Conclusions

The study successfully demonstrated that chemical modification of AG-3 using HNO_3 is an effective approach to enhance the adsorption capacity for acetone.

The optimal concentration of HNO_3, which lies around 2 M, significantly increased the adsorption capacity due to the introduction of polar functional groups that promote stronger interaction with acetone molecules. While the modification improved the kinetic parameters for adsorption, it was observed that excessive HNO_3 concentration could diminish the adsorbent's efficiency, emphasizing the need for a balanced approach in the modification process. The Kinetic studies further confirmed that the adsorption mechanism is primarily chemisorption, underlining the essential role of surface chemistry in VOC removal. This study contributes valuable insights into developing more effective and sustainable strategies for managing VOC emission in various industrial settings, Further research is recommended to explore the long-term stability and regeneration capabilities of HNO_3-modified AG-3 AC for practical application.

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