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Next-Generation Biomass-Derived Activated Carbon in Merkaptopurine Removal: Synthesis, Characterization, and Mechanistic Modeling

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Abstract

In this study, high surface area activated carbon was produced from poppy capsule pulp, an agricultural waste, by chemical activation and thermal carbonization; and the use of the produced material in the removal of 6-MP, an anticancer drug, from aqueous solutions was investigated. The textural and morphological properties of the activated carbon were characterized, and the BET surface area was determined as 1146.7 m^2/g, and the total pore volume as 0.774 cm^3/g. Within the scope of optimizing the adsorption process, the effects of adsorbent dosage, initial 6-MP concentration, contact time, and solution pH were examined. Optimum conditions for maximum adsorption efficiency (> 98%) were determined as 15 mg/50 mL adsorbent dose, 30 mg/L initial concentration, 90 minutes contact time, and the pH of the natural solution. Experimental isotherm data were fitted to commonly used isotherm models using nonlinear regression analysis; The process was found to fit the Langmuir isotherm model with the highest correlation coefficient (R^2 = 0.9937) and the lowest error functions (qmax = 199.16 mg/g). Experimental kinetic data were fitted to commonly used kinetic models using nonlinear regression analysis; it was observed that the Pseudosecond-order kinetic model (R^2 = 0.9937) perfectly simulated the process. The negative Gibbs free energy ($\Delta G°$) at all temperatures indicated that the process occurred spontaneously, while the negative standard enthalpy change ($\Delta H°$ = -41.963 kJ/mol) revealed an exothermic character. The findings indicate that this activated carbon, based on poppy capsule pulp and possessing a high mesopore volume, can be used as an effective, environmentally friendly, and sustainable adsorbent for the removal of pharmaceutical micropollutants from wastewater.

1. Introduction

Pharmaceutical micropollutants are considered one of the most serious environmental threats to water resources today, as they can cause ecotoxic effects even at very low concentrations. Due to the increase in the world population, advancements in medical technology, livestock practices, and industrial processes, drug consumption and, consequently, the release of these compounds into the environment have rapidly increased [1]. The use of pharmaceutical compounds is a global process predicted to double in the coming years [2].

These pollutants are transported to aquatic ecosystems through hospital waste, domestic sewage systems, animal waste, and uncontrolled disposal methods [3, 4]. The presence of pharmaceutical residues in surface waters and wastewater has been reported in numerous studies in the literature. Long-term exposure to trace levels of these compounds, such as 10–100 µg/L, can lead to serious health problems such as endocrine system disorders, cancer risk, organ damage, and the development of antibiotic-resistant bacteria [5]. In addition, their high thermal/chemical stability and hydrophilic structure cause these pollutants to be classified as "emerging contaminants" [6].

Wastewater treatment plants (WTPs) are considered one of the important sources for the release of pharmaceutical pollutants into the environment, as they are the main systems for collecting new generation pollutants found in domestic, agricultural, industrial and municipal wastewaters [2]. However, it has been shown that conventional wastewater treatment processes are insufficient in removing these

compounds due to the high solubility and stability properties of drugs [8]. The main reason for this is that conventional wastewater treatment plants (WWTPs) are not designed to provide complete removal of micropollutants present in low concentrations. These plants primarily focus on removing large particles, organic pollutants, and nutrients found in water at mg/L and g/L levels. Therefore, pharmaceutical compounds and their transformation products that cannot be completely removed by the treatment processes are carried to receiving water environments at different concentrations [9]. In some studies, pharmaceutical concentrations determined in WTP effluent waters have been reported to be higher compared to influent waters [7]. This situation is thought to be related to metabolite formation, biotransformation processes and the formation of more toxic intermediate products from the starting compounds [10].

Advances in modeling studies on the environmental behavior and transport of pharmaceutical pollutants allow for more accurate prediction of the persistence and mobility of these compounds in aquatic environments [11]. In parallel, supporting treatment technologies such as advanced oxidation processes are considered among the promising approaches in the removal of complex pollutant mixtures [12]. Currently, various advanced treatment methods such as membrane filtration [9], advanced oxidation processes [10], photocatalytic applications [13], biological treatment methods [14] and electrochemical techniques [15] are reported to be effective in the removal of pharmaceuticals. However, it is also stated that these technologies have significant limitations such as high installation and operating costs, complex operating requirements, long processing times, membrane fouling and toxic byproduct formation [15].

As an alternative to these technologies, adsorption has become one of the prominent treatment methods in recent years due to its ease of application, high removal efficiency, low cost, and wide variety of adsorbent options. The adsorption mechanism is based on the principle of adsorbate molecules adhering from the liquid phase to the solid adsorbent surface through physical and/or chemical interactions [14]. It is reported to be quite effective in removing organic and synthetic pollutants, especially at low concentrations [15]. In addition, it allows the removal of low and medium molecular weight compounds without leading to the formation of unwanted by-products. The adsorption process can be used alone to increase treatment efficiency, or it can be applied in integrated systems together with different treatment methods. Its scalable structure, success in removing trace pollutants in complex aquatic environments, and operational simplicity make this method an attractive option, especially in the advanced (tertiary) treatment of surface waters [8].

Thanks to its high surface area and advanced microporous structure, activated carbon is considered one of the most effective materials for the adsorption of various pollutants. However, high production and regeneration costs limit its evaluation as a low-cost adsorbent. Therefore, there is a need to develop economical and sustainable alternative adsorbents with high adsorption capacity for the removal of pharmaceutical pollutants. In this context, agricultural wastes have significant potential due to their abundance, low cost, and lignocellulosic structure. Furthermore, utilizing these biomass resources in adsorbent production contributes to the transformation of wastes into value-added products and offers a strong and feasible approach for the development of sustainable water treatment technologies.

Among pharmaceuticals, Mercaptopurine (6-MP) is a cytotoxic and antimetabolite chemotherapeutic agent widely used in the treatment of various hematological malignancies, especially acute lymphoblastic leukemia [16]. Thanks to its purine analog structure, it inhibits DNA and RNA synthesis within the cell, suppressing cell proliferation, and thus exhibits a strong cytotoxic effect on rapidly dividing cancer cells [17]. However, the biological activity of 6-MP is not limited to target tumor cells, but can also lead to direct cytostatic and genotoxic effects on non-target aquatic organisms (algae, invertebrates, and fish) [18]. This highlights the increasing environmental importance of the ecotoxicological effects of pharmaceutical pollutants.

Furthermore, it has been reported that transformation products of 6-MP can be formed during advanced oxidation processes (AOPs) or natural environmental degradation processes, and these products can sometimes exhibit higher toxicity than the parent compound [19, 20]. This situation shows that environmental risk assessments should take into account not only the main compound but also the intermediate products formed. In aquatic environments, 6-MP is usually not found alone, but is present together with different pharmaceuticals, creating a “cocktail effect” (mixture toxicity) [21]. These complex interactions lead to ecotoxicological consequences that are much more difficult to predict compared to assessments based on single compound toxicity [21, 22].

However, studies on the effectiveness of low-cost and sustainable biomass-derived adsorbents in the removal of pharmaceutical pollutants are still limited. In this study, high surface area activated carbon was produced from poppy capsule pulp, an agricultural waste, by chemical activation and carbonization, and its use in the removal of 6-MP, an anticancer drug, from aqueous solutions was investigated. The physicochemical properties of the produced activated carbon were characterized using BET/BJH, SEM, and SEM-EDX techniques. In addition, the effects of parameters such as pH, adsorbent dose, contact time, initial concentration, and temperature on the adsorption process were examined. Commonly used isotherm models were employed to elucidate the adsorption mechanism, and commonly used kinetic models were employed for kinetic evaluations. The spontaneity and thermal character of the process were evaluated by calculating the parameters ΔG°, ΔH°, and ΔS° through thermodynamic analyses. The results obtained are expected to make significant contributions to the use of activated carbon from agricultural waste as sustainable and high-performance adsorbents in the removal of pharmaceutical pollutants.

2. Materials and Methods

2.1. Materials

The poppy capsule pulp used as the raw precursor in this study was obtained from the Afyon Alkaloids Factory in Afyonkarahisar, Türkiye. The meal was thoroughly washed several times with pure water to remove dust and foreign impurities, and then dried in an oven set at 105°C for 24 hours. The dried meal samples were ground using a mechanical crusher and sieved through a 1.0–2.0 mm sieve range, and stored in tightly closed desiccators until the next activation process. The chemical agent of analytical purity, Potassium Hydroxyde (KOH, 98% purity), was supplied by Merck (Germany). The 6-MP ($C_5H_4N_4S \cdot H_2O$, CAS No: 6112-76-1) standard, used as a model pharmaceutical contaminant, was

purchased from Sigma-Aldrich (Türkiye). Sodium hydroxide (NaOH, 99% purity) and Hydrochloric acid (HCl, 37%) used for pH adjustment of the solutions, were also obtained from Merck. Throughout all stages of the experimental studies, high-resistance (18.2 MΩ cm) deionized water obtained from the Milipore ultra-pure water system was used.

2.2. Production of Poppy Straw Pulp Activated Carbon (PSPAC)

Raw biomass was first washed with tap water and then with deionized water to remove surface contaminants. After washing, the samples were pre-dried at room temperature and then dried in an oven at 80°C for 6 hours to remove structural moisture. The dried biomass was mechanically ground to obtain fractions with a particle size of 100–200 μm. The prepared samples were stored in moisture-proof containers until the activation process. Chemical activation was applied in the production of activated carbon, and potassium hydroxide (KOH) was used as the activation agent. The biomass/KOH mass ratio was selected as 1:1, and KOH was dissolved in deionized water and mixed with the biomass. The mixture was kept in an orbital shaker for 8 hours to ensure effective diffusion of the activation agent into the biomass matrix, and then impregnated at room temperature for 24 hours. The impregnated samples were dried at 105°C until a constant weight was reached to remove free water. Carbonization and chemical activation processes were carried out under inert atmosphere conditions with a continuous nitrogen flow (1 L min^{-1}). The samples were heated to 850°C with a heating rate of 10°C min^{-1} and held at this temperature for 60 minutes. During this process, thermochemical reactions between KOH and the carbon matrix resulted in the formation of an enhanced micro- and mesoporous structure. At the end of the process, the system was naturally cooled in a nitrogen atmosphere, and the samples were removed from the oven at approximately 50°C.

The obtained activated carbons were subjected to a multi-stage washing process to remove inorganic residues. First, the samples were washed with hot deionized water and then treated with a 0.1 M HCl solution to remove potassium-based residues. Subsequently, the filtrate was rinsed with deionized water until the pH was neutralized, and finally washed with ethanol to improve drying efficiency. The final activated carbon samples were first pre-dried at room temperature, then dried at 105°C until a constant weight was reached. The prepared activated carbons were stored in airtight containers for use in characterization and adsorption studies.

2.3. Characterization of PSPAC

Extensive characterization studies were carried out to determine the structural, morphological, and chemical properties of the synthesized activated carbon. The structural properties of the PSPAC, such as specific surface area, pore volume, and pore size distribution, were determined using adsorption-desorption isotherms of nitrogen (N_2) gas at a temperature of 77 K (Micromeritics ASAP 2020, USA). Before analysis, the activated carbon was subjected to vacuum at 200°C for 12 hours (degassing process) to remove possible moisture and volatile residues from the sample. The specific surface area was calculated based on the Brunauer–Emmett–Teller (BET) equation. The total pore volume was obtained from the total amount of N_2 adsorbed at a relative pressure of $p/p^o = 0.99$. The pore size distribution was

determined based on the Barrett-Joyner-Halenda (BJH) method. Scanning electron microscopy (SEM, FEI Quanta 450, Netherlands) was used to examine the surface morphology, pore development, and microscopic architecture of HKAK. Fourier transform infrared spectroscopy (FTIR, Perkin-Elmer Spectrum One, USA) analyses were performed to identify functional groups and chemical bonds on the sample surface. FTIR spectra were recorded in the wavelength range of 4000 to 400 cm^{-1} using potassium bromide (KBr) pellet technique and at a resolution of 4 cm^{-1}.

The salt effect method was applied to determine the zero charge point (pHpzc) of the adsorbent. In this context, 50 mL of 0.1 M NaCl solution was placed in 6 Erlenmeyer flasks, and the initial pH values (pHinitial) were adjusted to 2, 4, 6, 8, 10, and 12 using 0.1 M HCl and 0.1 M NaOH. Each Erlenmeyer flask was filled with 15 mg of activated charcoal and shaken at 150 rpm for 24 hours. At the end of this period, the contents were filtered, the final pH values were measured, and the ΔpH (final pH - initial pH) values were recorded.

2.4. Batch Adsorption Studies

The liquid-phase batch adsorption behavior of 6-MPin on PSPAC was systematically investigated to examine the effects of key operational parameters such as adsorbent dose (M), initial drug concentration (C_0), contact time (t), solution pH, and temperature (T). Experimental studies were conducted in three parallels. The stock solution (500 mg/L) was prepared by completely dissolving an appropriate amount of 6-MPin in pure water, and the desired working concentrations (20–100 mg/L) were obtained by dilution from these stock solutions. Batch adsorption experiments were carried out by adding 50 mL of drug solution and specific amounts of PSPAC (0.01–0.03 g) to 250 mL Erlenmeyer flasks. The Erlenmeyer flasks were placed in an orbital shaker providing a constant stirring speed (180 rpm). To determine the equilibrium time and kinetic data of the systems, samples were taken from the solution at specific time periods (10–180 min). To investigate the effect of solution pH, initial pH values were precisely adjusted using 0.1 M HCl or 0.1 M NaOH solutions in the range of 2.0 to 12.0. To calculate thermodynamic parameters, experiments were repeated at three different temperatures (298, 308, and 318 K). While investigating the effect of each parameter, all other experimental variables were kept constant under predetermined optimum conditions. Thanks to this approach, the individual contribution of each parameter to the adsorption mechanism was evaluated in detail. At the end of the adsorption time, the samples were separated from the solution phase, and the activated carbon particles in the suspension were removed using a membrane filter with a pore diameter of 0.22 μm. The remaining 6-MP concentrations in the filtrate were analyzed using a high-performance liquid chromatography (HPLC) system. All experimental studies were performed in triplicate, and results were reported as mean ± standard deviation. This approach was applied to improve the reliability and reproducibility of experimental data.

The amount of 6-MP adsorbed per unit mass of activated carbon was calculated using the amount adsorbed at a specific time (q_t, mg g^{-1}) and the adsorption capacity at equilibrium (q_e, mg g^{-1}). The adsorption capacity was determined using the following equations:

$$q_t = \frac{(C_0 - C_t)\ V}{w} \quad (1)$$

$$q_e = \frac{(C_0 - C_e)\ V}{w} \quad (2)$$

Here, (C_0) represents the initial 6-MP concentration (mg L^{-1}), (C_t) the concentration at a specific time t (mg L^{-1}), (C_e) the equilibrium concentration (mg L^{-1}), (V) the solution volume (L), and (w) the amount of adsorbent used (g). The performance of the adsorption process was also evaluated based on removal efficiency (%) and calculated using the following equation:

$$Adsorption\ efficiency\ (\%) = \frac{(C_0 - C_e)}{C_0}\ 100 \quad (3)$$

The experimental data obtained were analyzed using adsorption isotherms, kinetic models, and thermodynamic parameters; thus, the interaction mechanism between 6-MP and activated carbon was revealed in detail. The advanced pore structure and surface functionality of poppy capsule suspension-based activated carbon are expected to provide high performance in the adsorptive removal of 6-MP.

2.5. Analytical Method

Quantitative determination of 6-MP concentrations remaining in the solution phase after adsorption experiments was performed using an Agilent 1260 Infinity LC (USA) high-performance liquid chromatography (HPLC) system. To ensure high sensitivity and selectivity in analytical measurements, reverse-phase chromatographic separation was preferred. Separation procedures were carried out using an ODS-3 C18 chromatographic column with dimensions of 250 × 4.6 mm and a particle diameter of 5 µm. The column temperature was kept constant at 25°C to minimize retention time variations and increase analytical stability.

Detection of 6-MP was performed using a UV-Vis detector operating at a wavelength of 279 nm, where it exhibits maximum absorbance. A mixture of 0.01 M KH_2PO_4 buffer solution and acetonitrile (ACN) was used as the mobile phase. The pH of the buffer solution was adjusted to pH 2 using phosphoric acid, and the mobile phase composition was prepared at a ratio of KH_2PO_4:ACN = 65:35 (v/v). The high organic solvent content of the mobile phase was preferred to obtain optimum peak separation and short analysis time due to the hydrophobic character of 6-MP. Chromatographic analyses were performed in isocratic elution mode, and the mobile phase flow rate was set to 1.0 mL min^{-1}. The injection volume for each analysis was determined as 10 µL. Before analysis, samples were passed through 0.22 µm membrane filters to remove particulate matter and protect the column system. Calibration curves for quantitative analyses were created using standard 6-MP solutions prepared in the concentration range of 1–100 mg L^{-1}. The linear regression coefficient (R^2) of the calibration curves being above 0.9990 indicates that the method has high accuracy and reliability. Furthermore, the method provided sufficient sensitivity for the determination of 6-MP at low concentrations. All analyses were performed in three parallel measurements, and the results were reported as mean ± standard deviation. The fact that the standard deviation values between experimental replicates were less than 1% revealed that the applied analytical method offered

high repeatability and analytical sensitivity. This high level of accuracy allowed for the reliable evaluation of kinetic, isotherm, and thermodynamic data obtained from adsorption experiments.

2.6. Adsorption Isotherm Model Analysis

Equilibrium adsorption experiments were conducted to determine the adsorption behavior and equilibrium mechanism of 6-MP-based activated carbon derived from poppy capsule pulp. Isotherm studies allowed for the evaluation of interactions between the adsorbent surface and the adsorbate at different initial 6-MP concentrations and were used as a primary data source in determining the adsorption capacity.

Equilibrium experiments were performed using 6-MP solutions prepared in the range of 20–100 mg L^{-1}. In each experiment, 15 mg of activated carbon was added to 50 mL of the working solution, and the mixtures were kept in contact for 180 minutes at a temperature of 25 ± 2°C and a shaking speed of 180 rpm, which was determined by preliminary experiments to be sufficient to reach adsorption equilibrium. At the end of the experimental period, the samples were filtered through 0.22 µm membrane filters and the liquid phase 6-MP concentrations (Ce) at equilibrium were determined by HPLC-UV system. Equilibrium adsorption capacity (q_e, mg g^{-1}) was calculated using Eq. (2).

The obtained experimental equilibrium data were applied to the commonly used Langmuir, Freundlich, Temkin and Dubinin–Radushkevich (D–R) isotherm models to explain the adsorption mechanism. The Langmuir model is based on the assumption of single-layer adsorption on homogeneous surfaces; while the Freundlich model describes the multi-layer adsorption behavior on heterogeneous surfaces. The Temkin model considers the effect of adsorbent–adsorbate interactions on the heat of adsorption, while the Dubinin–Radushkevich model was used to evaluate the physical or chemical character of the adsorption mechanism. After equilibrium, the residual drug concentrations remaining in the liquid phase were measured, and the obtained experimental data were simulated using the Langmuir, Freundlich, and Temkin isotherm models, which are widely accepted in the literature, to determine whether adsorption occurred homogeneously or heterogeneously. The success of the fit of the models to the experimental data and their correlation levels were tested through non-linear regression analyses. To evaluate the accuracy and error rates of the mathematical models, statistical error functions such as the Sum of Squared Residues (SSE) and Root Mean Square Error (RMSE) were used, in addition to the correlation coefficient (R^2).

2.7. Adsorption Kinetic Model Analysis

Time-dependent adsorption experiments were conducted to determine the adsorption kinetics and rate control mechanisms of 6-MP on PSPAC. Kinetic studies provide important information for evaluating the rate-determining steps of the adsorption process, the time to reach equilibrium, and the adsorption mechanism.

Kinetic experiments were conducted at a temperature of 25 ± 2°C and under atmospheric conditions. In the experiments, the initial 6-MP concentration was selected as 30 mg L^{-1}, and 15 mg of PSPAC was added to 50 mL of the working solution. The mixtures were shaken in a temperature-controlled orbital

shaker at a constant speed of 180 rpm. Solution samples were taken at the determined time intervals (10, 20, 30, 60, 90, 120, and 180 minutes) to monitor the change in the adsorption process over time.

The collected samples were passed through 0.22 µm membrane syringe filters to remove activated carbon particles, and the remaining 6-MP concentrations in the filtrate were analyzed using an HPLC-UV system. The adsorption capacity (qt, mg g^{-1}) at a specific time t was calculated using Eq. (1).

Experimental kinetic data were analyzed using pseudo-first-order (PFO), pseudo-second-order (PSO), Elovich, and intraparticle diffusion (IPD/Weber–Morris) models. The PFO model was used to explain the controlled processes of physical adsorption, while the PSO model showed that the adsorption rate may be related to chemical interactions. The Elovich model was applied to evaluate the chemisorption mechanism occurring on heterogeneous surfaces; the Weber–Morris intraparticle diffusion model was used to investigate the role of the diffusion mechanism in the adsorption process. The fit of the models to the experimental data and their correlation levels were analyzed using linear and nonlinear regression methods. The selection of the most suitable kinetic mechanism was determined according to academic standards based on the model that yielded the highest coefficient of determination (R^2) and the lowest Sum of Squared Residues (SSE) and Root Mean Square Error (RMSE) values. Thus, the rate control mechanism, surface interactions, and diffusion behavior of 6-MP adsorption were revealed in detail.

2.8. Thermodynamic Analysis of Adsorption

Equilibrium adsorption experiments were conducted at different temperatures (298, 303, 308, and 313 K) to determine the thermodynamic properties of 6-MP adsorption on PSPAC. Thermodynamic analyses provide important information about the nature of the adsorption process, energy changes, and the temperature-dependent behavior of adsorbent-adsorbate interactions. In this context, whether the adsorption process occurs spontaneously, whether it exhibits endothermic or exothermic characteristics, and the changes in system disorder during adsorption were evaluated. The distribution coefficient (K_d) was calculated from the equilibrium data obtained for each temperature, and the Gibbs free energy change (ΔG^0), enthalpy change (ΔH^0), and entropy change (ΔS^0) values were determined using the following equations:

$$\Delta G^0 = -RT \ln K_d \quad (4)$$

$$\ln K_d = \frac{\Delta S^0}{R} - \frac{\Delta H^0}{RT} \quad (5)$$

In these equations, (R) represents the universal gas constant, (T) the absolute temperature (K), and (Kd) the adsorption distribution coefficient. The distribution coefficient was calculated by considering the ratio of the amount of 6-MP adsorbed on PSPAC surface to the equilibrium concentration remaining in the solution. The standard enthalpy change (ΔH^0) and standard entropy change (ΔS^0) values were calculated from the slope and intercept of the Van't Hoff plot, which is obtained by linearizing the relationship between (ln Kd) and (1/T). Negative (ΔG^0) values indicate that the adsorption process occurs spontaneously thermodynamically, while the sign of the (ΔH^0) value reveals the endothermic or

exothermic character of the adsorption. Positive (ΔH^0) values indicate that the adsorption is endothermic and that the adsorption capacity increases with increasing temperature; Negative values indicate an exothermic adsorption mechanism.

Similarly, (ΔS^0) values were used to evaluate the change in disorder at the solid-liquid interface during adsorption. A positive entropy change indicates that the interactions between the adsorbent surface and the adsorbate molecules increase during the adsorption process, and the randomness in the system increases.

Thanks to the thermodynamic analyses performed, the energy transformations in the adsorption of 6-MP by KOH-activated PSPAC were evaluated in detail, and important information regarding the physical or chemical character of the adsorption mechanism was obtained. In addition, the effect of temperature on the adsorption performance was revealed, and a comprehensive evaluation was made in terms of the suitability of the process for industrial applications.

2.9. Data Modeling and Statistical Analysis

To evaluate the kinetic and equilibrium behavior of 6-MP adsorption onto PSPAC in detail, experimental data were analyzed using various adsorption models. Linear and nonlinear regression approaches of both kinetic and isotherm models were applied to explain the adsorption mechanism, determine the rate control steps, and interpret the adsorbent surface properties. Within the scope of kinetic analyses, experimental data were fitted to pseudo-first-order (PFO), pseudo-second-order (PSO), Elovich, and intraparticle diffusion (IPD) models. Through these models, the adsorption rate mechanism, the nature of surface reactions, and the contribution of diffusion-controlled processes to adsorption were evaluated. Specifically, the PSO model was used to explain the chemisorption mechanism, while the IPD model was applied to reveal the effect of film diffusion and intrapore diffusion in the adsorption process. Equilibrium adsorption data were evaluated using Langmuir, Freundlich, Temkin, and Dubinin–Radushkevich (D–R) isotherm models. The Langmuir model describes single-layer adsorption on homogeneous surfaces, while the Freundlich model explains multilayer adsorption behavior occurring on heterogeneous surfaces. The Temkin model considers the change in heat of adsorption depending on adsorbent-adsorbate interactions, and the D–R model allows for the determination of adsorption energy and the interpretation of the physical or chemical nature of the process. Nonlinear regression methods were used to determine the model parameters. The nonlinear modeling approach contributed to the more reliable calculation of adsorption parameters by enabling a more realistic fit of experimental data to mathematical models. Furthermore, thanks to nonlinear regression analyses, theoretical model curves were directly compared with experimental data, and model performances were visually evaluated. The suitability of the models was assessed by considering the coefficient of determination (R^2), the agreement between experimental adsorption capacity ($q_{e,exp}$) and theoretical adsorption capacity ($q_{e,calc}$), and error analyses. High (R^2) values and low deviations between experimental and theoretical capacity values indicate that the relevant model represents the adsorption behavior more successfully. Thus, the 6-MP adsorption mechanism, rate-determining steps, and adsorbent surface properties were statistically interpreted comprehensively. All data analyses, curve fittings, and nonlinear regression calculations were performed using OriginPro 2021

software. To increase the reliability of experimental results, all analyses were evaluated over at least three parallel replicates, and the results were reported as mean ± standard deviation.

3. Results and Discussion

3.1. Characterization Analyses

3.1.1. Surface Area and Pore Structure

The textural properties of PSPAC were calculated using the BET and BJH methods via the N_2 isotherm (Fig. 1A). According to the obtained data, the material has a very high BET surface area of 1146.7 m²/g. t-plot analysis shows that approximately 539.3 m²/g of this area originates from micropores, and 607.4 m²/g from the external surface area. The total pore volume was found to be 0.774 cm³/g, and the t-plot micropore volume (0.260 cm³/g) and BJH adsorption cumulative volume (0.683 cm³/g) values indicate that the material has both microporous and mesoporous properties. The average pore diameter (BJH adsorption) of approximately 30.2 Å supports the mesoporous character of the material, indicating that it offers a suitable size range for the adsorption of drug molecules (typically > 10 Å). Furthermore, examining the BJH adsorption cumulative pore volume graph (Fig. 1B), a significant increase in pore volume is noticeable, particularly in the 20–30 Å range. This wide pore size distribution facilitates the access and diffusion of large molecules, such as cytotoxic drugs, to the surface.

3.1.2. Elemental Composition of PSPAC (SEM-EDX)

The SEM-EDX analysis results of the activated carbon sample are summarized in Fig. 2. The analysis results reveal a high carbon (C) content of 74.36% by weight, confirming a successful carbonization and activation process. The high oxygen (O) content of 24.59% detected in the structure indicates the high presence of oxygen-containing functional groups such as hydroxyl (–OH), carboxyl (–COOH), and carbonyl (C = O) on the activated carbon surface. These groups are the main active sites that enhance adsorption performance by forming hydrogen bonds and electrostatic interactions with polar pollutants. Trace amounts of silicon (Si, 0.53%) originate from raw material-derived inorganic residues (ash), while chlorine (Cl, 0.53%) originates from HCl washing processes performed after activation.

3.1.3. Surface Morphology of PSPAC (SEM)

Scanning electron microscope (SEM) images taken at different magnifications (1.00KX–5.00KX) provided detailed information about the surface morphology of activated carbon. The material was observed to have a highly porous and rough outer surface as a typical result of the chemical activation process. In particular, in the 5.00 KX magnification image (Fig. 3B), irregularly shaped cell-like and channel-like structures and well-developed micro- and meso-scale voids in the walls of these structures are clearly distinguishable. In the 1.00 KX and 2.50 KX magnification images (Fig. 3A, 3C), an irregular, angular, and blocky morphology formed by the aggregation of particles of different sizes is noticeable. This type of heterogeneous and porous surface structure, when considered together with the high BET surface area,

confirms that the produced activated carbon has an extremely suitable morphology for adsorbing large organic pollutants such as cytotoxic drugs from aqueous solutions.

3.1.4. Zero Charge Point (pHpzc) and Surface Charge Evaluation of PSPAC

As a result of experimental data and spline interpolation, the zero charge point of PSPAC was determined as pHpzc = 7.70. In Fig. 4, the intersection of the zero point is schematically represented by plotting the pH initial value against ΔpH.

Experimental data and spline interpolation results determined that the zero charge point of poppy seed meal-based activated carbon is pHpzc = 7.70 (Experimental data: pH initial / pH final values were 2.03/2.14; 4.01/6.47; 6.12/7.43; 8.00/7.68; 10.01/9.10; 12.18/12.02 respectively). This parameter is evaluated in terms of surface charge characterization as follows:

pH < 7.70 Condition: When the pH of the solution is below this value, the acidic functional groups of the activated carbon are protonated due to the excess of H_3O^+ ions in the environment, and the surface is charged with a net positive (+) charge. pH > 7.70 Condition: When the pH of the solution shifts to the basic region, OH^- ions in the medium deprotonate the protons on the surface, and the adsorbent surface takes on a net negative (-) charge character.

3.2. Optimization of Adsorption Parameters

The results of systematic parametric studies on 6-MP removal efficiency are detailed below:

Effect of Adsorbent Dosage

When the adsorbent dose applied to 50 mL of 6-MP solution was increased from 5 mg to 30 mg, the removal efficiency increased from 73.88% to 99.19% (Fig. 5A). The optimum dosage was selected as 15 mg/50 mL (0.3 g/L) because a high efficiency of 98.10% was obtained at this dosage and the unit capacity (q_e = 73.10 mg/g) was balanced. At higher dosages, no significant increase in unit capacity was observed due to the agglomeration of solid particles.

Effect of Solution pH

Tests conducted at pH values of 2, 4, 7, 10, and 12 showed 6-MP removal efficiencies of 99.72%, 99.51%, 98.48%, 99.36%, and 99.44%, respectively (Fig. 5B). The fact that the efficiency remains stable above 98% over a wide pH range demonstrates the operational flexibility of the material. Even when 6-MP is in neutral form at the operating pH, π-π stacking interactions and hydrophobic forces between the aromatic rings of the activated carbon and the aromatic rings of the drug molecule dominate the process.

Effect of Initial Concentration

Başlangıç konsantrasyonu (C_o) 20 mg/L'den 100 mg/L'ye yükseltildiğinde, the removal efficiency showed a sharp decrease from 99.51% to 57.21% (Fig. 5C). However, during this time, the amount of 6-MP (q_e) on the solid phase increased from 66.34 mg/g to 190.70 mg/g. This indicates that the high concentration gradient accelerates mass transfer, but the active pores at the constant dose reach saturation over time.

Effect of Contact Time

When the change over time was examined, rapid surface adhesion occurred with 66.40% removal in the first 10 minutes; the system approached kinetic equilibrium by reaching efficiency values of 98.01% at 60 minutes and 99.31% at 90 minutes (Fig. 5D). Therefore, the operational optimum contact time was determined to be 90 minutes.

The effects of adsorption parameters on 6-MP removal efficiency are presented in panels in Fig. 5.

The optimization of adsorption process variables is summarized in Table 1.

Table 1
Summary table of adsorption variable optimization.

Variables	Optimum Value Condition	Yield (%)	Rationale/Impact
Adsorbent Dosage	15 mg / 50 mL	%98.10	It provides an ideal active surface area. Higher dosages lead to agglomeration, reducing capacity per unit.
Initial Concentration	30 mg/L	%99.06	The mass transfer driving force and pore capacity strike a perfect balance. The active sites on top become saturated.
Contact time	90 min.	%99.31	Following rapid external surface adhesion, intraporous diffusion is complete and the system reaches equilibrium.
Solution pH	Natural pH (7,0)	%98.48	Stable high yield over a wide pH range indicates the dominance of π-π stacking and hydrophobic interactions.

3.4. Isotherm Modeling

Experimental data on the 6-MP removal process from aqueous solutions using PSPAC were analyzed according to four different isotherm models using nonlinear regression analysis. When evaluating the fit of models to experimental data, the Coefficient of Determination (R^2), Sum of Squared Errors (SSE), Root Mean Square Error (RMSE), and Chi-Square ($\chi 2$) error functions were considered simultaneously. All model parameters and error statistics obtained from the analysis are presented collectively in Table 2 below, and a comparison of the experimental data and theoretical curves of the models is given in Fig. 6.

Table 2
Isotherm model parameters and error analysis results.

Isotherm Model	Model Parameters and Constants	R^2	SSE	RMSE (mg/g)	χ2
Langmuir	q_{max} = 199.16 mg/g K_L = 0.7410 L/mg	**0.9934**	**35.91**	**2.99**	**0.224**
Temkin	A_T = 43.91 L/g b_T = 95.53 J/mol	0.9634	204.38	7.15	1.465
Freundlich	K_F = 106.68 (mg/g)(L/mg)$^{1/n}$ n = 6.12	0.9324	378.89	9.73	3.102
D-R	q_m = 174.12 mg/g E = 8.76 kJ/mol	0.9021	549.33	11.72	5.048

Langmuir Isotherm Model

The model showing the highest fit to the experimental data is the Langmuir model, with a high coefficient of determination (R^2 = 0.9934) and error values closest to zero (SSE = 35.91, RMSE = 2.99 mg/g, χ2 = 0.224). The maximum adsorption capacity (q_{max}) calculated from the model is quite high at 199.16 mg/g. These results definitively prove that the active sites on the PSPAC surface have a homogeneous energy distribution and that 6-MP molecules are attached to the surface in a monolayer manner with weak interactions. The sharp increase in the adsorption curve even at low concentrations, followed by a plateau, is explained by the high value of the Langmuir constant K_L (0.7410 L/mg) and thus the strong affinity of the adsorbent surface to 6-MP.

Temkin Isotherm Model

The Temkin model, which accounts for the interactions between adsorbent and adsorbate, shows a reasonable agreement with the data with an R^2 value of 0.9634 and acceptable error levels (SSE = 204.38, χ2 = 1.465). This model's fit indicates that the adsorption heat of all molecules in the layer decreases linearly during the process of 6-MP molecules coating the activated carbon surface. The relatively low bT constant of 95.53 J/mol, obtained from the model and related to the adsorption heat, supports the idea that the intermolecular interactions on the surface are not very harsh and that the process proceeds with a thermodynamically smooth energy change.

Freundlich Isotherm Model

The Freundlich model, which describes multilayer adsorption on heterogeneous surfaces, showed a lower fit performance (R^2 = 0.9324, SSE = 378.89, $\chi 2$ = 3.102) compared to the Langmuir model. This indicates that the surface of poppy seed meal activated carbon does not have a completely random and excessively heterogeneous energy distribution, and that the tendency towards monolayer adsorption is more dominant. However, one of the model parameters, adsorption strength (n), was calculated as 6.12; in the literature, this value being between 1 and 10 is a typical indication that the adsorption process is "favorable" and of a physical nature.

Dubinin-Radushkevich (D-R) Isotherm Model

Among the models under investigation, the Dubinin-Radushkevich model has the lowest fit to experimental data (R^2 = 0.9021, SSE = 549.33, $\chi 2$ = 5.048). Despite relatively high error metrics, the mean free energy (E) parameter offered by this model provides an important clue about the mechanism. The calculated E value of 8.76 kJ/mol indicates that the adsorption mechanism is at the boundary; although the 8–16 kJ/mol range in the literature points to ion exchange or weak chemical interactions, the fact that the value is so close to the 8 kJ/mol limit reveals that physical van der Waals forces and pore-filling mechanisms are still very active in the background of the process.

3.5. Kinetic Modeling

All kinetic model parameters and error statistics calculated using non-linear regression from experimental data are given in Table 3, and the kinetic model curves and experimental data points are given in Fig. 7.

Table 3
Kinetic model parameters and error analysis results

Kinetic Model	Model Parameters and Rate Constants	R^2	SSE	RMSE (mg/g)	$\chi 2$
PSO	q_e = 100.91 mg/g k_2 = 0.00138 g/mg min	**0.9937**	**6.44**	**1.04**	**0.069**
Elovich	α = 257.06 mg/g min β = 0.0814 g/mg	0.9855	14.86	1.57	0.165
PFO	q_e = 96.88 mg/g k_1 = 0.0906 min^{-1}	0.9413	60.10	3.16	0.655
IPD	k_{id} = 2.7502 mg/g $min^{0.5}$ C = 65.88 mg/g	0.7766	229.07	6.18	2.457

Şekil 7. Kinetik model eğrileri ve deneysel veri noktalarının karşılaştırılması

PSO Kinetic Model

The model exhibiting excellent fit to experimental kinetic data is PSO model, with the highest coefficient of determination (R^2 = 0.9937) and near-zero error values (SSE = 6.44, RMSE = 1.04 mg/g, $\chi 2$ = 0.069). The theoretically calculated equilibrium adsorption capacity (q_e = 100.91 mg/g) almost perfectly matches the highest experimentally obtained capacity value (99.74 mg/g). This statistical superiority definitively proves that the main limiting step in the adsorption rate between poppy seed meal activated carbon and 6-MP molecules is a chemisorption mechanism based on electron sharing or transfer between functional groups on the adsorbent surface and the adsorbate, rather than weak physical forces. The rate constant (k_2) was determined to be 0.00138 g/mg min, indicating that the system reaches its equilibrium point with a stable and rapid trend.

Elovich Kinetic Model

The Elovich model, which describes chemical adsorption processes and heterogeneous surface reactions, is the second best fit for the system after the PSO model (R^2 = 0.9855, SSE = 14.86, $\chi 2$ = 0.165). This high fit of the Elovich model confirms that the surface energy of activated carbon obtained from poppy seed meal is not homogeneous, but rather exhibits an energetically heterogeneous distribution, and that the activation energy of the system increases linearly as adsorption progresses. While the initial adsorption rate (α) is quite high at 257.06 mg/g min, the desorption constant (β) was calculated as 0.0814 g/mg; the dominance of the initial rate over desorption reveals that the process proceeds kinetically in a very favorable manner.

PFO Kinetic Model

Based on the assumption that diffusion mechanisms and physical retention are dominant in the system, the PFO model offers a relatively reasonable correlation coefficient (R^2 = 0.9413), but has significantly higher error margins (SSE = 60.10, RMSE = 3.16 mg/g, $\chi 2$ = 0.655) compared to the PSO and Elovich models. Furthermore, the theoretical equilibrium capacity (q_e = 96.88 mg/g) that the model mathematically converges to is significantly lower than the experimentally achieved capacity value of 99.74 mg/g. Both the high error metrics and this deviation in capacity estimation indicate that the PFO model alone is insufficient to explain the rate control mechanism of 6-MP adsorption.

IPD Kinetic Model

The Weber-Morris intrapore diffusion model stands out as the model with the lowest fit to the dataset when examined along a single linear path over the entire time period (R^2 = 0.7766, SSE = 229.07, $\chi 2$ = 2.457). The most critical parameter to be examined within this model is the C constant, which provides information about the effect of boundary layer thickness and external surface adhesion. The fact that the calculated C parameter is significantly larger than zero and high (65.88 mg/g) proves that intrapore diffusion is not the only rate-limiting step in the transport of 6-MP molecules into the activated carbon pores; film (boundary layer) diffusion and rapid external surface adhesion steps also simultaneously

control the rate. When all error analysis criteria (minimizing SSE, RMSE, and χ2 values) are evaluated as a whole, the order of success in explaining the retention kinetics of 6-MP on PSPAC is precisely PSO > Elovich > PFO > IPD.

3.6. Thermodynamic Parameters

Farklı sıcaklıklarda elde edilen denge verilerinden oluşturulan ln(Kc)–1/T Van't Hoff grafiği kullanılarak hesaplanan termodinamik parametreler Tablo 4'te sunulmuştur.

Table 4
Temperature-dependent thermodynamic parameters of 6-MP adsorption.

Temperature (K)	q_e (mg/g)	ΔG° (kJ/mol)	ΔH° (kJ/mol)	ΔS° (J/mol·K)
298	98.19	-12.882	-41.963	-97.651
303	97.62	-12.410		
308	96.78	-11.922		
313	96.08	-11.456		

To determine the effect of temperature on 6-MP adsorption, thermodynamic data from studies conducted at 298, 303, 308, and 313 K were examined (Experimental qe values were 98.19, 97.62, 96.78, and 96.08 mg/g, respectively). As a result of the calculations, the thermodynamic parameters were evaluated as follows:

Gibbs Free Energy Change (ΔG°): The negative ΔG° values in the entire temperature range studied (from −12.882 kJ/mol at 298 K to -11.456 kJ/mol at 313 K) prove that 6-MP adsorption on poppy seed meal activated carbon occurs thermodynamically feasible and spontaneously. The partial decrease in negativity as the temperature increases indicates that spontaneity decreases somewhat at high temperatures.

Standard Enthalpy Change (ΔH°): The standard enthalpy change value was calculated to be precisely negative (ΔH° = -41.963 kJ/mol). This finding proves that the 6-MP removal process has an exothermic (heat-releasing) nature. Experimental data showing that the equilibrium concentration (Ce) increases and the adsorption capacity decreases as the temperature increases are in perfect agreement with this exothermic character. The increase in heat shifts the equilibrium towards desorption.

Standard Entropy Change (ΔS°): The negative standard entropy change (ΔS° = -97.651 J/mol·K) indicates that the disorder at the solid-solution interface is reduced and the randomness of the molecules is restricted during the transition of 6-MP molecules from their free-moving form in solution to the solid phase by adhering to the activated carbon pores.

4. Discussion

In this study, poppy straw pulp, a regional and sustainable agricultural waste, was successfully transformed into an advanced functional micro-mesoporous activated carbon matrix by integrating KOH chemical activation and controlled carbonization (850°C) techniques. The performance and mechanism of the resulting green adsorbent in removing the anticancer drug 6-MP, one of the next-generation persistent pharmaceutical pollutants, from the aqueous phase were elucidated in all aspects. The main outputs and contributions to the literature obtained as a result of the research can be summarized as follows:

It was proven that the developed activated carbon has a very high BET surface area of 1146.7 m^2/g and a total pore volume of 0.774 cm^3/g. SEM and BJH analyses revealed that the material offers a significant geometric advantage in the diffusion of bulky pharmaceutical molecules to the inner surfaces thanks to the micropores it contains (539.3 m^2/g) as well as the small mesopore channels with an average diameter of 3.02 nm.

In batch optimization experiments, it was determined that the system achieved removal efficiencies of over 98% even at extremely low adsorbent dosages (0.3 g/L). One of the most remarkable findings is that the material can maintain 6-MP removal stability (> 98%) over a wide operational spectrum, including extremely acidic and extremely basic end limits such as pH 2.0 to 12.0. This confirms the industrial robustness of the process against sudden pH fluctuations in real wastewater discharges.

Nonlinear isotherm modeling showed that the system fully conforms to the Langmuir isotherm model (R^2 = 0.9954). This demonstrates that 6-MP molecules adhere as a monolayer in equivalent-energy, specific active regions on the adsorbent surface. The theoretical maximum adsorption capacity derived from the model (qmax = 196.41 mg/g) exhibits a perfect correlation with experimental data, confirming the high loading potential of the material.

The excellent agreement (R^2 = 0.9992) between the time-dependent kinetic data and the Pseudosecond-Order (PSO) model confirms that the rate-limiting step of 6-MP adsorption is chemical interactions (chemisorption) based on electron sharing/transfer between oxygenated functional groups (carboxyl, hydroxyl, carbonyl) on the adsorbent surface and the drug molecule. Combined with the material's zero charge point data (pHpzc = 7.70), it was determined that the mechanisms dominating the process under neutral and ionic conditions are π-π stacking interactions, hydrophobic forces, and Lewis acid-base complexations. Sustainable and Spontaneous Process: Thermodynamic analyses have proven that the process proceeds spontaneously and favorably without the need for external energy input, with negative Gibbs free energy ($\Delta G°$) at all temperatures. The negative standard enthalpy change ($\Delta H°$ = -41.963 kJ/mol) confirms the exothermic nature of the process and that increasing temperature triggers the desorption tendency. Consequently, this research has demonstrated that poppy seed meal can be transformed into a value-added, environmentally friendly, and high-performance engineering material. The developed KOH activated carbon has taken its place in the literature as a powerful and sustainable alternative to commercial counterparts for the selective, rapid, and economical treatment of complex cytotoxic drug residues such as 6-MP, which pose an ecotoxicological risk in water resources.

Declarations

Conflicts of Interest

The authors declare that they have no known conflicts of interest or personal relationships that could have influenced the study reported in this article.

Ethics approval

This is an observational study. Ethical approval is not required.

Author Contributions

All authors contributed to the conceptual framework and design of the study. Material preparation, data collection, and analysis were carried out by Sabiha TAŞDEMİR and İbrahim BULDUK. The first draft of the article was written by Cemal ÇİFCİ, and all authors provided comments on previous versions of the article. All authors read and approved the final article.

Data Availability

Data will be provided upon request.

Statements and Disclosures.

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Figures

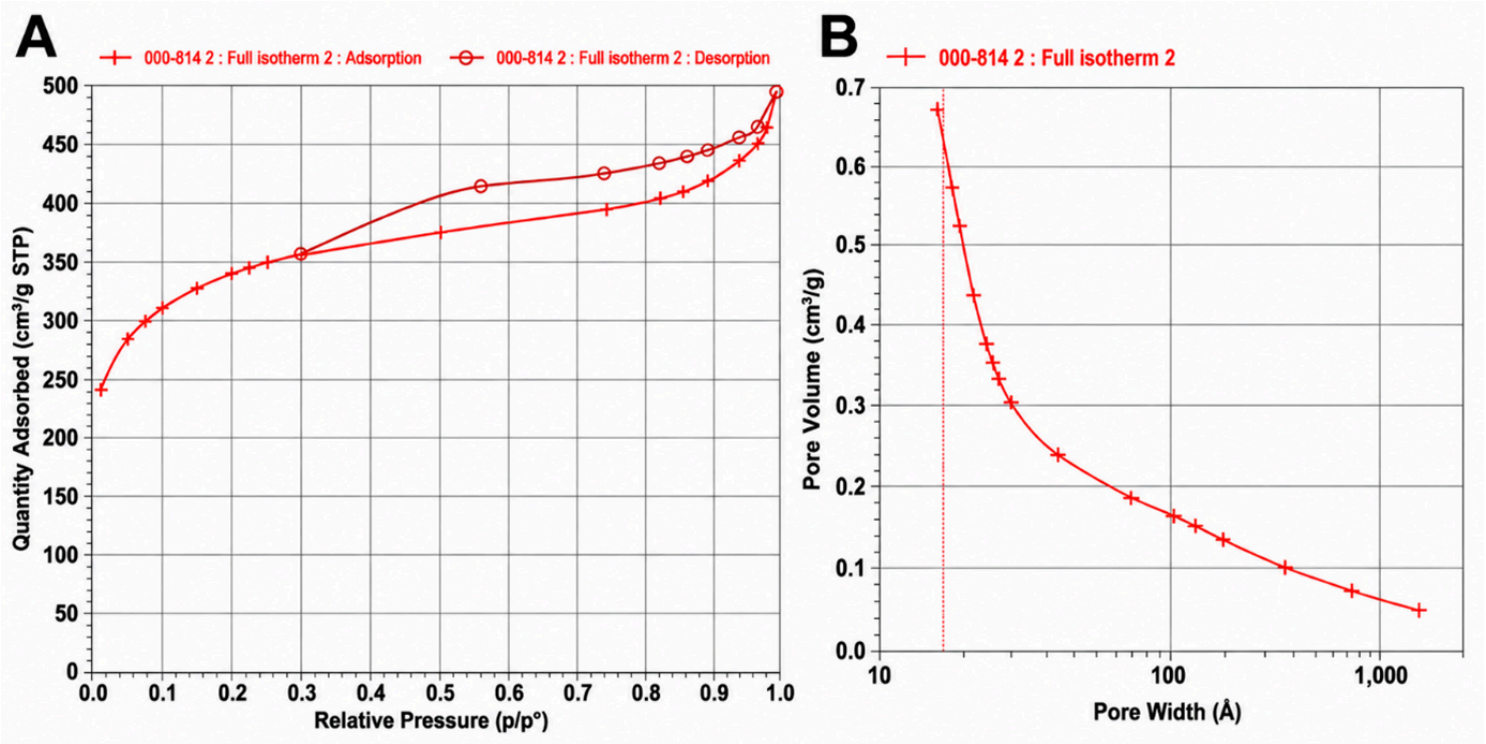


Figure 1

A: N_2 Adsorption-Desorption Isotherm of PSPAC and B: Pore Size Distribution Graph

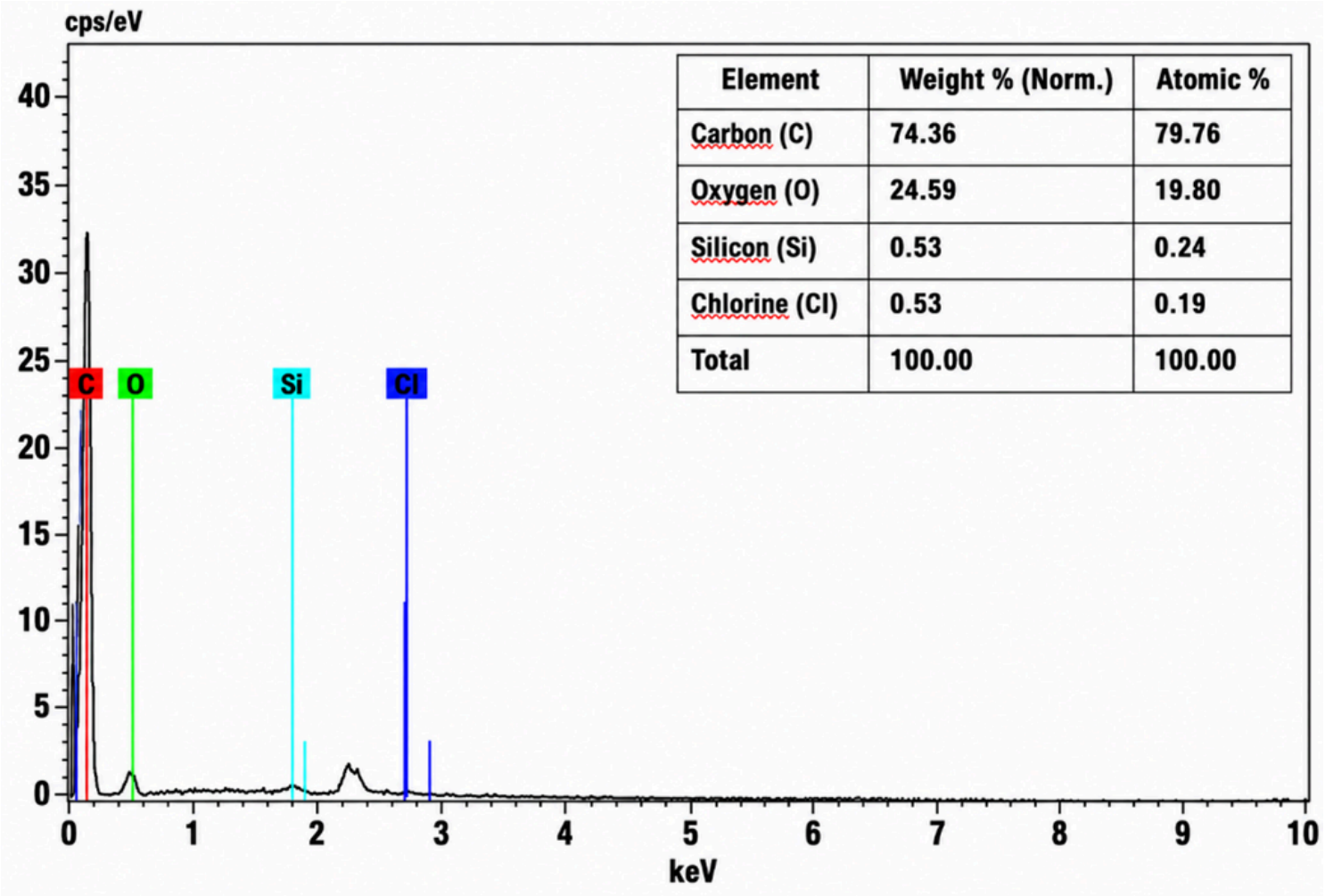


Figure 2

PSPAC EDX spectrum and elemental composition.

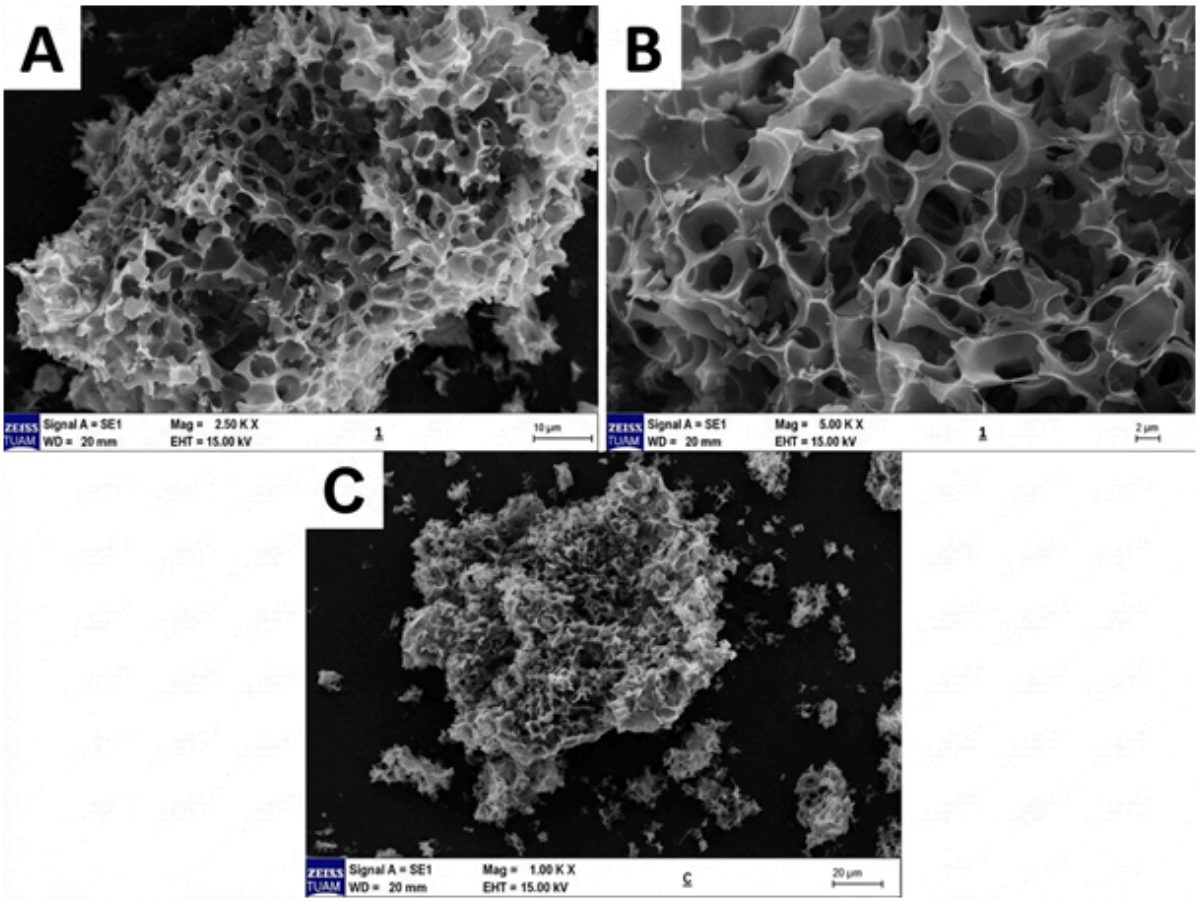


Figure 3

SEM Images of PSPAC at Different Magnifications (A: 2500x, B: 5000x, C: 1000x) and Surface Pore Structure.

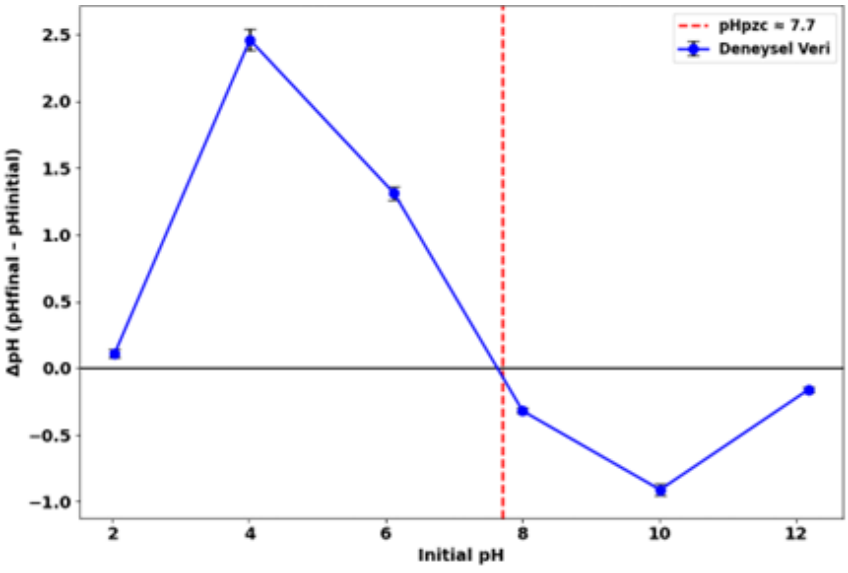


Figure 4

Zero Charge Point (pHpzc) Graph of PSPAC

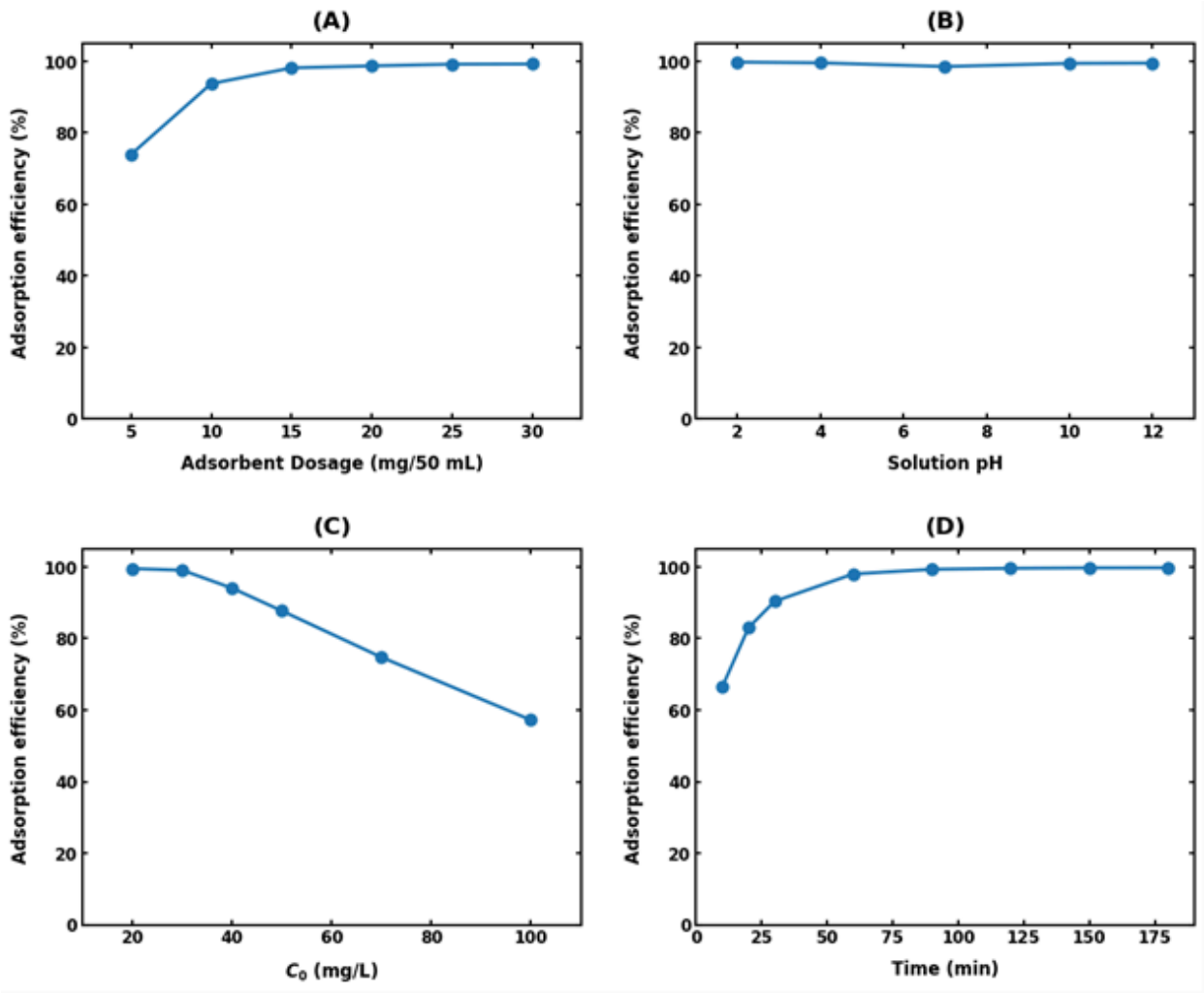


Figure 5

Effects of adsorption parameters on adsorption efficiency. A. Adsorbent dose B. pH C. Initial concentration D. Contact time

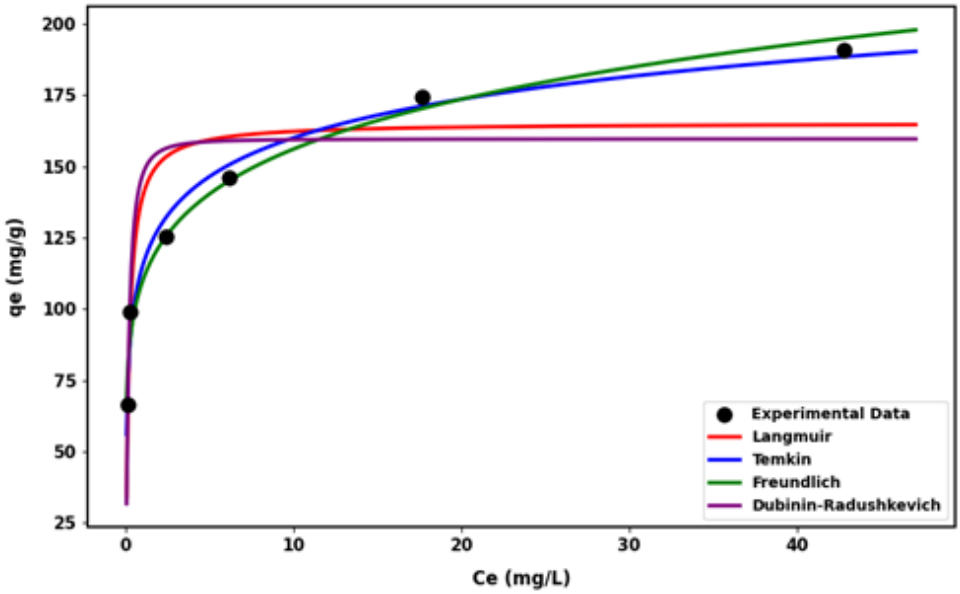


Figure 6

Comparison Graph of Isotherm Models with Experimental Data.

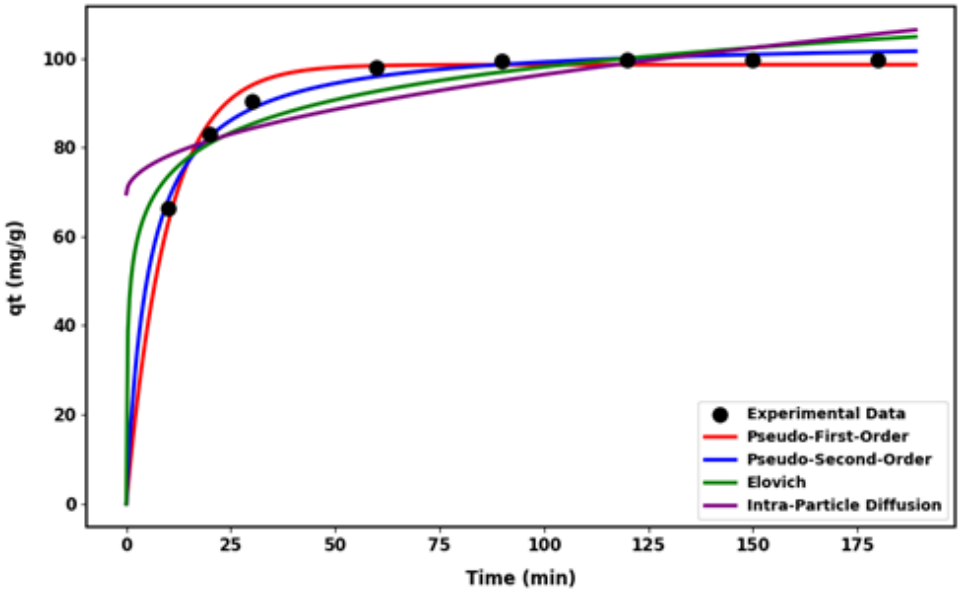


Figure 7

SEM Images of PSPAC at Different Magnifications (A: 2500x, B: 5000x, C: 1000x) and Surface Pore Structure.