

Review Article 

A Perspective on Ibuprofen Adsorption Studies from Aqueous Solutions by Activated Carbon-Based Adsorbents: A Review

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ABSTRACT

The persistent presence of Ibuprofen (IBP) in surface and wastewater represents a growing environmental and public health concern, prompting extensive research into effective removal strategies. Among available treatment approaches, adsorption using activated carbon and other carbon-based materials has proven to be efficient, versatile, and economically feasible. This review provides a critical analysis of recent progress in the synthesis and modification of activated carbons, biochars, metal-organic framework-derived carbons, and magnetic composites for the adsorption of IBP from aqueous solutions. Key aspects discussed include synthesis methods, surface functionalization techniques, adsorption isotherms, and kinetic modeling, and the influence of operational parameters such as pH, temperature, adsorbent dosage, and the presence of competing substances. The adsorption mechanism is predominantly governed by π - π stacking, hydrogen bonding, hydrophobic interactions, electrostatic attraction, and pore-filling effects, with enhanced removal generally occurring under acidic conditions. Although many newly developed adsorbents demonstrate high capacity and satisfactory regeneration performance, most reported studies are limited to laboratory-scale conditions with IBP concentrations significantly higher than those typically found in real wastewater. Future research should focus on developing low-cost, waste-derived adsorbents, conducting experiments under realistic environmental conditions, optimizing regeneration processes, and integrating adsorption with complementary treatment technologies to achieve practical, scalable, and sustainable removal of pharmaceutical contaminants from aquatic environments.



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1. Introduction

Population growth, urban sprawl, agricultural and industrial expansion, and excessive human interference in nature have led to degradation and widespread physical, chemical, and biological pollution diversification. Today, the presence of different pollutants in water and soil resources caused by urban and industrial wastewater has raised a significant concern. Pharmaceutical compounds are one of the most important environmental pollutants that, after administration are released as metabolites [1-4]. If pharmaceutical compounds are not removed or decomposed in the wastewater treatment stage, they will be discharged into the

environment and ultimately enter the water. These substances cause changes in the microbial ecology of surface and groundwater [5]. Surveys show that most people take pharmaceutical compounds arbitrarily [6], also expired and redundant pharmaceutical compounds, along with pharmaceutical factories are other sources of environmental pollution. Most pharmaceutical compounds are directly or indirectly dumped into urban sewage without undergoing metabolism and decomposition. Some pharmaceutical compounds accumulate in the environment due to their long half-life [7]. The most crucial reason for investigating and controlling pharmaceutical pollution in the environment is the entry of these pollutants into the food cycle, which can cause drug resistance

and pose many environmental risks. Due to the great variety of pharmaceutical compounds in terms of physical and chemical properties, their investigation presents many problems and challenges. In this work, research on pharmaceutical compounds such as painkillers has been prioritized [8].

Various physical and chemical methods have been proposed to remove some pharmaceutical compounds. These methods include electrochemical methods, membrane processes, biological methods, advanced oxidation processes, and adsorption processes. The adsorption process is a very effective and efficient method used today to remove toxic pollutants [2,9-11]. In the adsorption process, pollutants that move slowly toward the adsorbent surface are called adsorbates. The surface on which the adsorption process takes place is called the adsorbent. An adsorbent must adsorb significant amounts of an adsorbate. The adsorption ability depends on the interaction between the adsorbent and the adsorbate and the nature of the adsorption surface [12-15]. One of the best adsorbents is activated carbon which can remove the pharmaceutical compounds well from aqueous solutions. Activated carbon and carbon-based materials usually have a large surface area, small pores, high adsorption capacity, and good structural properties [16]. One of the main advantages of activated carbon compared to other adsorbents is its ability to be derived from a wide range of organic materials, including by-products and agricultural residues [17,18].

In recent years, various studies on Ibuprofen (IBP) removal have been reviewed [19-21]. Oba *et al.* reviewed experimental findings on the adsorption of IBP from aqueous solutions. Their reviews reveal that activated carbon and carbon-based materials are the best adsorbents for the adsorption of IBP [14,22]. Ayati *et al.* reviewed various studies and showed that the

IBP adsorption of some carbon-based adsorbents is appreciably better than that of commercial activated carbons [23-27]. In a review, Osman *et al.* showed that carbon-based adsorbents, biochar, and metal-organic frameworks appear favorable for IBP removal owing to their high surface areas and unique properties. They reported the highest IBP removal, from 10.8 to 408 mg/g for activated carbon and 2.5 to 1,033 mg/g for biochar [15,25]. Due to the importance of this type of adsorbent in Ibuprofen removal from an aqueous environment, this review paper aims to study recent achievements in the IBP adsorption by activated carbon-based adsorbents. The adsorption behavior and mechanisms, maximum IBP-binding capacities, process factors, optimum conditions, and reusability are reviewed. Finally, prospects in the development of IBP adsorbent are also outlined.

2. Search Strategy and Data Collection

2.1. Research methods

This review was conducted by systematically collecting, screening, and analyzing published studies related to the adsorption of Ibuprofen (IBP) from aqueous solutions using activated carbon and carbon-based adsorbents. Relevant literature was searched in major scientific databases, including Scopus, Web of Science, and ScienceDirect, covering the period from approximately 2000 to 2025. The keywords applied during the search included: "Ibuprofen adsorption," "activated carbon," "carbon-based adsorbents," "wastewater treatment," and "pharmaceutical pollutants."

The inclusion criteria comprised experimental and review papers that reported on the synthesis, modification, or application of activated carbon and related materials for Ibuprofen removal. Articles focusing exclusively

on non-carbon adsorbents or degradation processes without adsorption were excluded. Studies were compared based on adsorbent preparation methods, physicochemical properties, adsorption capacities, kinetic and isotherm models, and regeneration potential.

Data from the selected publications were carefully examined to identify trends in adsorption mechanisms, operational parameters (pH, temperature, adsorbent dosage, and competing solutes), and thermodynamic behavior. Where available, quantitative results such as maximum adsorption capacities, equilibrium constants, and kinetic rate constants were extracted and contrasted.

By adopting this structured approach, the review ensures a comprehensive and unbiased synthesis of recent progress, challenges, and future perspectives in using activated carbon-based adsorbents for Ibuprofen remediation from water systems.

2.2. Ibuprofen

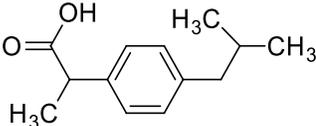
Ibuprofen (IBP) is one of the most popular and widely used drugs worldwide. IBP is a crystalline and colourless compound [14]. Some details of its specifications and chemical structure are given in **Table 1**. The IUPAC name of IBP is 2-[4-(2-methylpropyl) phenyl] propanoic acid [23,25-29]. In 1969, Ibuprofen was introduced as a better alternative to Aspirin.

It was the first member of the propionic acid derivatives [30]. By acting on a group of compounds called prostaglandins, IBP not only reduces fever, but also reduces inflammation and pain [14,26-28,31]. Some research has revealed that Ibuprofen and its degraded products can disturb the endocrine system and the central nervous system [30,31]. The drug poses a significant environmental challenge because 85% of Ibuprofen ends up in urine and reaches wastewater at 0.22 µg/L concentrations. Research teams have found Ibuprofen in wastewater and rivers of many countries. The concentrations range from 3.5 to 8600 ng/L [15,23]. A closer look at this without a prescription drug shows the potential disadvantages of its release from various sources in the environment. The adsorption process can be the best choice for removing pharmaceutical compounds and personal care products from aqueous solutions. Research has shown that activated carbon and carbon-based adsorbents can remove Ibuprofen effectively [30-36].

2.3. Activated carbon and novel activated carbon materials

Carbon-based materials offer a promising solution through adsorption technology for removing contaminants. These materials excel at removing pharmaceutical compounds from aqueous solutions. Adsorption by activated

Table 1. Specifications of Ibuprofen

Compound	Chemical formula	Chemical structure	Molecular weight (gmol ⁻¹)	λ _{max} (nm)
Ibuprofen	C ₁₃ H ₁₇ O ₂ H		206.00	221

carbon leads to pharmaceutical waste treatment technologies.

In some research, the process achieved surface adsorption rates between 83.12% and 87.12%. Pore adsorption ranges varied from 12.88% to 16.88% [34]. It seems regular wastewater treatment processes cannot completely remove pharmaceutical compounds. All the same, research has shown that activated carbon-based systems work better, especially when pharmaceutical compounds are at low concentrations [35]. Granular activated carbon (GAC) systems, which were first used in treatment plants across America and Canada, show exceptional adsorption capabilities [36]. The combination of activated carbon with biological treatment or hybrid membrane systems improves removal efficiency [37]. The pharmaceutical industry creates large amounts of Ibuprofen-containing waste that needs proper management. Activated carbon quickly deactivates medications, and studies show desorption rates stay below 0.5% [35]. It also stops the formation of toxic byproducts or pharmacologically active compounds [36]. Modern disposal systems that use activated carbon are a secure and quick way to dispose of unused medication. These systems achieve more than 99% deactivation efficiency, and leaching rates stay below 1.3% in washout studies [35]. Activated carbon works better than deactivating agents like sodium percarbonate and zeolite because it can deactivate almost any drug [35]. Setting up activated carbon systems requires careful attention to process parameters. System performance relies on particle diameter, mass transfer coefficient, and porosity [38]. Therefore, optimizing these parameters will maximize Ibuprofen adsorption, especially at the particle center [38]. Recent breakthroughs in carbon-based materials have created new methods to remove Ibuprofen molecules. Scientists have developed innovative

adsorbents that perform better and have enhanced surface properties [25,39]. Agricultural and industrial waste materials make promising precursors for activated carbon production. Waste coffee-derived adsorbents created at 850 °C for 100 minutes demonstrate remarkable adsorption capabilities [32]. Green practices utilizing biomass sources like olive waste cake, cork powder, watermelon rind, rice husk, and coconut shell have become effective adsorbents [32,40,41]. The surface area of these materials varies significantly. Some bio-derived carbons reach up to 3116 m²/g [42]. Waste-derived carbons from recycled textile biochar show adsorption capacities of 53.9 mg/g [43]. Their superior performance comes from their well-laid-out pore structure and high surface reactivity. Metal-organic framework (MOF) derived carbons mark a breakthrough in composite material development. These materials blend high porosity with well-defined pore structures [44]. Magnetic nickel ferrite/activated carbon composites with surface areas of 564 m²/g achieve maximum adsorption capacities of 261 mg/g [44]. Silica-carbon composites created through pyrolysis at 700 °C show improved adsorption properties [32]. Spherical carbons prepared through hydrothermal treatment and activation deliver promising results from various precursors. A summary of the types of precursors and key properties of carbon-based composite materials is given in **Table 2**.

Chemical modification techniques have boosted adsorption performance. Surface oxidation treatments paired with agents like phosphoric acid, sulfuric acid, and potassium carbonate improve the material's affinity for Ibuprofen molecules [44]. Ethylamine and ethylenediamine functionalization create basic and hydrophobic surfaces that enhance adsorption kinetics [44]. The modification relies on donor-acceptor mechanisms between

Table 2. Summary of precursor types, hydrothermal processing methods, and key features of carbon-based composite materials

Precursor type	Processing method	Key features
Carbohydrates	Hydrothermal+ Chemical activated	High surface area, controlled porosity
Saccharides	Hydrothermal+ KOH activated	Enhanced pore distribution
Agricultural waste	Direct hydrothermal carbonization	Cost-effective, sustainable

Ibuprofen's π aromatic ring and resulting carbonyl groups [44]. Advanced treatments like ozonation and sonication create other binding sites on the activated carbon surface. This increases adsorption capacity by 25% compared to unmodified versions [44].

3. Overview and Interpretation of Findings

3.1. Studies conducted on Ibuprofen removal

A brief look at the history of IBP removal shows this issue was studied by Melillo and colleagues for the first time [23]. Ibuprofen removal from protein-free and bovine serum albumin-containing aqueous solutions was accomplished by activated carbon adsorbent that possessed a varied pore sizes [45]. The Ibuprofen in the liquid phase was removed by AC prepared from cork waste. The adsorption process followed pseudo-second-order kinetics and Langmuir isotherm [32]. Two activated carbon adsorbents were prepared from cork waste. The chemical activation of cork (CAC) and physical activation of CAC (CPAC) adsorbents were prepared by chemical activation method using K_2CO_3 and physical activation of CAC with N_2 steam, respectively. The maximum adsorption capacity of Ibuprofen was estimated by the Langmuir isotherm. The findings showed that q_m was 153.2 mgg^{-1} and 416.7 mgg^{-1} for CAC and CPAC adsorbents, respectively, at 40°C . The results of this research show adsorption capacity for CPAC is better than that of CAC [32]. The annual consumption of plastic materials, especially plastic bottles, is increasing rapidly worldwide.

A kind of AC was prepared from municipal waste and used to remove Ibuprofen from the solution. Polyethylene terephthalate (PET), found in plastic bottles, could be used for preparing AC [46]. PET adsorbent derived from municipal waste has delicate pores and a high surface area. The municipal waste was converted to AC at 925°C under a CO_2 atmosphere [46]. Table 3 summarizes some studies on the adsorption of IBP by activated carbon-based adsorbents.

Sisal, which comes from the leaves of a tropical plant called *Agave sisalana*, is a strong fiber used to make rope and sacking. A certain amount of saturated aqueous solution of K_2CO_3 was added to sisal waste at room temperature. After drying at 100°C , the adsorbent was activated under N_2 flow. The removal efficiency depended on the volume of the micropores, and it changed from 65 to 75 percent [47]. The activated carbon was prepared using as a precursor a by-product of cork and was activated by KOH. This adsorbent was used to remove some pharmaceutical compounds, and IBP was removed better than other substances. It was revealed that the diffusion of IBP towards adsorbent active sites depends on the dimension of IBP and the larger micropores of the adsorbent [33].

Guedidi *et al.* conducted two types of research on IBP removal. They modified granular AC by oxidation with H_2O_2 and $NaOCl$, which was performed in the presence or absence of ultrasound. The IBP removal is strongly dependent on pH. When pH 7 predominates, the dispersive interactions increase and IBP removal decreases. At pH 3, the adsorption of

IBP was increased and the adsorption process was reported as endothermic and spontaneous. When the AC surface was treated with NaOCl, the phenolic and carbonyl groups were formed, resulting in decreased IBP removal. In contrast, treatment with H₂O₂ activated the lactonic or quinone groups on the adsorbent surface to be activated, leading to increased IBP adsorption [48]. In another study, they evaluated the performance of an AC cloth for the removal of IBP. Increased IBP removal occurred at the lower pH of 3 with rising temperature. The intraparticle diffusion model stated that the adsorption of IBP on AC cloth is controlled by three stages. In the first stage, the adsorbate is placed on the external surface of the adsorbent, then it diffuses into the larger porous network, and finally, intra-particle diffusion of compounds into the adsorbent ultramicropores [49]. A study was conducted to prepare microwave-assisted activated carbon from bamboo waste. In this work, the parameters such as contact time, adsorbent dose, pH, and temperature were evaluated, and the experimental data accommodated the Langmuir isotherm and pseudo-second-order kinetic model. The adsorption process began with the diffusion of adsorbate to the surface of the AC, which was accelerated for one hour. Then, IBP removal was performed slowly [50]. One study investigated the adsorption of IBP, a common pharmaceutical contaminant, onto granular activated carbon through batch experiments. The effects of IBP concentration, pH, and temperature on adsorption capacity were examined. Results indicate that adsorption is most effective at low pH (around 2) and high temperatures, conditions that favor the non-ionized form of IBP, which has a higher affinity for activated carbon. The research also highlights the role of the activated carbon's surface charge and proposes a Langmuir-based multicomponent adsorption model. This model

accurately explains the experimental results, showing that adsorption is exothermic and influenced mainly by the speciation of IBP in solution [51]. In another study, the conditions for IBP removal were optimized, and synthesized magnetic-carbon nanocomposite was used. In this work, in addition to experimental work, modeling based on experimental design was performed. Experimental conditions depended on concentration, temperature, pH, and adsorbent dose. The synthesized magnetic nanocomposite can remove IBP better than its precursor carbon from the water. The modeling method predicted that the maximum of IBP removal is 65.81% of the solution. This value is close to the experimental value of 65.12%. The modeling method predicted that the maximum IBP removal is 65.81% of the solution. This value is close to the experimental value of 65.12% [52]. Mukoko *et al.* investigated activated carbon from rice hulls using phosphoric acid for adsorbing paracetamol, aspirin, and Ibuprofen from hospital effluent. The rice hull activated carbon was characterized using SEM, XRD, and FT-IR, with an iodine number of 815.0 ± 2.52 mg/g. Aspirin adsorption fits the Freundlich isotherm, while IBP and paracetamol fit the Langmuir isotherm, and adsorption kinetics follow a pseudo-second order. Aspirin, paracetamol, and IBP were found in hospital wastewater, and the activated carbon effectively removed these compounds [53].

A method of preparation for magnetic AC using palm shell waste was evaluated to remove IBP. Experimental results showed that the magnetic adsorbent has a sorption density of about 2.5 times that of AC. [54]. Wong *et al.* synthesized another magnetic adsorbent based on palm to remove several pharmaceutical compounds. The magnetic strength of desired composite decreased, when the AC was functionalized by triethoxyphenylsilane. The values of different

Table 3. Findings of carbon-based adsorbents in the removal of IBP from the aqueous solution

Adsorbent	Activation method or AC modification	Surface area (m^2g^{-1})	Maximum adsorption capacity (mgg^{-1}) or Removal	Adsorption optimum Condition	Kind of Kinetics	Kind of isotherm	Thermodynamics		Ref.
							ΔG (kJ/mol)	ΔH (kJ/mol)	
AC	Covered with cellulose	2,330	1,009.4	310 K, pH=6.5, 5-1000 μgml^{-1} 30 min	Not reported	Langmuir	-0.33	Not reported	[45]
Cork	Chemical activated	891	153.2	313 K, pH=2, 20-60 mg^{-1} 0.5-6 h	Pseudo-second order	Langmuir	Not reported	Not reported	[32]
	Physical activated	1,060	416.7	313 K, pH=2, 20-60 mg^{-1} 0.5-6 h	Pseudo-second order	Langmuir Freundlich	Not reported	Not reported	
Municipal waste	Polyethylene terephthalate (PET)	1,426	266.6	303 K, pH=2, 20-120 mg^{-1} 2-6 h	Pseudo-second order	Langmuir Freundlich	Not reported	Not reported	[46]
Sisal	Chemical activated	1,038	75% Removal percentage	303 K, pH=4, 120 mg^{-1} 6 h	Pseudo-second order	Not reported	Not reported	Not reported	[47]
AC-magnetic nanocomposit	Chemical activated	335	60.39%	293-358 K, pH=2.5-10.5, 80-100 mg^{-1} 60 min	Not reported	Not reported	Not reported	Not reported	[52]
AC	AC (NaOCl)	709	Not reported	298-328 K, pH=3 & 7, 100 mg^{-1} 5 days	Pseudo-second order Elovich	Langmuir Freundlich	Not reported	Not reported	[48]
	AC (H_2O_2)	781	159.9				-7.3	8.1	

Table 3. Continued

Adsorbent	Activation method or AC modificati	Surface area (m ² g ⁻¹)	Maximum adsorption capacity (mgg ⁻¹) or Removal percentage	Adsorption optimum Condition	Kind of Kinetics	Kind of isotherm	Thermodynamics		Ref.
							Not reported	Not reported	
Pre-treated cork	Chemical activated with KOH	729	138.3	303 K, pH=5, 30 mgl ⁻¹ 24 h	pseudo-second order	Langmuir	Not reported	Not reported	[33]
Bamboo Waste	Microwave	722.27	278.55	298-333 K, pH=5, 80- 100 mgl ⁻¹ 60 min	Pseudo-second order	Langmuir Freundlich	-6.15	-21.20	[50]
Rice hull AC	Chemical activated		1,100	298-318K, pH=4, 20 mgl ⁻¹ 120 min	Pseudo-second order	Langmuir	-	-	[53]
Magnetized AC	Sonicated AC	666.5	157.3	298-318 K, pH=4- 7, 20 mgl ⁻¹ 7 days	Pseudo-second order	Langmuir Freundlich	-7.99	6.35	[54]
Granular Activated	Made from bituminous coal	1,000	35	307 K, pH=2, 10 mgl ⁻¹	-	Langmuir-based multicomponent	-	-	[51]
magnetic palm AC	Hydrothermal method	960.9	102.9	298-318 K, pH=2- 12, 10-50 mgl ⁻¹ 360 min	Pseudo-second order	Freundlich	Not reported	Not reported	[55]

Table 3. Continued

Adsorbent	Activation method or AC modification	Surface area (m ² g ⁻¹)	Maximum adsorption capacity (mgg ⁻¹) or Removal percentage	Adsorption optimum Condition	Kind of Kinetics	Kind of isotherm	Thermodynamics		Ref.
							Not reported	Not reported	
Granular AC	Commercial AC	1,036	105	298-318 K, pH=2-10, 20-80 mg ^l -1 12 h	-	Langmuir	Not reported	Not reported	[56]
AC cloth	Chemical activated	1,910	492	303-323 K, pH=3 & 7, 100 mg ^l -1 7 days	Pseudo-second order	Langmuir-Freundlich	-5.8	45.0	[49]
AC with TiO ₂	Sol-Gel UV-vis	-	92 %	298K, pH=4.3, 15 mg ^l -1, 4 h	Pseudo-second order	-	-	-	[58]
NiFe ₂ O ₄ /activated carbon	Hydrothermal method	564.4	261.35	298 K, pH=2, 25 mg ^l -1 240 min	Pseudo-second order	Sips	-34.18	20.27	[59]
AC embedded in chitosan-polyvinyl alcohol	Chemical activated	224.5	18.5	323 K, pH=3, 40 mg ^l -1 180 min	Pseudo-second order	Langmuir	-7.1	51.6	[56]
AC modified using FeCl ₃ .6H ₂ O and Na ₂ SO ₃	Co-precipitation method	-	95%	319 K, pH=7.22, 10 mg ^l -1 120 min	Pseudo-order n, with n = 2.5	Two-site Langmuir	-	-	[61]
AC with Beverage industry wastewater	Chemical activated	642	105.91	298 K, native pH, 50 mg ^l -1 120 min	Pseudo-first-order	Sips	-	-	[63]

Table 3. Continued

Adsorbent	Activation method or AC modification	Surface area (m ² ·g ⁻¹)	Maximum adsorption capacity (mg·g ⁻¹) or Removal	Adsorption optimum Condition	Kind of Kinetics	Kind of isotherm	Thermodynamics		Ref.
AC	Activated carbon	641	84.5%	298 K, pH=2, 100 mg·l ⁻¹ 300 min	-	-	-	-	[64]
	Sonicated activated carbon	732	92.5%						
AC	Purchased from Trace Elemental	870	96%	pH=6, 1 mg·l ⁻¹ 10 mins	-	Langmuir Freundlich	-	-	[65]
Magnetic Activated Carbon	Microwave assisted pyrolysis process	795	Ultrapure water: 711 Wastewater r: 273	298 K, pH=5.5-8, 20 µmol ⁻¹ 120 min	Elovich	Langmuir	-	-	[66]
AC-RGL	Chemical Activated	17.69	113.76	318 K, pH=5, 75 mg·l ⁻¹ 105 min	Pseudo-first-order	Freundlich	-3.8	-2.34	[67]
AC-nZVI-clay	nZVI-clay sonicated with AC	-	87.1%	298 K, pH=7, 50 mg·l ⁻¹ 150 min	Pseudo-second order	Freundlich	-	-	[31]
AC	Purchased from Norit (Utrecht, The Netherlands)	523	0.45 mmol·g ⁻¹	298 K, 0.298mmol·L ⁻¹ 355.9 min	Pseudo-first-order	Generalized Langmuir	-3.07	22.73	[69]
TiO ₂ -NPs-GNSAC composite	Chemical Activated	395.92	82%	303 K, 5 mg·l ⁻¹ , 50 min	Pseudo-second order	Langmuir	-5.416	12.385	[68]

hydrogel activated carbon polypyrrole/act CuO-	Chemical Activated and precipitati on method	190.3	96.7%	293 K, pH=6 5 mg ^l -1, 60 min	Pseudo- first- order	-	-	-	[70]
Carbon Activated Biomass	Chemical Activated	1424.8 8	99.14%	303 K, pH=3 50 mg ^l -1, 120 min	Pseudo- second order	Langmuir	-	-	[25]

pH and the presence of electrolytes affected the removal percentage of pharmaceutical compounds [55]. Research on removing Ibuprofen and diclofenac from water by metal-organic framework (MOF) derived porous carbon and activated carbon was published in 2017. The maximum adsorption capacities of IBP by commercial activated carbon and porous carbons derived from MOFs (PCDMs) were 105 mg/g and 320 mg/g, respectively. The results of adsorption fitted well with the Langmuir isotherm [56]. Bahamon *et al.* focused on the removal of Ibuprofen from water using adsorption in activated carbons, employing advanced molecular simulations. This work utilizes Grand Canonical Monte Carlo (GCMC) simulations to explore how Ibuprofen interacts with activated carbons. Findings confirm the effectiveness of GCMC simulations for understanding and optimizing drug removal in water treatment. The interaction strength between IBP and the surface of ACs is influenced by the acid-base characteristics of the surfaces. Functional groups can alter the electronic density on the carbon surfaces, affecting how well IBP is adsorbed compared to water molecules. The hydrophobic nature of the ACs also impacts the preferential adsorption of IBP over water. The adsorption capacities at different concentrations of IBP (1, 10, and 100 ppm) ranged from 0.15 to 0.8 mmol/g, increasing at higher concentrations [57].

A document discusses the removal of Ibuprofen from wastewater using activated carbon (AC) composites impregnated with TiO₂ (ACxTy) in a flow reactor under UV irradiation. The key findings are: 1. The composite AC90T10 showed the highest removal of Ibuprofen (92%) owing to the synergistic effect of adsorption and photodegradation. 2. The weight ratio of composite to Ibuprofen had a limited effect on the removal efficiency within the concentration range of 5-25 mg/L, but reaction time under UV light and solution pH were essential factors. 3. Kinetic studies showed the data fitted well with pseudo-second order, pseudo-first order, and Elovich models, indicating a combined adsorption and photodegradation mechanism. 4. Intraparticle diffusion was the rate-limiting step, with faster initial diffusion followed by a slower final equilibrium stage [58]. Fröhlich *et al.* synthesized the NiFe₂O₄/activated carbon composite (NiAC) using a hydrothermal method to remove some pharmaceutical compounds like Ibuprofen and ketoprofen from diluted aqueous solutions. The adsorption of Ibuprofen and ketoprofen was evaluated under different pH conditions, and the best results were obtained at acidic pH (pH 2). Adsorption was favored at higher temperatures, with equilibrium reached after 240 minutes. Kinetic data were modeled using the pseudo-second-order model, while the equilibrium adsorption was best described by the Sips model. The maximum adsorption

capacities were 261.35 mg/g for Ibuprofen and 97.75 mg/g for ketoprofen [59]. One study investigates the efficiency of using activated carbon (AC) and graphene oxide (GO) embedded in chitosan-polyvinyl alcohol (CS-PVA) biocomposites for the removal of Ibuprofen, a common pharmaceutical pollutant, from wastewater. The research addresses the challenges of pharmaceuticals and personal care products (PPCPs) in aquatic environments. AC and GO significantly improved the Ibuprofen removal rates from 11% to 83% and 94%, respectively. Removal percentages were highest at acidic pH (around pH 3.0). The optimum conditions determined through experiments included a biocomposite amount of 100 mg, an Ibuprofen concentration of 40 mg/L, and a temperature range of 20 °C to 60 °C. The Temkin and Freundlich models fit the data better than the Langmuir model, indicating heterogeneous adsorption on the biocomposite surfaces [41]. Kinetic studies indicated that the Ibuprofen adsorption followed a pseudo-second order model, suggesting that the adsorption process is chemisorption [42,60]. Vargues *et al.* investigated a new method for removing pharmaceuticals from wastewater using a magnetic-activated carbon adsorbent. Magnetite NPs were synthesized via a modified procedure using $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$ and Na_2SO_3 . The hybrid adsorbent was characterized by FTIR and XRD methods and tested for Ibuprofen and amoxicillin adsorption, achieving 95% and 90% removal rates, respectively. The adsorbent proved effective in spiked urban wastewater and maintained adsorption ability upon regeneration. The two-site Langmuir model and the pseudo-order n model of kinetics, with $n = 2.5$, best described IBU's adsorption [61]. Guedidi *et al.* researched how effective adsorption on activated carbon can be for removing ionic liquids and Ibuprofen from wastewater. This study investigates the

adsorption of two pyridinium ionic liquids (IL1 and IL2) and IBP on activated carbon cloth. Adsorption kinetics and isotherms were examined at pH 3 and 7.5, revealing an exothermic physisorption process. IL1 adsorption kinetics was faster at pH 3 than pH 7.5, while IL2 adsorption equilibrium was similar at both pH levels. Adsorption isotherms indicated an exothermic process, with the Langmuir-Freundlich model providing the best fit for the experimental data. In this study, competition between Ibuprofen and IL2 during adsorption kinetics in mixtures was identified, and the location of adsorbed molecules within the activated carbon's porosity was determined [62]. One study focused on the preparation and characterization of activated carbon derived from the sludge of a beverage industry effluent treatment plant (ETP), and its application for the adsorption of pharmaceuticals (Ibuprofen, ketoprofen, and paracetamol) from aqueous solutions. The study involved the production of two types of activated carbon: Beverage Sludge Activated Carbon (BSAC) and Acid-Treated Beverage Sludge Activated Carbon (ABSAC). The acid treatment significantly improved the properties of ABSAC, resulting in a higher surface area and total pore volume than BSAC, making it more efficient in adsorbing pharmaceutical contaminants. It was found that increasing the adsorbent dosage led to higher removal efficiencies for all the pharmaceutical compounds. ABSAC, in particular, showed better performance than BSAC, due to its enhanced surface characteristics, which included a greater number of active sites and a higher porous structure. The maximum adsorption capacity for Ibuprofen was 105.91 mg/g, based on the Sips model for equilibrium data. The kinetic studies indicated that adsorption followed the pseudo-second-order model, and equilibrium was achieved after 180 minutes. Additionally, using sludge from the beverage industry as a

precursor material for producing activated carbon represents a sustainable solution for managing wastewater treatment plant sludge, which is otherwise costly and challenging to dispose of. The results suggest that ABSAC could be effectively applied to the treatment of pharmaceutical contaminants in industrial wastewater, offering an environmentally friendly alternative to conventional waste disposal methods [63]. A study developed a mathematical model to investigate Ibuprofen removal from pharmaceutical wastewater using the adsorption process with activated carbon (AC) and sonicated activated carbon (SAC). The model evaluated how operating parameters, including particle porosity, particle diameter, and Ibuprofen diffusion coefficient, affect the adsorption process. This research aimed to understand better the role of particle characteristics and solute properties on Ibuprofen adsorption. SAC outperforms regular AC due to its higher porosity and external mass transfer coefficient. Furthermore, particle diameter, porosity, and diffusion coefficient are crucial factors in determining the efficiency of the adsorption process. The maximum IBP removal was 84.5% and 9.5% for the AC and SAC, respectively [64]. The activated carbon purchased from Trace Elemental Instruments demonstrated high efficiency in removing common non-steroidal anti-inflammatory drugs (NSAIDs) from wastewater. In this work, the analysis of drug removal was done by high-performance liquid chromatography (HPLC) with a diode array detector (DAD). Activated carbon was highly effective in removing NSAIDs from wastewater, with removal efficiencies up to 98% for acetaminophen and 96% for Ibuprofen under optimal conditions [65]. A magnetic activated carbon (MAC) was prepared from paper mill sludge for the adsorptive removal of carbamazepine (CBZ), sulfamethoxazole (SMX), and Ibuprofen (IBU)

from water and wastewater. Here, the benefits of using magnetic activated carbon (MAC) over traditional activated carbon were investigated. This study indicated that the adsorption capacity of IBU is 711 and 273 in ultrapure water and wastewater, respectively [66]. The other research evaluates the potential of rose geranium leaves for producing low-cost activated carbon (AC-RGL) using orthophosphoric acid (H_3PO_4) to adsorb Ibuprofen. AC-RGL was characterized using TGA, SEM, and FTIR, and its performance was compared to natural rose geranium leaves (Raw-RGL). AC-RGL exhibited a maximum sorption capacity of 113.76 mg/g. In comparison, Raw-RGL had a capacity of 74.12 mg/g, confirming the potential of rose geranium leaves as an adsorbent for Ibuprofen. BET analysis showed that AC-RGL had a surface area of 17.69 m²/g, with a high micropore volume, and pH(PZC) values for Raw-RGL and AC-RGL were 7.32 and 6.61, respectively. Ibuprofen adsorption increased with concentration, with AC-RGL showing performing better than Raw-RGL, and the Freundlich model best fit the adsorption data. Kinetic studies showed that Ibuprofen removal was rapid initially and slowed down as active sites filled, with the pseudo-first-order model providing the best fit [67]. Azizpourian *et al.* investigated the removal of metronidazole (MNZ) and Ibuprofen (IBP) from aqueous solutions using clay-based adsorbents like activated carbon-nZVI-clay nanocomposite. In this study, zero-valent iron nanoparticles (nZVIs) were prepared and then used to create nZVI-clay and activated carbon-nZVI-clay nanocomposites. The effects of parameters such as pH, adsorbent dose, initial concentration, and contact time were evaluated for removing MNZ and IBP. The results showed that the 20% activated carbon-nZVI-clay (20-AC-nZVI-clay) nanocomposite had the highest removal efficiency of 87.11% for MNZ and

87.1% for IBP under optimum conditions. The adsorption data fitted well with the Langmuir isotherm model and followed the pseudo-second-order kinetic model. This adsorbent can be reused up to three cycles with adequate efficiency [31]. A study aimed to develop eco-friendly and cost-effective adsorbents for removing pharmaceutical pollutants from wastewater. Titanium dioxide nanoparticles (TiO₂-NPs) were biosynthesized using *Cola nitida* pod extract and impregnated onto groundnut shell-derived activated carbon (GNSAC). The TiO₂-NPs-GNSAC composite exhibited a mesoporous structure with an average pore size of ~5 nm and high carbon content. Batch adsorption experiments for Ibuprofen removal were optimized via Box-Behnken design and response surface methodology (RSM), investigating temperature, contact time, and adsorbent dosage as key factors. Under optimal conditions, Ibuprofen removal efficiencies reached ~68% for GNSAC and ~82% for TiO₂-NPs-GNSAC. Langmuir isotherm provided the best fit for equilibrium data, while the pseudo-second-order kinetic model accurately described the adsorption process. Thermodynamic analysis revealed that adsorption was spontaneous, endothermic, and predominantly physical. Additionally, the modified adsorbent maintained performance after three regeneration cycles.

These findings highlight the potential of utilizing agricultural waste and green-synthesized nanomaterials for efficient pharmaceutical wastewater treatment and environmental pollution mitigation [68]. Another study investigates the adsorption behavior of Ibuprofen sodium (IBP), naproxen sodium (NPX), and diclofenac sodium (D) on granular activated carbon (GAC), focusing on equilibrium, kinetics, thermal stability, and electrokinetic properties. These compounds are commonly found pollutants in water due to the widespread

use of pharmaceuticals. Activated carbon is highly effective at adsorbing non-steroidal anti-inflammatory drugs (NSAIDs) due to its large surface area and porous structure. The adsorption process was reported to be spontaneous, endothermic, and physical (physisorption). Temperature increases (15 °C to 35 °C) enhanced adsorption rates and capacities for all drugs. Among the medicines, IBP showed the lowest adsorption capacity due to its high water solubility, making it less prone to interact with hydrophobic activated carbon surfaces. The negative values of ΔG° indicate that the adsorption process is spontaneous. Also, the positive values of ΔH° confirm that the adsorption process is endothermic and has a physisorption mechanism [69]. Alqahtani *et al.* introduced a novel and sustainable photocatalyst, CuO-polypyrrole/activated carbon hydrogel (Cu@Ppy/AC), designed for the efficient removal of Ibuprofen (IBU) from aqueous environments under visible light. The photocatalyst was synthesized using rice husk-derived activated carbon and polypyrrole hydrogel, and characterized by XRD, FTIR, SEM, and BET analyses, confirming a high surface area (190.3 m²/g) and enhanced charge separation. Optimal conditions were established at 0.5 g/L catalyst dosage, pH 6, and 5 mg/L IBU concentration, achieving complete degradation in 40 minutes and total mineralization into CO₂ and H₂O within 80 minutes. The degradation pathway involved hydroxylation, decarboxylation, and aromatic ring cleavage, with OH• and O₂•⁻ radicals as dominant reactive species. Toxicity tests indicated transient cytotoxicity of intermediate products, which disappeared upon complete mineralization. The catalyst retained over 85% efficiency after seven reuse cycles, demonstrating excellent stability and recyclability. Comparative evaluation showed superior performance and cost-effectiveness compared to previously reported

photocatalysts, making Cu@Ppy/AC a promising candidate for large-scale pharmaceutical wastewater treatment. Future work will focus on real wastewater testing, scalability via immobilized or continuous systems, and assessment against other pharmaceutical pollutants [70]. Su *et al.* explore using waste Ginkgo biloba leaves to prepare nitrogen-doped biochar via a one-step carbonization process using KOH and urea as activators. The resulting biochar exhibits a high surface area (1,424.88 m²/g) and a hierarchical porous structure, making it highly efficient for adsorbing Ibuprofen (IBU) from water. Adsorption experiments demonstrated a maximum removal rate of 99.14% and an adsorption capacity of 160 mg/g under optimal conditions (pH 3, 30 °C, 0.04 g/L biochar, 120 min contact time). The adsorption process conforms to pseudo-second-order (PSO) kinetics and Langmuir isotherm models, suggesting uniform monolayer adsorption. Mechanistic analysis reveals that hydrogen bonding, π - π interactions, electrostatic forces, and van der Waals interactions contribute to the adsorption. Molecular dynamics simulations confirmed enhanced interaction energy due to nitrogen doping, especially from graphitic and pyrrolic nitrogen groups. Furthermore, the biochar retained 92% efficiency after five cycles, highlighting its reusability. The estimated treatment cost is only 0.0003 USD/L, making this approach economically viable and environmentally friendly. This research proposes Ginkgo biochar as a promising adsorbent for wastewater purification and resource utilization of forestry waste [25].

3.2. Removal of Ibuprofen by activated carbon-based adsorbents

Pharmaceutical removal efficiency depends on several factors: adsorbent properties (surface

area, pore structure, and functional groups), adsorbate properties (solubility, molecular size, and charge), and operating conditions (pH, temperature, AC dosage, and competing substances). Adsorption equilibrium is typically described using isotherm models such as Langmuir, Freundlich, and Sips. Kinetic models like pseudo-first-order, pseudo-second-order, and Elovich equations help explain adsorption rates [2,31,39,71].

In studying the operating conditions of the adsorption process, it is essential to know the characteristics of the adsorbent. Also, research has often shown that the adsorption process of IBP is more effective at acidic to neutral pH levels [60,65,67]. Temperature frequently influences the adsorption capacity. In some cases, higher temperatures generally lead to increased IBP adsorption, meaning an endothermic process occurred, indicating that thermal energy facilitated the mobility and interaction of IBP with adsorbents [57].

Some of the equations of the adsorption isotherm models used for all the studies presented in Table 4 are listed in Table 3. In the adsorption process, the study of the amount of adsorbed compound on the adsorbent at a specific temperature was described by the adsorption isotherm. The type of isotherm can show beneficial information about the nature of adsorbents and adsorption [31,72].

The Langmuir isotherm explains that the adsorption process strongly depends on the active sites of the desired adsorbent surface. In this model, the adsorbent surface is uniform and homogeneous, and all sites have the same priority for adsorption. The desired adsorbent has active sites with the same energy. No interaction occurs between two adjacent adsorbed molecules, and ultimately, a monolayer coating is formed on the adsorbent surface. The Freundlich isotherm is an empirical equation and can be used well when

experimental data do not fit the Langmuir isotherm. In this model, the active sites of the adsorbent have different energies and a heterogeneous surface. The adsorption occurs in multilayers. The Sips model is an adsorption isotherm that combines aspects of the Langmuir and Freundlich isotherms to make it helpful in describing heterogeneous adsorption systems. [31,59,71,75]. The Sips model can be used when the interactions between the adsorbate and

adsorbent are complex or when the active sites are not uniformly distributed [24,31,59,63,71,73,74]. The Langmuir-Freundlich model is a special type of the Sips model. In this model, when the heterogeneity parameter approaches 1, the adsorption conditions approach the Langmuir model. Conversely, when this parameter is less than 1,

Table 4. Linear equations of some of the adsorption isotherm models

Isotherm models	Linear equation	Parameters
Langmuir isotherm	$\frac{1}{q_e} = \left(\frac{1}{q_{max}K_L} \right) \frac{1}{C_e} + \frac{1}{q_{max}}$	<p>q_e: The amount of drug adsorbed at equilibrium (mg g⁻¹)</p> <p>q_{max}: The maximum amount of drug adsorbed (mg g⁻¹)</p> <p>K_L: Adsorption equilibrium constant (L mg⁻¹)</p> <p>C_e: The equilibrium concentration of drugs in solution (mg L⁻¹)</p>
Freundlich isotherm	$\ln q_e = \ln K_F + \left(\frac{1}{n} \right) \ln C_e$	<p>K_F: Adsorption capacity</p> <p>n: Adsorption intensity</p>
Sips	$\frac{q_{mS}}{q_e} = 1 + \frac{1}{K_S C_e^\beta}$	<p>q_e: The amount of drug adsorbed at equilibrium (mg g⁻¹)</p> <p>q_{mS}: The Sips maximum capacity (mg g⁻¹)</p> <p>K_S: The Sips equilibrium constant (L mg⁻¹)</p> <p>C_e: The equilibrium concentration of drugs in solution (mg L⁻¹)</p> <p>β: The Sips model exponent</p>
Langmuir-Freundlich	$\frac{q_{mLF}}{q_e} = 1 + \frac{1}{(K_{LF} C_e)^\beta}$	<p>q_e: The amount of drug adsorbed at equilibrium (mg g⁻¹)</p> <p>q_{mLF}: The Langmuir-Freundlich maximum capacity (mg g⁻¹)</p> <p>K_{LF}: The equilibrium constant for a heterogeneous solid</p> <p>C_e: The equilibrium concentration of drugs in solution (mg L⁻¹)</p> <p>β: The heterogeneity parameter perches between 0 and 1</p>

Table 5. Linear equations of some of the adsorption kinetic models

Kinetic models	Linear equation	Parameters
Pseudo-first-order	$\ln(q_e - q_t) = \ln q_e - k_1 t$	q_e : Equilibrium adsorption capacity q_t : Adsorption capacity at time t k_1 : Rate constant
Pseudo-second-order	$\frac{t}{q_t} = \frac{t}{q_e} + \frac{1}{k_2 q_e^2}$	q_e : Equilibrium adsorption capacity q_t : Adsorption capacity at time t k_2 : Rate constant
Elovich	$q_t = \frac{1}{\beta} \ln(\alpha\beta) + \frac{1}{\beta} \ln(t)$	q_t : Adsorption capacity at time t α : Initial adsorption rate β : Elovich constant
Intra-particle diffusion	$q_t = k_{dif} t^{0.5} + C$	q_t : Adsorption capacity at time t C: A constant that gives about the thickness of the boundary layer k_{dif} : Diffusion constant

the adsorption conditions approach the Freundlich model [76,77]. The Langmuir and Freundlich models showed the best fit for IBP adsorption. In some studies, the Sips model analyzes data when the IBP-adsorbate interactions are complex. The kinetic studies indicated that adsorption followed the pseudo-first-order, pseudo-second-order, and Elovich models. The used kinetic models are listed in **Table 5**.

Adsorption kinetics explains the rate at which a solute is adsorbed onto an adsorbent. This concept is often represented graphically as an adsorption curve, showing the amount of adsorbate over time. The shape of this curve represents the essential kinetics of the adsorption process [78]. The pseudo-first-order and pseudo-second-order are two widely used experimental approaches in studying the adsorption kinetics of solutions. The adsorption kinetics depend on factors such as adsorbate material, adsorbent, temperature, and pH. The pseudo-first-order kinetics model is valid when the time to reach adsorption equilibrium is long. When a chemical interaction occurs between the adsorbent and the adsorbate, pseudo-second-

order kinetics can be used to describe the rate of surface adsorption [78,79]. Another kinetic model that can explain the adsorption process well is the Elovich model. This model is usually applied when the adsorption process involves adsorption on a heterogeneous surface, and is complex [80]. The result of the kinetic studies demonstrated that IBP adsorption mostly followed the pseudo-second-order model. Studies on the pseudo-second-order kinetic model showed that in the rate-limiting step, electron sharing and exchange occur between the adsorbent and IBP [2,80]. To investigate the nature of surface adsorption, changes in Gibbs energy, ΔG , and enthalpy changes play crucial roles. Thermodynamic findings have shown that low values of ΔG up to about -20 kJ/mol can indicate physisorption, and higher values of ΔG in the range of -80 kJ/mol and above indicate chemisorption [15,50].

According to **Table 3**, the ΔG values were negative, indicating the spontaneity of the adsorption process. The adsorption process can be endothermic or exothermic. When the process is exothermic, the adsorbent releases heat during the adsorption process. Unlike it, the

endothermic process needs to obtain energy from the surroundings. The negative values of ΔH for the IBP removal process indicate that this process has a physical nature involving weak attractive forces [46]. The positive values of ΔH indicate that the adsorption process and the interaction force between the adsorbent and IBP are physisorption, but also demonstrate that an increase in temperature promotes the adsorption process [59,60].

3.3. Proposed mechanism of Ibuprofen removal

The various agents that affect the adsorption mechanism include the nature of the adsorbate and the properties of the adsorbent. Significant adsorption can consist of four main steps: adsorbate transport in the liquid phase, liquid film mass transport, intra-particle diffusion, and adsorption onto active sites of the surface [2,81]. Both intra-particle diffusion and liquid film mass transport have a significant impact on the adsorption process [82]. Additionally, the interactions between the adsorbent and the adsorbate play an essential role in the adsorption.

The forces that influence physical adsorption consist of: hydrophobicity, Van der Waals forces, dipole-dipole interactions, hydrogen bonding, steric interaction, polarity, and π - π interaction. Also, the functional groups on the surface and their charges influence adsorption through wettability, alteration of electron-donating nature, and electrostatic interactions [2,54].

Wong *et al.* prepared a magnetic AC adsorbent for IBP removal. They reported that the primary removal mechanism of IBP could arise from dispersive π - π interactions between the hexagonal graphite of AC and the aromatic ring of IBP. The chemical properties of the adsorbent surface and the functional groups on the surface can be effective factors in the adsorption mechanism.

The donor-acceptor complexes are formed between the carbonyl group and the aromatic ring of IBP [54]. A study investigated the efficiency of using AC and graphene oxide (GO) embedded in chitosan-polyvinyl alcohol (CS-PVA) biocomposites to remove Ibuprofen. In this study, hydrogen-bond interactions between IBP molecules and the biocomposites and π - π interactions between π electrons of IBP and π electrons of benzene rings of carbonaceous biocomposites were essential factors that affected adsorption [60]. Thabede *et al.* assessed various mechanisms for the adsorption of IBP onto adsorbents, such as hydrophobic hydrogen bond, interactions, cation exchange, and electrostatics. **Figure 1** shows this mechanism [67].

Sandoval- Gonzalez *et al.* reported that physicochemical characteristics of the adsorbents, driving force, temperature, pH, contact time, and the interaction between adsorbate and adsorbent can determine the adsorption mechanism. The physicochemical characteristics of the AC consist of pore filling, interactions n - π and π - π , hydrogen bonds, Van der Waals forces, and electrostatic attraction. IBP is a small molecule with one aromatic ring containing hydrophobic and hydrophilic parts. The π - π interactions between the AC and the IBP solution can create high binding energy [9]. When the pH decreases, the hydrogen bonds are formed between carbon and IBP are made, while the π - π interaction decreases due to the reduction of the electron density in the carbon planes. The results show that the adsorption capacity increases in the range of $2 < \text{pH} < 4$ [51]. Bhadra *et al.* discussed the adsorption of two pharmaceutical and personal care products (PPCPs), Ibuprofen (IBP) and diclofenac (DCF), on porous carbon-derived materials (PCDMs). The researchers focused on IBP adsorption on PCDM-1000 as a representative material to

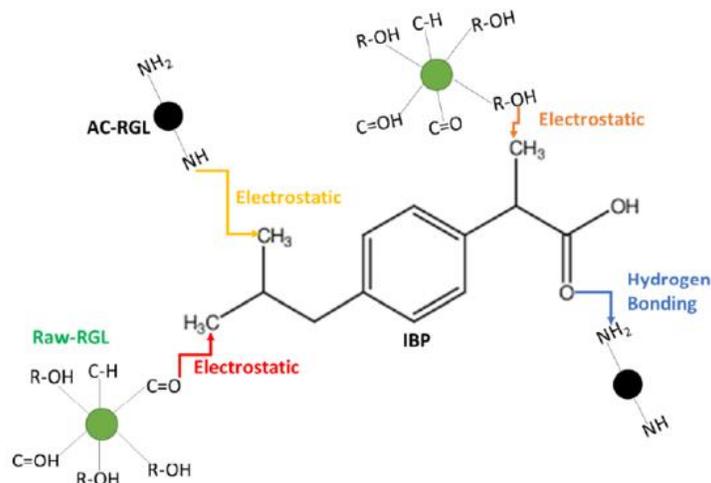


Figure 1. Proposed interaction between activated carbon from rose geranium leaves adsorbent (AC-RGL) and IBP compared to natural rose geranium leaves adsorbent (Raw-RGL) [67]

investigate the possible interaction mechanisms. The effect of solution pH on the adsorption capacity (q_t) was analyzed, and it was found that the q_t values decreased with increasing pH. Conventional electrostatic interaction could not explain the observed adsorption behavior, particularly at high pH values. As conventional electrostatic interaction could not fully explain the observed adsorption behavior, especially at high pH values where IBP is anionic and the PCDM-1000 surface is also negatively charged, the interaction mechanism suggested to explain the adsorption of IBP on PCDM-1000 was hydrogen bonding. The IBP has one hydrogen bond donor (COOH group) and two hydrogen bond acceptor sites. Meanwhile, PCDM-1000 has acidic (O-H-containing) and basic (N-containing) functional groups. The analysis suggests that IBP can interact with the PCDM-1000 surface through hydrogen bond formation, with the PCDM-1000 acting as the hydrogen bond donor [56]. Su *et al.* indicated that the adsorption mechanism of Ibuprofen onto Ginkgo biochar involves both physical and chemical interactions. Nitrogen doping (graphitic, pyrrolic, and pyridinic nitrogen) introduces active sites and enhances adsorption

energy. Molecular dynamics simulations reveal strong van der Waals forces (86.29%) and moderate electrostatic interactions (13.71%), along with hydrogen bonds per IBU molecule. Hydrogen bonding mainly occurs between biochar's -OH/pyrrole groups and Ibuprofen's carboxyl groups, while π - π stacking arises from aromatic structures. Under acidic conditions (pH 3), protonation enhances these interactions, increasing adsorption capacity. The hierarchical porous structure facilitates rapid diffusion and pore-filling, leading to efficient removal of IBU. **Figure 2** shows this mechanism [25].

In general, it can be concluded that the primary factors influencing the adsorption mechanism of IBP onto carbonaceous materials include the nature and molecular structure of the adsorbent, the surface charge of the carbonaceous adsorbents, and the electrostatic interactions between the IBP molecule and the carbonaceous material. Additionally, the pH, pKa of the adsorbate, and pH_{pzc} of the adsorbent are also important parameters that influence the adsorption mechanism. The main interactions of organic pollutant adsorption onto biochar and activated carbon include electrostatic

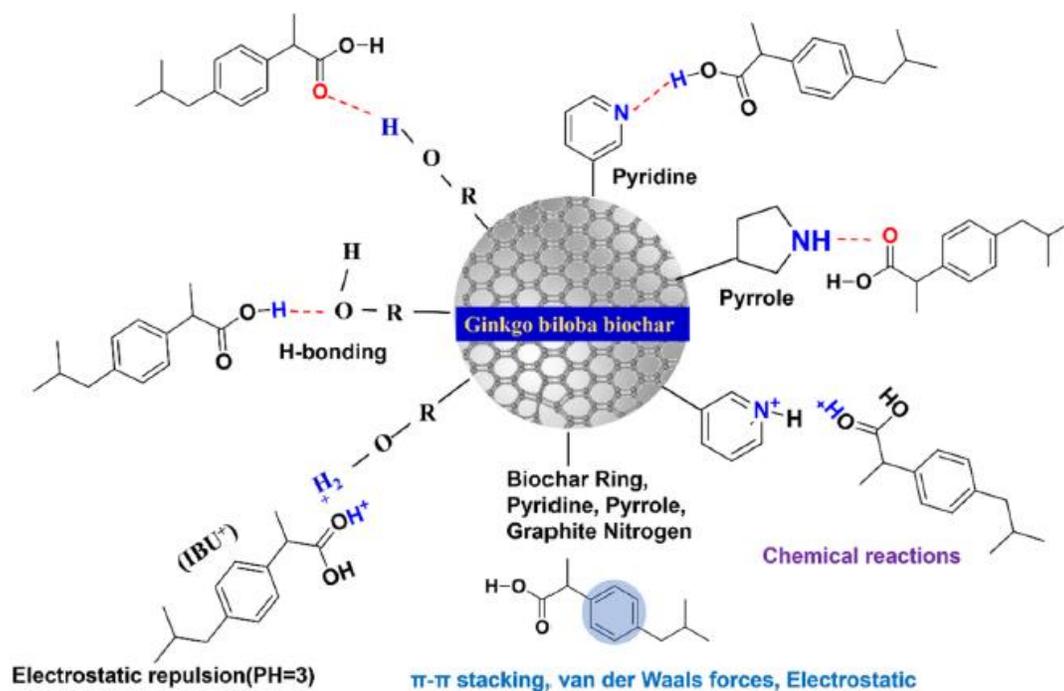


Figure 2. Proposed molecular interaction mechanism between biochar and IBP [25]

interactions, hydrogen bonding, π - π interactions, hydrophobic interactions, and pore filling. The key characteristics of the IBP molecule that contribute to the adsorption mechanism are its two acceptor sites (from the $-\text{COOH}$ group) and one H-bond donor. These characteristics enable predominantly electrostatic interactions to govern the adsorption of IBP onto carbonaceous materials. The incorporation of acidic oxygen-containing functional groups (*e.g.*, carboxylic, phenolic) due to oxidation can decrease the surface pH of the adsorbent. These acidic oxygen functionalities can facilitate hydrogen bonding, dipole-dipole interactions, and π - π stacking with organic pollutants, enhancing adsorption. The surface acidity of the adsorbent, as determined by the pH at the point of zero charge (pHpzc), can influence the electrostatic interactions between the adsorbent and the organic pollutants. At pH values above the pHpzc, the adsorbent surface becomes negatively charged, leading to electrostatic

repulsion with anionic organic pollutants and reduced adsorption. Conversely, at pH values below the pHpzc, the adsorbent surface may be positively charged, facilitating electrostatic attraction with anionic organic pollutants and enhancing adsorption. The surface acidity of adsorbents can vary depending on the synthesis conditions and can lead to differences in the dominant adsorption mechanisms for organic pollutants such as Ibuprofen [2,23].

3.4. Recovery and regeneration processes

The economic success of activated carbon systems depends on how well they can be regenerated. Thermal and chemical regeneration methods allow multiple reuse cycles, though efficiency changes between cycles [37]. Surface modification techniques, such as chemical oxidation with phosphoric or sulfuric acid, improve Ibuprofen's adsorptive removal. Recent work with magnetic carbon

composites offers promising solutions for recovery processes. For example, magnetic nickel ferrite/activated carbon composites, with surface areas reaching 564 m²/g, achieve maximum adsorption capacities of 261 mg/g. These materials make separation easier with external magnets, which optimizes the recovery process [37]. Some research discusses methods for regenerating activated carbon (AC) for pollutant removal. Various chemicals such as sodium hydroxide, sodium chloride, hydrochloric acid, methanol, and ethanol have been tested for desorption efficiency. Some research discusses methods for regenerating activated carbon (AC) used for pollutant removal. Chemicals such as sodium hydroxide, sodium chloride, hydrochloric acid, methanol, and ethanol have been tested for desorption efficiency. Findings demonstrated that sodium hydroxide and methanol are the most effective regenerating agents. Reza *et al.* indicated that IBP desorption via different eluents, especially methanol, can be effective with 96% reusability. It should be noted that after each regeneration cycle, the adsorption capacity decreases but remains acceptable for reuse. Chemical regeneration methods are cost-effective and practical, but may not be universally applicable for all pollutants. It is recommended to evaluate regeneration efficiency for individual pollutants or specific pharmaceutical groups to optimize the process [2,50,83]. Some reconstruction methods include: thermal regeneration (heating AC at high temperatures), chemical regeneration (using solvents or acids), and electrochemical regeneration (applying an electric current to break bonds between pharmaceuticals and AC). However, high costs, energy consumption, and reduced adsorption efficiency after several regeneration cycles must be considered [2].

4. Conclusion and Perspectives

This paper reviewed the experimental findings on the adsorption of Ibuprofen (IBP) using activated carbon-based adsorbents from aqueous solutions. IBP contamination in wastewater poses significant environmental and health risks due to its extensive use. Adsorption has proven to be an effective, economical, and promising technique for IBP removal, with carbon-based materials such as activated carbons, biochar, magnetic adsorbents, and single-walled carbon nanotubes exhibiting high adsorption capacities.

Key factors influencing adsorption performance include initial IBP concentration, adsorbent porosity, and surface functionalization methods such as grafting and crosslinking. The predominant adsorption mechanisms involve hydrophobic interactions, π - π stacking, hydrogen bonding, and electrostatic attractions, with optimal removal generally achieved under acidic conditions (approximately pH 3). Kinetic studies align with the pseudo-second-order model, suggesting that chemisorption and pore availability govern the uptake process.

Despite these advances, most research remains confined to laboratory-scale experiments using IBP concentrations much higher than those typically found in real wastewater (mg/L vs. μ g/L or ng/L). Additionally, competitive adsorption with coexisting pollutants, such as organic matter, metals, and dyes, is rarely addressed in practical scenarios.

Research on the regeneration of spent activated carbon, particularly from agricultural wastes, is scarce but critical for sustainable application. Cost-effective chemical and physical regeneration methods are essential to maximize adsorbent reuse.

Challenges remain in scaling up adsorption systems, ensuring economic feasibility, safety, and proper disposal of spent adsorbents. Future research should focus on developing low-cost, high-efficiency adsorbents tailored for real wastewater treatment, integrating adsorption with biological or mechanical processes, and addressing practical implementation issues to enable sustainable and effective IBP removal.

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Conflict of Interest

The authors declared that there are no conflicts of interest in this work.

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