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Analysis of Biochar Adsorption of Heavy Metal Ions in Water

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Abstract

At present, heavy metal ion pollution in water bodies has become a major challenge in global water environment governance. Although conventional treatment technologies such as chemical precipitation, membrane separation, ion exchange, and electrochemical methods are widely applied, they are often constrained by high operational costs, secondary pollution risks, and complex processing procedures. Against this background, biochar has attracted increasing attention as a promising material for water pollution remediation. This paper compares the physicochemical differences between plant-based biochar and solid waste-based biochar, with a focus on their implications for adsorption performance in different environmental conditions. The results indicate that the adsorption of heavy metal ions by biochar is governed by the combined effects of physical adsorption, chemical interactions, and ion exchange processes. These mechanisms together provide a more integrated explanation of the adsorption behavior of biochar in aquatic environments.

Keywords

biochar, heavy metal adsorption, adsorption mechanisms

1. Introduction

With the expansion of industrial activities such as mining, metal smelting, electroplating, and chemical manufacturing, increasing volumes of wastewater containing heavy metal ions are being discharged into aquatic environments. As a result, elements such as lead, cadmium, chromium, copper, and mercury continue to accumulate in water bodies. Due to their non-degradable nature, these contaminants pose persistent risks to both ecosystems and human health.

Biochar is a carbon-rich porous material produced through the pyrolysis of agricultural and forestry residues under oxygen-limited conditions. Compared with conventional adsorbents such as activated carbon, it offers advantages in terms of low cost, wide raw material availability, and abundant surface functional groups, all of which contribute to its adsorption capacity.

Existing studies have shown that biochar can remove heavy metal ions from water through multiple mechanisms, including physical adsorption, surface complexation, and ion exchange [1]. However, differences in raw materials and operational conditions lead to variations in adsorption performance, and the underlying mechanisms are not yet fully unified in quantitative terms. Against this background, this paper examines the

adsorption behavior of heavy metal ions by biochar, focusing on the relationship between material types and adsorption performance, and discusses the current limitations and potential directions for further improvement.

2. Physicochemical Properties and Structural Characteristics of Biochar

Biochar derived from plant sources includes a wide range of feedstocks such as crop straw (e.g., corn, wheat, rice, and sunflower residues), woody and bamboo materials, fruit shells, and aquatic emergent plants including reed, cattail, and calamus. These materials generally produce biochar with a well-developed pore structure. Woody and fruit shell-derived biochars tend to contain a higher proportion of micropores, whereas straw-derived biochars are relatively richer in mesopores. Their ash content is typically low, ranging from approximately 15% to 30%, although reed-derived biochar may fall below 20%. In addition, plant-based biochar is characterized by strong thermal stability and a highly aromatic carbon structure, allowing it to remain stable in soil over long time scales. It usually has a low apparent density (around 0.2–0.6 g/cm³) and comparatively lower pyrolysis yields than solid waste-derived biochar. Carbon content is relatively high, typically within 56%–65%, while hydrogen and nitrogen contents are generally below 5%. Among mineral components, potassium is often dominant, whereas phosphorus, calcium, and magnesium are present at lower levels. The surface chemistry is typically weakly to moderately alkaline, with abundant oxygen-containing functional groups such as carboxyl, phenolic hydroxyl, and carbonyl groups, which contribute to its redox activity. Functionally, plant-based biochar tends to show stronger adsorption toward non-polar organic contaminants (e.g., polycyclic aromatic hydrocarbons and petroleum hydrocarbons), but relatively weaker affinity for heavy metal ions compared with solid waste-derived biochar.

In contrast, solid waste-derived biochar includes materials such as livestock and poultry manure (pig, cow, and chicken manure), municipal sludge, and other residues such as eggshells and kitchen waste. Compared with plant-based biochar, its pore structure is generally less uniform and its specific surface area tends to be lower. A defining characteristic is its very high ash content, typically ranging from 45% to 90%, with eggshell-derived biochar exceeding 90%. It also shows lower thermal stability, as its carbon matrix is more prone to gradual oxidation. Apparent density is higher, generally between 0.5 and 1.2 g/cm³, and pyrolysis yield is significantly greater than that of plant-based materials. Carbon content varies considerably depending on the organic composition of the feedstock, while mineral elements such as phosphorus, calcium, magnesium, iron, and zinc are present at much higher levels, often several times those found in plant-based biochar. The material is generally strongly alkaline. In some sludge-derived biochars, sulfur- and nitrogen-containing functional groups also enhance anion exchange capacity. Overall, solid waste-derived biochar tends to exhibit stronger adsorption capacity for heavy metals, often reported to be 2–5 times higher than that of plant-based biochar, as well as better performance for polar organic pollutants such as antibiotics and pesticides.

3. Adsorption of Heavy Metal Ions in Water by Biochar

3.1 Physical Adsorption

Physical adsorption is widely regarded as a basic pathway for the removal of heavy metal ions by biochar, driven primarily by intermolecular interactions associated with its porous carbon structure. This mechanism is generally manifested through pore-filling effects, van der Waals interactions, and electrostatic attraction.

3.1.1 Pore-Filling Effect

Biochar is a porous carbonaceous material formed through the pyrolysis and carbonization of biomass under oxygen-limited conditions. Its pore system spans micropores (<2 nm), mesopores (2–50 nm), and macropores (>50 nm), forming a hierarchical structure. Reported studies indicate that its specific surface area typically ranges from 50 to 800 m²/g, and may exceed 1500 m²/g in activated biochars [1]. This highly developed pore network provides abundant accessible sites for ion accommodation. When the hydrated diameter of heavy metal ions is smaller than the effective pore size, ions can migrate into internal pore structures via liquid film diffusion and intraparticle diffusion processes, where they become physically confined. This phenomenon is commonly referred to as the pore-filling effect.

3.1.2 Van der Waals Forces

Van der Waals interactions represent weak, non-specific forces arising from transient dipole effects between atoms or molecules. Although the interaction energy of a single bond is relatively low (generally below 10 kJ/mol), their cumulative contribution across the large surface area of biochar can become significant in the overall adsorption process [2]. As a result, adsorption driven by van der Waals forces typically exhibits low enthalpy changes ($\Delta H < 40$ kJ/mol), rapid kinetics, weak selectivity, and reversibility, which are consistent with characteristics of physical adsorption [2]. This type of multilayer adsorption on heterogeneous surfaces is often described using the Freundlich isotherm model [1].

3.1.3 Electrostatic Attraction

Electrostatic attraction arises from the interaction between surface charge sites on biochar and ionic species in solution, and is strongly influenced by solution chemistry. Oxygen-containing functional groups on the biochar surface undergo protonation and deprotonation reactions depending on pH, thereby determining the net surface charge. When the solution pH exceeds the point of zero charge of biochar, deprotonation dominates and the surface becomes negatively charged. Under these conditions, positively charged heavy metal ions such as Pb^{2+}, Cd^{2+}, Cu^{2+}, and Zn^{2+} can be attracted to the surface through Coulombic forces [3]. Experimental evidence suggests that electrostatic interactions contribute approximately 15%–40% of total adsorption capacity. However, this contribution is sensitive to ionic strength. As noted by Shaheen et al., background electrolytes such as Na^{+} and Ca^{2+} compete with heavy metal cations for adsorption sites, leading to a shielding effect that reduces electrostatic attraction with increasing ionic concentration [4].

3.2 Chemical Complexation

Chemical complexation (also referred to as surface complexation) describes the formation of relatively stable coordination structures between functional groups on biochar and heavy metal ions. Compared with physical adsorption, this process involves stronger binding interactions (generally 200–400 kJ/mol) and lower reversibility, and is therefore considered a key mechanism in the long-term immobilization of heavy metals [2].

3.2.1 Coordination with Oxygen-Containing Functional Groups

Oxygen-containing functional groups are widely distributed on the surface of biochar. The lone pair electrons on oxygen atoms allow these groups to function as Lewis bases, enabling coordination with heavy metal ions acting as Lewis acids. Comparative studies have shown that carboxyl and phenolic hydroxyl groups are among the most active binding sites for metal ions such as Cu^{2+}, Ni^{2+}, and Cd^{2+}, although their relative contributions vary with feedstock type. In some cases, they can account for more than 60% of total adsorption capacity [5]. Similar findings have been reported in modified biochar systems. For example, phosphorus-modified corn straw biochar (2PBC550) exhibited a maximum adsorption capacity of 145.48 mg/g for Pb^{2+}, and spectroscopic analyses (FTIR and XPS) confirmed that coordination between Pb^{2+} and oxygen-containing groups such as —OH and —COOH plays a dominant role in the adsorption process [6].

3.2.2 Complexation with Nitrogen- and Sulfur-Containing Functional Groups

In addition to oxygen-based sites, biochar surfaces may also contain nitrogen- and sulfur-containing functional groups, including amino (—NH_2), amide (—CONH—), pyridinic nitrogen, and sulfhydryl (—SH) groups. Compared with oxygen, nitrogen and sulfur atoms generally exhibit stronger electron-donating ability, which enhances their affinity for soft acid metal ions such as Hg^{2+}, Cu^{2+}, and Ag^{+} [7]. In recent years, introducing nitrogen-rich precursors into biochar has been widely adopted as a modification strategy to increase the density of active sites and improve adsorption selectivity toward specific heavy metals.

3.2.3 Surface Precipitation

Under certain chemical conditions, surface complexation may further evolve into precipitation processes. When heavy metal ions interact with anions either originating from biochar ash (e.g., PO_4^{3-}, CO_3^{2-}, silicates) or present in solution (e.g., OH^{-}), insoluble mineral phases may form and accumulate on the biochar surface or within its pores. The role of intrinsic mineral components in this process has been emphasized in previous studies. Xu et al. highlighted that minerals such as $CaCO_3$, MgO, KCl, and $Ca_3(PO_4)_2$ embedded in biochar

significantly contribute to heavy metal immobilization, with phosphate and carbonate precipitation alone accounting for approximately 30%–50% of Pb^{2+} removal [8].

3.2.4 Redox Reactions

For variable-valence metals such as Cr(VI) and As(III), biochar can participate in redox reactions through surface functional groups including phenolic hydroxyl and quinone structures. These groups act as electron donors, enabling the reduction of high-valence, highly mobile species into lower-valence forms with reduced toxicity and solubility [9]. Xu et al. further demonstrated that biochar not only directly reduces Cr(VI) but may also function as an electron shuttle, facilitating electron transfer during the reaction process [9]. This redox-mediated pathway provides an additional mechanism for heavy metal detoxification beyond simple adsorption.

3.3 Ion Exchange

Ion exchange refers to a chemical adsorption pathway in which heavy metal ions in solution replace exchangeable ions originally associated with biochar surfaces or its mineral components. The process is primarily driven by differences in binding affinity between heavy metal ions and surface-bound cations [10].

3.3.1 Exchange with Mineral Cations

Biochar ash typically contains abundant alkali and alkaline earth metal cations, including K^+, Na^+, Ca^{2+}, and Mg^{2+}. When biochar is introduced into a heavy metal ion solution, these exchangeable cations may be displaced as heavy metal ions exhibit stronger interactions with surface sites and become immobilized on the biochar [8]. Quantitative evidence supports the significance of this pathway. He et al. investigated Ni(II) adsorption on industrial alkali lignin biochar and found that soluble minerals and soluble organic fractions accounted for 93.76% of total adsorption, whereas contributions from carbon skeleton-related mechanisms such as surface complexation and ion exchange were relatively limited at 6.3% [11]. These results highlight the dominant role of the mineral phase in governing ion exchange behavior in certain biochar systems.

3.3.2 Proton Exchange of Surface Functional Groups

In addition to mineral-driven exchange, oxygen-containing functional groups such as carboxyl (—COOH) and phenolic hydroxyl (—OH) also participate in ion exchange through proton dissociation in aqueous environments. As these groups deprotonate, H^+ is released and negatively charged sites are generated on the biochar surface, which can subsequently interact with heavy metal ions through electrostatic attraction or coordination. This process is strongly dependent on solution pH. Under acidic conditions, excessive H^+ suppresses deprotonation and reduces the availability of exchange sites, thereby inhibiting adsorption. In contrast, under higher pH conditions, increased deprotonation enhances the density of negatively charged sites, leading to improved ion exchange capacity and higher overall adsorption performance [12].

4. Limitations and Future Prospects

Despite substantial progress in the study of biochar-based removal of heavy metals, several structural limitations in the existing literature remain evident.

A first limitation concerns the understanding of adsorption mechanisms. Although physical adsorption, chemical complexation, and ion exchange are widely recognized as the main pathways, most studies still rely on qualitative descriptions. A lack of systematic quantitative approaches makes it difficult to compare the relative contribution of each mechanism to overall adsorption performance under different conditions.

A second issue lies in the gap between experimental design and real environmental conditions. Current research is still largely dominated by batch experiments involving single-metal systems. In contrast, natural and engineered wastewater systems are typically more complex, involving multiple coexisting heavy metals as well as competing influences from background electrolytes, natural organic matter, and suspended particles. As a result, the applicability of many laboratory findings to real-world scenarios remains uncertain.

A further concern relates to environmental safety and long-term stability. Although biochar is generally considered an environmentally friendly material, its raw biomass sources may contain trace heavy metals or other impurities that could potentially be released after application. In addition, the long-term aging behavior

of biochar—including physical fragmentation, surface oxidation, and microbial transformation—may gradually alter its adsorption performance, yet this process remains insufficiently understood.

Future research should therefore move beyond isolated laboratory-scale characterization toward more integrated and environmentally realistic frameworks. One important direction is the development of more quantitative and standardized approaches for mechanism identification, potentially combining advanced spectroscopic techniques such as X-ray absorption fine structure (XAFS) with multi-method validation. Another priority is the evaluation of adsorption behavior under complex multi-contaminant conditions and the expansion of studies to pilot-scale and field applications. Finally, greater attention should be given to the long-term environmental behavior of biochar, including the fate of potential contaminants and its ecological impacts during aging, in order to ensure both effectiveness and environmental safety in practical applications.

5. Conclusion

Biochar has shown considerable potential in the remediation of heavy metal-contaminated water due to its porous structure, surface functionality, and relatively low production cost. Differences in feedstock lead to notable variations in physicochemical properties between plant-based and solid waste-derived biochars. In particular, solid waste-derived biochar often exhibits stronger adsorption performance for heavy metals, which can be associated with its higher mineral content.

The adsorption process is governed by the combined effects of physical adsorption, chemical complexation, and ion exchange. These mechanisms are interrelated rather than independent, with chemical processes such as complexation and surface precipitation generally playing a more decisive role in the immobilization of heavy metals in aqueous systems.

At the same time, current research still faces several limitations, including the predominance of qualitative mechanism descriptions, the gap between laboratory-based studies and real environmental conditions, and insufficient assessment of long-term environmental risks. These issues restrict the direct translation of laboratory findings into practical applications.

Future progress will likely depend on more quantitative approaches to mechanism analysis, as well as a stronger focus on system complexity and environmental relevance. In parallel, attention should also be given to the long-term stability and ecological safety of biochar under real-world conditions, so as to support its more reliable application in heavy metal pollution control.

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Conflicts of Interest

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