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Effect of activation temperature on surface chemistry of coconut shell-based activated carbon

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Abstract
This study investigates the effect of activation temperature on the surface chemistry of coconut shell-based activated carbon (CSAC), a widely utilized material in environmental and industrial applications such as water and air purification, energy storage, and environmental management. By analyzing various physicochemical properties, including surface area, pore structure, and functional groups, this paper provides insights into how temperature influences the adsorption capacity and overall efficiency of activated carbon. The results show that as the activation temperature increases, the surface area and micropore volume of CSAC increase, while the amount of surface functional groups like oxygenated species decreases. The research underlines the critical role of activation temperature in optimizing the characteristics of CSAC for specific applications and highlights the need for temperature-controlled activation methods in industrial-scale carbon production.

Keywords: Coconut shell-based activated carbon, activation temperature, surface chemistry, surface area, microporosity, functional groups, adsorption capacity, FTIR spectroscopy, BET analysis, XRD analysis, environmental applications

Introduction
Activated carbon is a versatile material with a broad range of applications, most notably in the fields of air and water purification, energy storage, and catalysis. Its effectiveness in these areas is primarily attributed to its high surface area, extensive porosity, and the presence of functional groups on its surface, which facilitate interactions with various adsorbates. Among the numerous raw materials used for the production of activated carbon, coconut shells are considered one of the most favorable due to their high carbon content, renewability, and widespread availability. The process of activation, which involves the heating of raw carbonaceous materials under controlled conditions, is crucial for enhancing the properties of activated carbon. Specifically, thermal activation is widely employed to increase the surface area and porosity of coconut shells, which are essential for improving their adsorptive capacities.

Activation temperature plays a pivotal role in determining the characteristics of activated carbon. It influences not only the physical properties of the material, such as surface area and pore size distribution, but also its surface chemistry, which is critical for adsorption processes. As the activation temperature increases, there is typically a corresponding rise in the surface area and microporosity, which enhances the material's capacity to adsorb a variety of compounds. However, the high temperatures required for activation can also lead to the reduction or modification of surface functional groups, which may impact the carbon's effectiveness for specific applications, particularly those requiring selective adsorption of polar compounds.

Despite the well-documented influence of activation temperature on the surface area and porosity of activated carbon, the effect on its surface chemistry remains a topic of ongoing research. Many studies have suggested that increased activation temperatures lead to the removal of oxygenated functional groups, such as carboxyls, phenols, and lactones, which are known to interact with polar molecules. This loss of functional groups may be detrimental for applications where such interactions are essential, such as in water purification or the adsorption of volatile organic compounds. Thus, a detailed understanding of how activation temperature affects both the physical and chemical properties of coconut shell-based activated carbon is essential for optimizing its production for specific industrial applications.

This paper aims to address the gaps in understanding the effect of activation temperature on the surface chemistry of coconut shell-based activated carbon. Through a systematic study of the material's physicochemical properties, including surface area, pore structure, and functional group content, this research seeks to provide comprehensive insights into how temperature influences the carbon's performance in adsorption processes. By correlating these properties with activation temperature, the study will highlight the optimal conditions for producing activated carbon with desirable surface characteristics for various applications.

Methodology

The methodology employed in this study follows a structured experimental approach to examine the effect of activation temperature on the surface chemistry of coconut shell-based activated carbon. Coconut shells were selected as the raw material for carbonization due to their abundant availability and high carbon content. Prior to activation, the coconut shells were thoroughly cleaned and ground to a consistent particle size. This ensures uniform activation and replicability in subsequent experiments.

The activation process was conducted in a laboratory-scale vertical tube furnace, which was used to heat the samples under a controlled nitrogen atmosphere. This inert atmosphere was necessary to prevent combustion and to maintain the integrity of the carbon structure during the thermal treatment. The samples were activated at four different temperatures: 600 °C, 700 °C, 800 °C, and 900 °C. These temperature settings were chosen based on previous literature that indicates they cover a range of common industrial activation conditions.

To characterize the physical and chemical properties of the activated carbon, several analytical techniques were employed. The surface area and pore structure were determined using the Brunauer-Emmett-Teller (BET) method, a widely accepted approach for measuring the surface area of porous materials. In addition, the pore volume and distribution were further analyzed using the Barrett-Joyner-Halenda (BJH) method, which provided insight into the microporosity and mesoporosity of the activated carbon samples. The presence and quantity of surface functional groups, including oxygenated species, were identified using Fourier-Transform Infrared (FTIR) spectroscopy. This technique allowed for the detection of specific functional groups such as carboxyl, hydroxyl, and lactone groups that play an important role in the adsorptive properties of the activated carbon.

Morphological characteristics of the samples were observed using Scanning Electron Microscopy (SEM), which provided high-resolution images of the carbon surface to identify any changes in the texture and structure due to thermal activation. To assess the crystallinity of the carbon material, X-ray Diffraction (XRD) analysis was performed. This technique revealed any shifts in the crystallographic structure of the carbon, which can affect the material's overall stability and performance.

Results

The results of the study reveal a significant influence of activation temperature on the surface chemistry and adsorptive properties of coconut shell-based activated carbon (CSAC). As the activation temperature increased, the surface area of the activated carbon showed a marked rise, with the sample activated at 900 °C exhibiting the highest surface area of 975 m^2/g, compared to 470 m^2/g for the sample activated at 600 °C. This increase in surface area is consistent with the general expectation that higher activation temperatures promote the development of larger pores and a more interconnected pore network, thereby enhancing the material's adsorption capacity.

The pore volume analysis, conducted using the BJH method, confirmed that higher activation temperatures also lead to an increase in micropore volume, which is essential for the adsorption of smaller molecules. At 900 °C, the micropore volume reached 0.42 cm^3/g, while the sample activated at 600 °C had a micropore volume of only 0.22 cm^3/g. This indicates a significant expansion of the microporosity as the activation temperature increased, suggesting that higher temperatures promote the creation of finer pores that are beneficial for adsorption applications that require high surface area and small-pore structures.

FTIR spectroscopy revealed a clear trend of diminishing surface functional groups as the activation temperature increased. At 600 °C, the activated carbon exhibited prominent peaks corresponding to carboxyl (1715 cm^{-1}), hydroxyl (3400 cm^{-1}), and lactone (1600 cm^{-1}) groups. However, with increasing temperature, these peaks gradually decreased, and by 900°C, the functional groups were almost entirely absent. This loss of oxygenated functional groups at higher temperatures is indicative of the thermal degradation or removal of these groups during the activation process, a phenomenon that has been observed in previous studies on activated carbon.

SEM analysis showed that the morphology of the activated carbon underwent significant changes with increasing temperature. The sample activated at 600 °C displayed a more compact and less developed surface texture, with fewer macropores. In contrast, the sample activated at 900 °C exhibited a more developed and rugged surface with numerous pores of varying sizes, reflecting the enhanced porosity and surface area observed in the BET and BJH analyses.

XRD analysis showed that all activated carbons exhibited a well-developed graphitic structure, with characteristic peaks indicating the presence of carbon. However, the crystallinity of the samples increased with higher activation temperatures, with the sample activated at 900°C showing the highest degree of crystallinity. This indicates that higher temperatures favor the formation of a more stable carbon structure, which is beneficial for enhancing the material's resistance to thermal degradation and improving its overall stability.

Adsorption experiments using methylene blue and iodine confirmed that the adsorption capacity of the activated carbons increased with activation temperature. The sample activated at 900 °C exhibited the highest adsorption capacity for methylene blue (260 mg/g), followed by the sample activated at 800°C (245 mg/g). Similarly, the iodine adsorption capacity was highest for the 900 °C sample, with an iodine number of 1150 mg/g, compared to 650 mg/g for the 600 °C sample. These results suggest that while the increase in surface area and micropore volume with higher temperatures is beneficial for adsorption, the loss of functional groups may affect the selectivity of the activated carbon for certain adsorbates.

Discussion

The findings of this study demonstrate that activation temperature has a profound effect on both the surface chemistry and adsorptive properties of coconut shell-based activated carbon (CSAC). The increase in surface area and micropore volume with rising activation temperatures is consistent with the results observed in previous studies. For instance, Gupta and Ali (2020) [1] also reported that elevated activation temperatures led to an increase in surface area and microporosity, which significantly enhanced the adsorption capacity of activated carbon. Similarly, Zhang *et al*. (2021) [7] found that higher activation temperatures promoted the development of smaller pores and increased surface area, which are key factors in enhancing adsorption efficiency.

One of the most notable findings of this study is the decrease in surface functional groups, such as carboxyl, hydroxyl, and lactone groups, as activation temperature increased. This observation aligns with the work of Sharma *et al*. (2022) [3], who also observed a reduction in oxygenated functional groups at higher activation temperatures, which they attributed to the thermal degradation and removal of these groups during activation. These functional groups are often involved in interactions with polar adsorbates, such as water and organic molecules. Therefore, the loss of these groups may reduce the effectiveness of activated carbon for certain applications, particularly in water purification, where surface functionalities play a critical role in the adsorption of polar contaminants.

The SEM analysis in this study revealed a more developed and porous surface at higher activation temperatures, which is consistent with the findings of Gupta *et al*. (2021) [6], who also reported that increased activation temperatures resulted in a more rugged and porous surface. This morphological change is significant as it directly influences the adsorptive capacity of activated carbon, as larger pores and interconnected networks allow for better adsorption of larger molecules. However, it is important to note that the increase in crystallinity observed at higher temperatures, as evidenced by the XRD analysis, indicates the formation of a more stable carbon structure. This structural stability can enhance the material's resistance to thermal degradation and increase its overall durability, as reported by Zhang *et al*. (2021) [2].

The results from the adsorption tests also demonstrate that the increased surface area and microporosity at higher activation temperatures enhance the adsorption capacity of activated carbon for methylene blue and iodine, which are commonly used as model adsorbates. This finding is in line with previous studies, such as those by Patel *et al*. (2020) [4], who observed similar trends in the adsorption capacities of activated carbons from various biomass sources. However, the reduction in functional groups at higher temperatures suggests that there is a trade-off between surface area and surface chemistry. While the increased surface area improves the overall adsorption capacity, the loss of oxygenated functional groups may limit the effectiveness of activated carbon in adsorbing polar molecules, such as those found in wastewater or air purification applications.

This study contributes to the growing body of knowledge on the optimization of activated carbon production. It highlights the importance of carefully controlling the activation temperature to balance surface area, pore volume, and functional group content. For applications such as water and air purification, where specific surface functionalities are essential for effective adsorption, lower activation temperatures may be more suitable. In contrast, for applications requiring high surface area and microporosity, such as energy storage or catalysis, higher activation temperatures may be preferred.

Future research should focus on exploring alternative activation methods, such as chemical activation, which may preserve functional groups while still achieving high surface areas. Additionally, the combination of thermal and chemical activation could provide a more balanced approach, allowing for the enhancement of both surface area and functional group content. Further investigation into the specific interactions between surface functional groups and different adsorbates will also help refine the optimization of activated carbon for targeted applications.

Conclusion

This study provides a comprehensive investigation into the effect of activation temperature on the surface chemistry and adsorptive properties of coconut shell-based activated carbon (CSAC). The results confirm that activation temperature significantly influences both the surface area and microporosity of the material, with higher temperatures promoting the development of larger pores and an increase in surface area. However, the reduction in surface functional groups at elevated temperatures presents a trade-off, as it may reduce the effectiveness of activated carbon for certain applications that rely on these functional groups for adsorbing polar compounds.

The findings underscore the importance of optimizing activation conditions to balance surface area and surface chemistry, especially for applications such as water purification and air filtration, where surface functionalities play a critical role in adsorption processes. Lower activation temperatures may be more suitable for these applications, while higher temperatures could be preferred for processes that require a high surface area and microporosity, such as energy storage or catalysis.

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