



Significance of microporosity on the interaction of phenol with porous graphitic carbon

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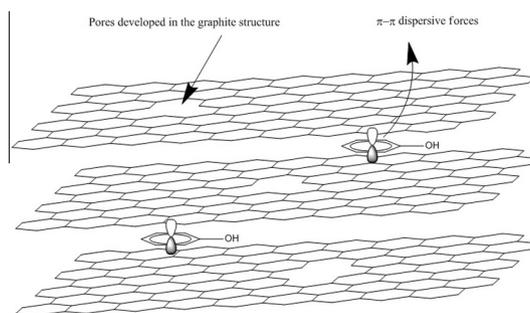
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HIGHLIGHTS

- Production of tyre char activated carbons under various experimental conditions.
- Determination of effective surface area as a measure of accessible pores for certain adsorbate.
- Evaluation of the phenol adsorption onto the produced activated carbons.
- Determination of the significance of microporosity in phenol adsorption.
- Elucidation of the phenol molecule orientation onto activated carbons using the model molecule.

GRAPHICAL ABSTRACT



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ABSTRACT

Many researches have produced porous activated carbons from various precursors for phenol removal from wastewater. A number of literature focus on the optimization of activation conditions to obtain adsorbents with higher specific surface areas as a result of the general misconception that higher surface areas result in higher adsorption capacities, disregarding the effect of the pore geometry. The aim of this study is to demonstrate the significance of micropore surface area, rather than total surface area, in the adsorption of phenol. It has been confirmed that for activated carbons with similar surface areas, the one with higher fraction of microporosity leads to higher phenol uptake. This has been attributed to the π - π London dispersion forces between the graphitic carbon basal planes and the phenol aromatic ring. Thus, it is hypothesized that hydrogen bonding does not occur between the phenol molecules and the functional groups on the carbon surface.

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1. Introduction

The presence of phenol in the environment has been of great concern for public health due to the carcinogenicity and toxicity of this compound [1]. One of the major discharge routes of phenols into the environment is through the improperly-treated

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phenol-laden industrial wastewater, released from petrochemical, pharmaceutical, steel, paint, and plastic industries [2]. Hence, stringent regulations have been enacted to control the discharge of phenol-containing wastewater into surface water bodies or even drainage canals [3]. In order to meet the discharge standards, several techniques, such as membrane separation, chemical coagulation, photocatalytic degradation, and adsorption, have been developed and widely used [4], among which the latter has been found to be the most promising and efficient technique [5–8].

Although many researches have been devoted to the study of phenol removal by various adsorbents, only limited articles have

been concerned with in-depth understanding of phenol adsorption mechanism [9]. The utmost importance of the phenol adsorption mechanism originates from its essentiality for the design of the porous structure of the adsorbents.

It is generally acknowledged that the porous structure of activated carbons, as the most commonly-used adsorbent materials, can be manipulated by altering the activation conditions, such as activating agent, activation temperature and time [10,11]. Tyre char is a viable material to be used as precursor for the production of activated carbons, due to the carbon-rich nature of this material [12,13].

On the other hand, there is a general misconception that higher specific surface area of activated carbons leads to enhanced phenol adsorption capacities, disregarding the crucial effect of pore size, which results in improper design of activated carbons. The aim of this study is to produce a *mesoporous* activated carbon from tyre char with a surface area close to that of the commercial *microporous* activated carbons and compare their phenol adsorption capacities. Although the primary role of micropores of activated carbons has already been studied by few other researchers [14,15], no relationship between the geometry of the phenol and the pores has been presented. Accordingly, the role of the pore geometry in the adsorption of phenol has been investigated and the mechanism of phenol adsorption has been discussed in detail.

2. Materials and methodologies

2.1. Materials

Tyre char, obtained by the conversion of the waste tyre rubber into hydrocarbon fuel and tyre char in a fixed bed pyrolysis reactor at an average temperature of 823 K, was provided by Global Power and Energy Company Limited, Guangzhou, China.

Ultra-pure phenol was supplied by Invitrogen. The properties and molecular size of phenol are summarized in Table S1.

2.2. Steam activation

Approximately 30 g tyre char was loaded into a horizontal Carbolite furnace. Before commencing the experiment, nitrogen (N₂ with a purity concentration of 99.7, v/v%), with a flowrate of 200 ml min⁻¹ was purged into the furnace for an hour to remove residual air. During the heat-up process, using a heating rate of 15 K min⁻¹, N₂ was purged into the reactor. While the target activation temperature was reached, the gas supply was switched to the activation gas, steam and N₂ in a volume ratio of 85:15 with a total flowrate of 700 ml min⁻¹.

2.3. Activated carbon characterization

2.3.1. Elemental analysis

An elemental analyzer, model ELEMENTAR VARIO EL III, was used to determine the mass fractions of the carbon, hydrogen, nitrogen and sulphur content (in weight%) of the tyre char activated carbons.

2.3.2. Nitrogen gas adsorption–desorption

The textural characterization of the prepared activated carbons was conducted using an automated volumetric gas adsorption apparatus, model Autosorb-I, Quantachrome, at a constant temperature of 77 K. Before analysis, all carbon samples were outgassed at 473 K for 6 h in a vacuum condition.

The obtained N₂ adsorption–desorption data were then analyzed according to the Brunauer–Emmett–Teller (BET) equation [16], t-plot method [17], and Barrett–Joyner–Halenda (BJH) equa-

tion [18] for the determination of the specific surface area, micropore surface area and pore size distribution, respectively.

2.3.3. Equilibrium phenol adsorption

The phenol adsorption capacities of the produced carbons and the commercial activated carbon were investigated by varying the initial concentration of the phenol (50–1000 ppm) at an adsorbent dosage of 1 g L⁻¹. The bottles were sealed and shaken at a speed of 150 rpm in a thermostatic shaker bath at a constant temperature (298 K) until reaching equilibrium. The initial and equilibrium concentrations of the phenol were measured by a UV-visible Spectrophotometer, model CARY 100 VARIAN. The concentrations were measured three times and the average value was taken as the result.

The amount of adsorption at equilibrium was obtained by the mass balance of the adsorbate in liquid and solid phase as follows:

$$m \cdot (q_e - q_0) = V \cdot (C_0 - C_e) \quad (1)$$

For fresh adsorbents, $q_0 = 0$. Therefore, rearrangement gives:

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

where q_e is the adsorption capacity of the adsorbent (mmol g⁻¹; C_0 and C_e are the initial and equilibrium adsorbate concentrations (mmol L⁻¹; V is the volume of the solution (L); and m is the mass of adsorbent (g).

2.4. Adsorption modelling

Three adsorption isotherm models, namely Langmuir [19], Freundlich [20], and Redlich–Peterson [21], have been used to fit the experimental data (see Eqs. (3)–(5)). Due to the abundance of information on the assumptions of these models, they are not repeated here [22–24]:

$$\text{Langmuir: } q_e = \frac{K_L C_e}{1 + a_L C_e} \quad (3)$$

$$\text{Freundlich: } q_e = K_F C_e^{\frac{1}{n}} \quad (4)$$

$$\text{Redlich–Peterson: } q_e = \frac{K_R C_e}{1 + a_R C_e^\beta} \quad (5)$$

Two error functions, the sum of the squares of the errors (SSE) and the average relative error (ARE), have been selected in order to evaluate the quality of the fit of the isotherm model to the experimental data:

$$\text{SSE function: } \sum_{i=1}^n (q_{e,exp} - q_{e,cal})^2 \quad (6)$$

$$\text{ARE function: } \frac{100}{n} \sum_{i=1}^n \left| \frac{q_{e,exp} - q_{e,cal}}{q_{e,exp}} \right|_i \quad (7)$$

Ho and McKay suggested a meaningful comparison between the parameter sets and a procedure of normalizing and combining the error results was adopted producing a “sum of normalized errors”, SNE, for each parameter set for each isotherm. The calculation method for the SNE has been described in detail elsewhere [25].

3. Results and discussion

3.1. Textural properties of the activated materials

The main objective of the activation study is to produce activated carbons with different textural characteristics and yields,

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