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### **RESEARCH PAPER**

#### **TITLE:**

### **THERMODYNAMICS OF BISPHENOL: A REMOVAL FROM AQUEOUS SOLUTION**

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## THERMODYNAMICS OF BISPHENOL: A REMOVAL FROM AQUEOUS SOLUTION

### Abstract

Discharge of bisphenol A (BPA) and other phenolic compounds by the industries in to water bodies has adverse effects on wildlife and human health. It is necessary to treat this wastewater before draining. The present work is evaluated the cheap and environmental technique for the removal of BPA by different adsorbents. Recent studies have been reported that the ability of Peanut husk (PH) as an adsorbent to eliminate BPA from the surface water. Study of different experimental conditions like pH (6 for native and 7 for its composites), contact time, temperature, adsorbent dose 0.05 g and initial BPA concentration (25 ppm) have been done. The pseudo second-order kinetics equations fit in the adsorption data of BPA. The Thermodynamic parameters including  $\Delta S$  (entropy changes),  $\Delta H$  (enthalpy change), and  $\Delta G$  (Gibbs free energy change) were studied to determine the spontaneity of adsorption. The nature of adsorption is exothermic for the adsorption of BPA onto peanut husk and its composites. Adsorption data has also been analyzed by regression model.

### 1. INTRODUCTION

Water is vital to our health thus its quality must be improved. But our valuable water resources are polluted by different sources. With time, the value of our water resources are declining due to the nonstop addition of unwanted substances. Most of water-polluting sources are industries, cultivated actions, and other ecological and

worldwide changes. Hundreds of inorganic and organic pollutants are found that spoil water resources. The organic pollutants effluence is very hazardous because they cause numerous effects and cancer-causing in nature (Yang et al., 2011). Water bodies containing contain different types of organic pollutants. These organic pollutants are Water bodies contain different types of organic pollutants. These organic pollutants are fertilizers, pesticides, hydrocarbons, phenols, plasticizers, biphenyls, cleansers, lubricants, fats, drugs etc (Ali and Enein, 2004). They have many side effects. Some of the general characteristics of organic pollutants are: one or more cyclic ring existence that may be aromatic or aliphatic, polar functional groups absence, and the presence of a number of halogen substitutions commonly chlorine. Because of these features organic pollutants remain persistent in the atmosphere (Ali et al., 2012). Recently, the extensive diversity of chemicals are released from industries disturb the endocrine structure of advanced life forms, for example, fish, the natural world, and even human beings have appealed attracted significant attentions attention in from all over the world. Such chemicals have huge effect upon human beings so it is essential to develop technologies for their removal from the environment (Hoshiyama et al., 2016). Manufacturing of BPA by the condensation of phenol and acetone with catalyst. Polycarbonate (PC) and epoxy resins, unsaturated polyester-styrene, resins,

and flame retardants can be prepared by the use of BPA (Hoshiyama et al., 2016). While polycarbonate have been used for the manufacturing of various user products for example medical devices, drinking and food covering, vehicles lenses, motorbike helmet, protection eyeglasses and solid disk (Oke and Ogundugba et al., 2014).

#### **Characteristics of BPA including:**

- It has a low vapor pressure
- It has a high melting point
- It reasonably solubilized in water (300mg/L at room temperature)
- It dissociates in alkaline environment pKa 10-11.4 (Oke and Ogundugba et al., 2014)

#### **The current study paid particular attention to the following purpose:**

1. To investigate the elimination of BPA from aqueous media by using peanut husk and its composites
2. To evaluate the impact of different parameters such as adsorbent dose, pH, initial concentration, Contact period, temperature etc on the removal of BPA.
3. To investigate kinetic models and examine which kinetic model is best.

## **2. MATERIALS AND METHOD**

The experiment is conducted in research lab of Agriculture University Faisalabad, material and chemical used for analysis is Funnel, Conical flasks, Beakers, Aluminum foil, Conical flask , Test tube, Micro Pipettes, Burette, Stand, Measuring flasks, Octagon, siever, Orbital Shake, Analytical balance, pH Meter Polypyrol , Na Alginate, poly aniline (adsorbent) , Agriculture waste. The waste industrial water is collected from waste water canal of Faisalabad for analysis. The experiment will be planned in Completely Randomized Design (CRD).

Statistical data will be obtained and analyzed through Analysis of Variance (ANOVA).

#### **Preparation of Adsorbent**

Peanut husk was collected and ground in an electric ball mill then powdered was sieved to get a particular size. The powder was washed with distilled water to remove color and the powder was dried in the oven at 60°C and then stored in a container for further use.

#### **Preparation of stock solution of BPA**

The BPA soluble in water to a certain extent. Take 0.1g of BPA in a conical flask and add 10 ml of methanol to the conica flask . Shake it well so that BPA completely dissolved in it then make the volume up to 1000 ml. That is the 100 ppm stock solution of BPA. Store it and use it for further studies. The stock solution of BPA was prepared in distilled water. Altogether 1000 mgL<sup>-1</sup> stock solution of BPA was ready in 6% methanol and 94% distilled water combination. The desired concentration of BPA solution was prepared by diluting with distilled water (Balci and Erkurt, 2016).

#### **Study the effect of different adsorbent doses on removal of BPA**

Different amounts of adsorbent 0.05, 0.1, 0.15, 0.2, 0.25, and 0.3 were added in a 50 ml solution of BPA. In order to check the adsorption agitate the solutions for 90 min at 30 0 C with shaking speed 120 rpm.

#### **Study the effect of different pH on the removal of BPA**

Bisphenol A by means of native and its composites (Polyaniline, Polypyrole and Na Alginate) was conceded out at the pH range of 4 to 9. This pH range was varying with HCl and NaOH. The particle size (300□), dosage (0.05) of preliminary BPA concentration (25ppm), contact period (90 min), temperature

(30 0 C), and shaking speed (120 rpm) and then agitate the mixture after that concluded the reading at spectrophotometer.

**Study the effect of various contact times on the removal of BPA**

Add the maximum adsorbent dose of 0.05 g in 50 ml of BPA solution. Then shake this solution in a shaker for 90 min at 30 0 C in order to find the optimum interaction period by withdrawing the samples at intervals of 5, 10, 15, 20, 30, 60, 90, and 120 minutes

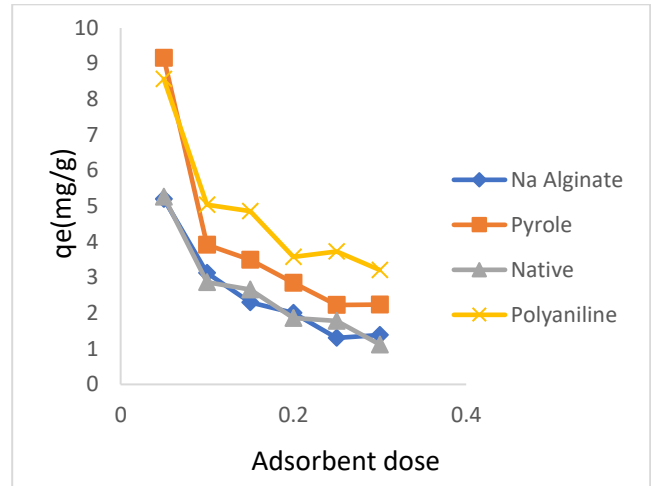
**Determine the behavior of BPA at different Temperature**

Temperature is a significant factor studying the exclusion of BPA. It influences on the adsorption capability. The experiment was accomplished at 30, 35, 40, 45, 50, and 55 0 C for optimal quantity of adsorbent 0.05g added into 50 ml of BPA solution under all adjusted conditions.

**3. RESULTS AND DISCUSSION**

**Effect of Bioadsorbent Dose**

The bio-sorbent dose is a significant factor that was plays a fundamental role in biosorption method. The bio-sorbent dose influence with a dose of (0.05, 0.1, 0.15, 0.2, 0.25, and 0.3 g) (Figure 1). The greater adsorption capacity was gained at 0.05 g quantity of adsorbent. It can be detected that the amount of adsorption capacity was diminished by raising the amount of adsorbent

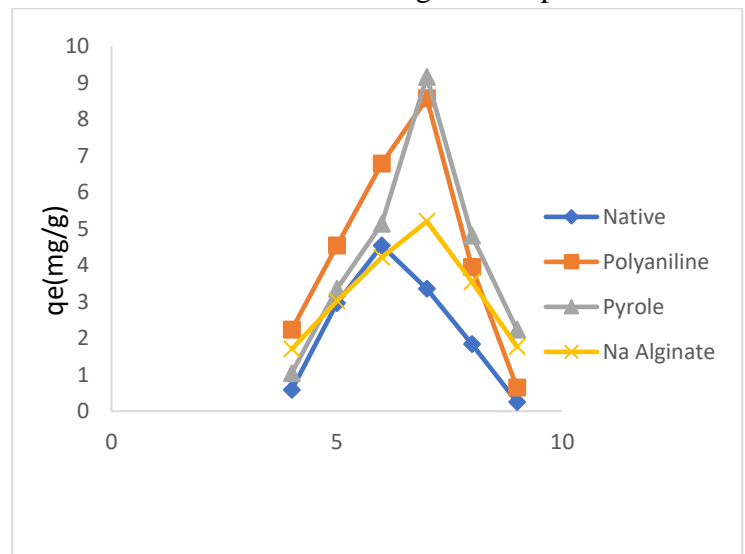


**Figure 1:** Effect of adsorbent dose on removal of BPA by using native and its composites

**Effect of PH**

Bisphenol A by means of native and its composites (Polyaniline, Polypyrole, and Na Alginate) was conceded out at the pH range of 4 to 9. This pH range was varying with HCl and NaOH.

When the pH was from 3 to 7 the adsorption capability displayed minor alteration (**Figure 2**). When the pH was more than 7 the adsorption capability was decreased. So the extreme exclusion of BPA was gained at pH 7.



**Figure 2:** Effect of pH on the removal of BPA by using native and composites

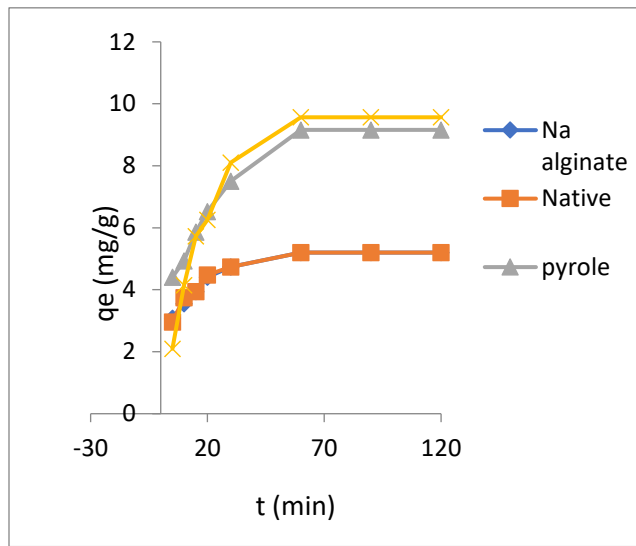
**Effect of contact time**

The contact period is a vital factor for the abolition of contaminants from wastewater. The contact time influence on the elimination of BPA by using native and its composites as adsorbent (**Figure 3**). Sixty minutes are desirable to attain equilibrium for the BPA adsorption. Sixty minutes was the best contact time for the elimination of BPA. So for more trials, sixty minutes were used.

$q_e$  (mg/g) is the preliminary adsorption capability of BPA

$q_t$ (mg/g) is the adsorption of BPA at time  $t$

The  $k_1/2.303$  denote slope. The preliminary adsorption capacity  $q_e$  and rate constant  $k_1$  originate from the slope and intercept resolute from  $\ln (q_e - q_t)$  versus  $t$  (Yang et al., 2016).



**Figure 3:** Effect of contact time on removal of BPA by using native and its composites

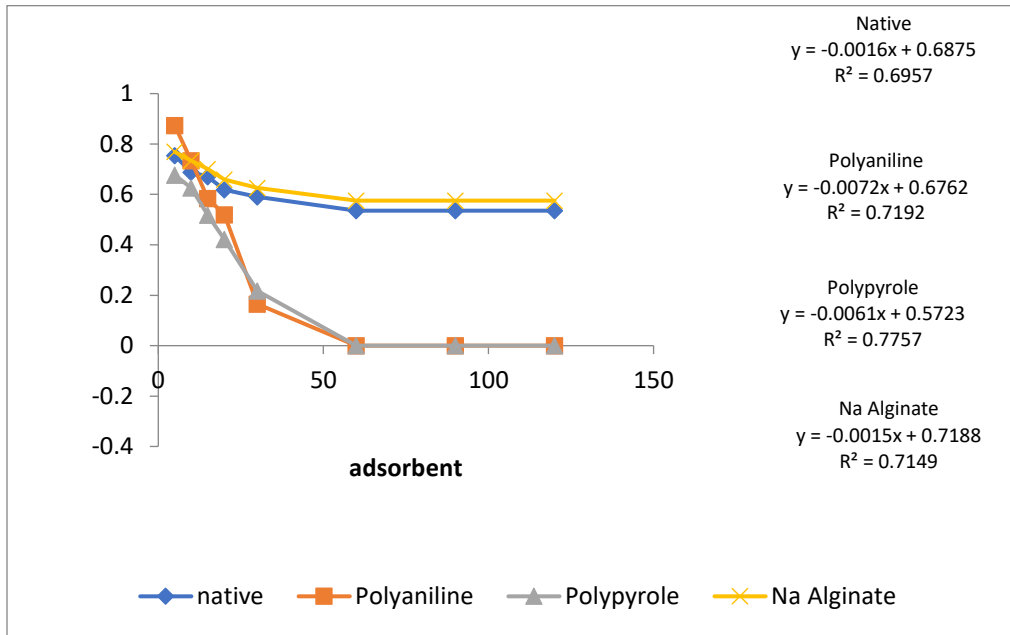
**Kinetic modeling**

Kinetic models are widely used to regulate the adsorption method, adsorption mechanism, and ability of adsorbent for the eradication of contaminants. Kinetic modeling created on investigational data.

Different models presented in order to investigate the sorption procedure (Figure 4).

- Lagergren Pseudo first order kinetics model
- Pseudo second order kinetics model  $\log (q_e - q_t) = \log (q_e) - k_1 t / 2.303$

**In this equation**



**Figure 4:** Graphical representation of Pseudo first-order kinetics for adsorption of BPA by native, Polyaniline, Polypyrrole and Na Alginate

**2 Pseudo second ordersecond-order kinetic study**

The subsequent equation signify signifies the pseudo second-order kinetics (**Figure5**).

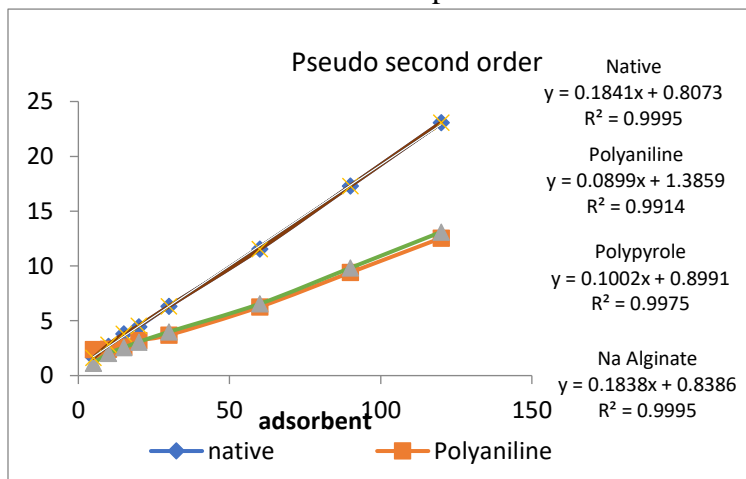
$$(t/q_t) = 1/k_2 q_e^2 + 1/q_e t$$

In the above equation

$q_t$  denote denotes the adsorption of BPA at time  $t$

$q_e$  represent represents the preliminary adsorption capacity of bisphenol A

$k_2$  denote denotes the rate constant of pseudo-second order adsorption



**Figure 5:** Graphical representation of Pseudo second order kinetics for adsorption of BPA by native, Polyaniline, Polypyrrole and Na Alginate

**READING ABOUT KINETIC MODEL FOR GRAPHICAL REPRESENTATION**

<b>Kinetic models</b>	<b>Native</b>	<b>Polyaniline</b>	<b>Polypyrrole</b>	<b>Na Alginate</b>
<b>Pseudo First order</b>				
<b>k1</b>	-0.0036	-0.016	-0.014	-0.0035
<b>qe cal (mg/g)</b>	4.86	4.74	3.73	5.23
<b>qe exp (mg/g)</b>	5.2	9.56	9.16	5.2
<b>R<sup>2</sup></b>	0.6957	0.7192	0.7757	0.7149
<b>Pseudo second order</b>				

<b>k2</b>	0.042	0.0058	0.011	0.040
<b>qe cal (mg/g)</b>	5.43	11.12	9.98	5.44
<b>qe exp (mg/g)</b>	5.2	9.56	9.16	5.2
<b>R<sup>2</sup></b>	0.9995	0.9914	0.9975	0.9995

**4. RESULTS**

BPA is used as a material in the production of epoxy gums and polycarbonate plastics. It is also used in food cans, storage bottles, dental fillings, and medical tools. In the environment, BPA causes

health effects. So it is necessary to remove the BPA from the environment. Agriculture wastes are important and low-cost adsorbents for the removal of BPA from wastewater. Among these agro wastes, peanut husk showed the best results for the elimination of BPA so prepared the composites of peanut husk that enhance the adsorption capacity. It

is necessary to check the maximum adsorption capacity in batch mode with a BPA solution. Solution pH, preliminary BPA concentration, and adsorbent amount can also expressively influence the complete adsorption method. Adsorption capacity decreases with an increase in temperature. In order to search and comprehend the depth the pseudo-first-order, the pseudo-second-order kinetic model describe describes the accurate sorption mechanism. The optimum conditions were determined as pH of 6 for native and 7 for its composites, temperature 30 0 C, and adsorbent dosage of 0.05 g. The thermodynamic study proposed that the BPA sorption method was spontaneous and exothermic

## 5. CONCLUSION

In conclusion, peanut husk is an effective and low-cost adsorbent for removing BPA from wastewater, with its performance influenced by factors such as solution pH, initial BPA concentration, and adsorbent amount. The adsorption capacity decreases with increasing temperature, and the sorption mechanism can be accurately described using the pseudo-first-order and pseudo-second-order kinetic models. Optimal adsorption conditions are achieved at a pH of 6.

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