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RESEARCH PAPER

Preparation of Micro/Nano Polyaniline Structures Deposited on Recycled Polyethylene Terephthalate (r-PET) for PCP Removal: Thermodynamic Investigation

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ABSTRACT

This research aims to examine the adsorption behavior of composite polymers (PAn- PET) (polyaniline with recycled polyethylene terephthalate (r-PET) were made from plastic bottles that had already been used, nanofibers adsorbing contaminants from a solution containing pesticides. XRD diffraction and SEM were used to characterize this nanofiber composite. Using batch adsorption studies, adsorption variables including contact time, starting pesticide dosage, and adsorbent dose were optimized. Under optimum conditions, the maximum removal efficiency was 81%. In addition, the three Langmuir, Freundlich and Temkin isothermal adsorption models were also applied and the Langmiur isothermal model (R^2 = 0.9857) better described the adsorption equilibrium data. Using experimental data, the feasibility of recycled polyethylene terephthalate-recycled polyethylene terephthalate nanofibers in the removal of PCP indicates a promising option for the removal of pollutants from water.

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INTRODUCTION

Pentachlorophenol) PCP (is utilized worldwide as a pesticide and in high doses in disinfectants. PCP is very toxic to a range of microorganisms [1,2] and human exposure to PCP is regarded as toxic. Toxic substances also pose serious health risks that will emerge in the future [3,4]. Presently, PCP contamination of the environment is widespread, and traditional cleaning strategies have included the using of granular activated carbon (GAC) for the purification of water [5,6]. Using the old method, on the other hand, will result in the use of organic solvents and hence the challenge of handling these solvents [7]. Due to the high surface area of these nanostructures in their various forms [8], several nanomaterials such as oxides and their composites [9] and polymeric materials have been employed to remove pollutants as a result of advancements in nanotechnology [10,11].

Even though there are a lot of commercial polymers, almost all of them are antimicrobial, Polymers have a lot of problems, and they could

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cause changes in the environment. So, the goal of the research right now is to create a new type of nanopolymer that can absorb some pesticides, dyes, and toxic elements from dirty water that has pollutants in it [12]. Polyaniline (Pan) is a key material in contemporary nanotechnologies because of its high electronic conductivity, stability in water, air and other unique physical and chemical features. Graphene is a good material because its physical and chemical properties can be changed at low cost by changing its structure, design and shape.

there is a considerable amount of interest in investigating polyaniline [13]. These characteristics suggest PAn's broad applicability this polymer has a variety of advantages, but it also has a number of downsides, including weak mechanical stability and a high degree of simplicity to increase stability mixed with inorganic oxides (such as TiO_2) are predominantly applied to the surface [14].

When forming a composite of PAn, not only inorganic substrates [15], but also organic polymer substrates have been actively employed. Polyethylene terephthalate (PET) is among the ideal organic substrates because of its versatility and low cost [16]. PET is a chemically inert, amorphous, glassy material with exceptional pliability and tensile strength. It is possible to increase its crystallinity through PET heated and changed into molten additions; at temperatures above 323K, Particles of PET can be stretched in one direction to create fibers making the material highly plastic [17].

In this study, a suitable polymer for the adsorption process was synthesized, distinguished by its tiny crystalline size, large surface area, and ease of removal, as well as the inclusion of polymeric material derived from the reuse of plastic bottles in its composition.

MATERIALS AND METHODS

Materials

Synthesis of (PAn- PET) nanopolymer

An in situ aniline polymerization process was used to make polyaniline nanocomposites [18]. After quickly adding a trace volume of ammonium persulphate in 1 M Hydrochloric acid, a magnetic bar was used to stir the mixture, which contained PET residues [19].

After five hours, the product was filtered and washed with distilled water, ethanol, and acetone to get rid of any remaining aniline or other contaminants. Then, they were dried in an oven at 80°C for 8 hours and put in a container that kept air out, results shown in Table 1.

Adsorption experiments

Sigma-Aldrich pesticide solutions of 0.016 g (PCP) were produced with deionized water for batch adsorption tests. Experiments on the kinetics of the reaction between the nanopolymer and PCP were conducted by introducing 0.01 g of nanopolymer to 50 mL of PCP solution at various times ranging from 0 to 300 minutes, with a standard duration of 30 minutes included.

Glass tubes were shaken on an HZQ-C shaker at 25, 35, 45, and 55 °C. Absorbance was evaluated using 665 nm UV-visible spectroscopy both before and during the adsorption process. Eq. 1 computes the adsorbed pesticide solution.

$$Q_e = \frac{(C_O - C_e)V_{sol}}{M} \quad (1)$$

Where Q_e the equilibrium adsorption capacity (mg/g) is now, C_O is the PCP concentration at the beginning, C_e is the pesticide concentration at

Table 1. Physicochemical Properties of Pentachlorophenol (PCP).

Property	Value
Chemical Name	Pentachlorophenol (PCP)
Molecular Formula	C6Cl5OH
Molecular Weight	266.34 g/mol
Appearance	White to light tan crystals
Melting Point	190 – 192 °C
Boiling Point	Decomposes before boiling
Solubility in Water	14 mg/L at 25 °C
pKa	4.7
Log Kow (Octanol/Water)	5.01
Vapor Pressure	1.7×10^{-4} mmHg at 25 °C
Density	1.98 g/cm³

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equilibrium, V_{sol} is the volume of the solution (L) and M is the amount of nanopolymer (g).

RESULTS AND DISCUSSION

XRD of nanopolymer

Fig. 1 illustrates the X-ray diffraction of polymers (PAn-PET). The pattern of diffraction exhibits a significant peak. In general, crystalline polymer diffraction bands are broad and include amorphous phase and crystalline plane reflections. The broad distribution of the peaks at 22.59 and 25.69 ° is due to the overlapping of the amorphous structure and crystal phase of polyethylene terephthalate and polyaniline [20]. The peaks at 17.37 ° correspond to the (010) A lattice reflection of polyaniline. While the peaks at 38°, 44°, and 77° are impurities caused by plastic trash, the peaks at 38.21°, 44.72°, and 77.29° are noted [21].

Debye-Scherer (Eq. 2) was used to figure out the average crystallite sizes (D) from the hight intensity diffraction peaks, D was 21.67 nm.

$$\text{Where } D = \frac{K\lambda}{FWHM \cos(\theta)} \quad (2)$$

Where (λ) equal to wavelength of Cu Kα radiation, (k) represent as constant (0.9), (FWHM) mean full width at half maximum of peak and (θ)

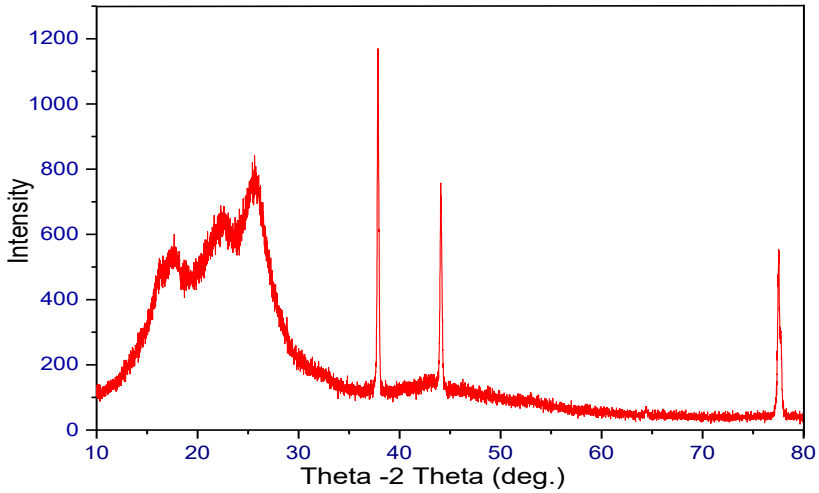

Fig. 1. XRD pattern of PAn- PET nanofibers.

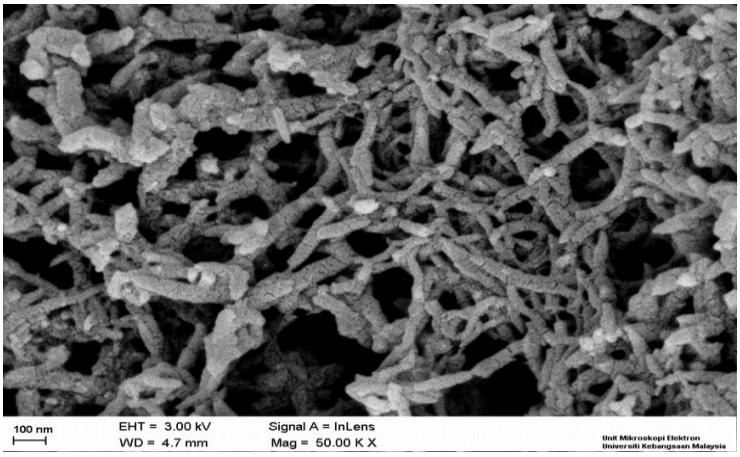

Fig. 2. FE-SEM image PAn- PET nanofibers.

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equal to Bragg angle. Based on the Debye-Scherer equation.

Broad diffractograms of the crystallographic pattern and smaller crystal sizes demonstrated that nanosized synthesis seems to have a successful quality.

FE-SEM images of PAn- PET

Fig. 2 The composite FE-SEM images revealed fibers consisting of a small group of nanofibers with an overall composition of (48.45 nm) nanofibers.

Effect of temperature on adsorption

The manipulation of temperature through absorption influences both absorption and behavior. The adsorption effectiveness improves up to a specific temperature and then declines as a result of the adsorption process. The influence of adsorption temperature is dependent on whether the process is exothermic or endothermic [22]. In endothermic adsorption, molecules migrate toward the active adsorption sites as the temperature rises. Higher temperatures made the adsorption process more accessible. The high temperature of adsorption raised the removal rate to 75.4% as can see in Fig. 3.

Effect of time on adsorption

Studies conducted on the effect of contact time on the removal of pesticides showed that

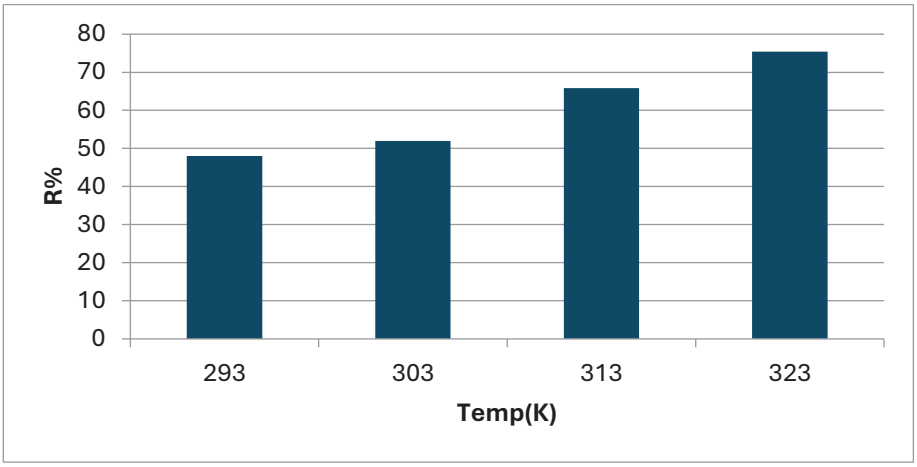

Fig. 3. relation of temperature vis R%.

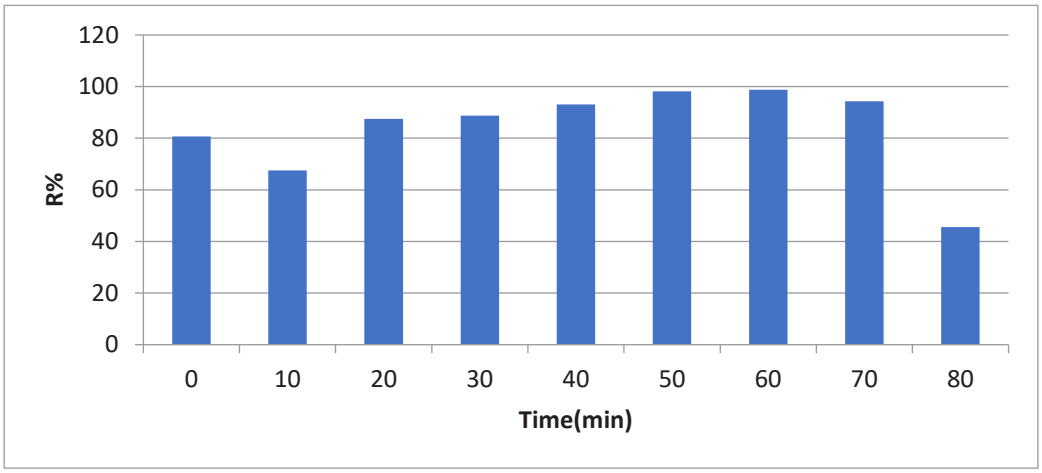

Fig. 4. relation of time Vis R%.

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the adsorption rate was 67.5% at 10 min. of adsorption then increased gradually until it reached equilibrium. It was found that the q (amount of pesticide) absorbed was high, as shown in Fig. 4. After 60 minutes, most of the pesticides were absorbed, and there were only slight changes between 50 and 60 minutes. After 60 minutes, the removal percentage decreased because the effective areas of the nanosurface became full [23].

Effect of Pentachlorophenol (PCP) concentration

(PCP) concentration is related to the absorbance of the polymer. To conduct the experiment, the pesticide content was increased from 10 ppt to 60 ppt, while the pH, contact time, and observed intensity remained unchanged. Fig. 5 displays the results, which indicate that as PCP concentration increases, adsorption efficiency declines. Since the active parts of the nanopolymer surface are filled up when there are more pesticides in the solution, PCP can't be taken from the solution and stuck to the polymer anymore [24].

Adsorption of pollutants on PAn- PET nanofibers

Langmuir, Freundlich and Temkin isotherms can be used to model the experimental data for the adsorption of the pesticide PCP from their solution.

We can express the Langmuir isotherm as an Eq. 3.

$$\frac{C_e}{Q_e} = \frac{1}{a} + \frac{b}{a} C_e \quad (3)$$

Where Qe is the adsorption capacity as a function of monolayer coverage, b is constant and Ce is the equilibrium concentration of (PCP). In Fig. 6A, represent the relationship between (Ce) and (Ce/Qe) shows that the adsorption curves of the pesticide (PCP) in their solutions were measured using the Langmuir equation, this is right for surface monolayer sorption since there are so few matching sites and the adsorbent energies are all the same. The isotherm was then used with the Freundlich equation, as shown in Eq. 4:

$$\log (Q_e) = \log(k_f) + \left(\frac{1}{n}\right) \log (C_e) \quad (4)$$

KF and n constants, which represent amount of adsorption and the strength. The Freundlich equation was made for adsorption on heterogeneous surfaces, but it doesn't suggest anything about how monolayer adsorption actually works. In solutions, the PCP pesticide adsorption curves (Fig. 6B) were changed to the Freundlich equation, which can be notice in relationship between (ln Q e) and (ln C e). In this equation, the results demonstrate that those that

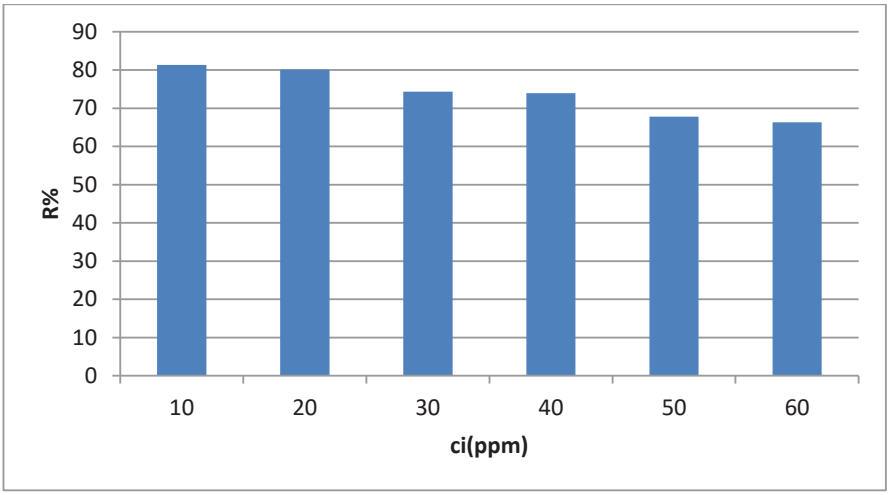

Fig. 5. relation of Ci Vis R%.

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do not undergo adsorption [4].

Additionally, the Temkin adsorption isometric expression provided a graphical representation of the interaction between adsorbent and adsorbing particle as can seen in (Fig. 6C). The equations provided below indicate the results of applying this model to the data [5,25]:

$$(Q_e) = B_T \, Ln \, K_T + B_T \, Ln \, C_e \quad (5)$$

The constants A and B, the Temkin isotherm constant (L/g) and the adsorption heat constant (J mol^{-1}), were determined by graphing Qe versus lnce. The gas constant is 8.314 mol/K. B is Temkin. Is the constant isothermal temperature, whereas is the Kelvin absolute temperature. The adsorption Temkin graph of qe versus ln Ce is drawn, and its parameters are obtained using a pectrophotometer to assess adsorption and the following relation.

Thermodynamic parameter

At different temperatures (25, 35, 45, and 55 °C), researchers looked at how the PCP pesticide stuck to the surface of PAn-PET nanofibers. The results of the experiments show that the amount of pesticide adsorbed goes up as the temperature goes up. This indicates that the adsorption process appears endothermic, as well as the mean value of H is positive. It also demonstrates that there is a strong link between the adsorbate and the adsorbent, which is consistent with the findings of a number of research studies [26,27].

Thermodynamic parameters tell us everything we need to know about how the energy changes during adsorption, so they need to be evaluated correctly. This study use Eqs. 6 and 7 to estimate the changes in free energy (G), enthalpy (H) and entropy (S) of adsorption in order to predict how adsorption works.

$$\log x_m = \frac{-\Delta H}{2.303R} + \frac{\Delta S}{R} \quad (6)$$

$$\Delta G = \Delta H - T\Delta S \quad (7)$$

Where Xm represents the maximum quantity of adsorbate (mg/g), R represents gas constant (8.314 J/mol K) and T represent the temperature (K). As shown in Fig. 7,

(ΔH) was calculated using the slope of the

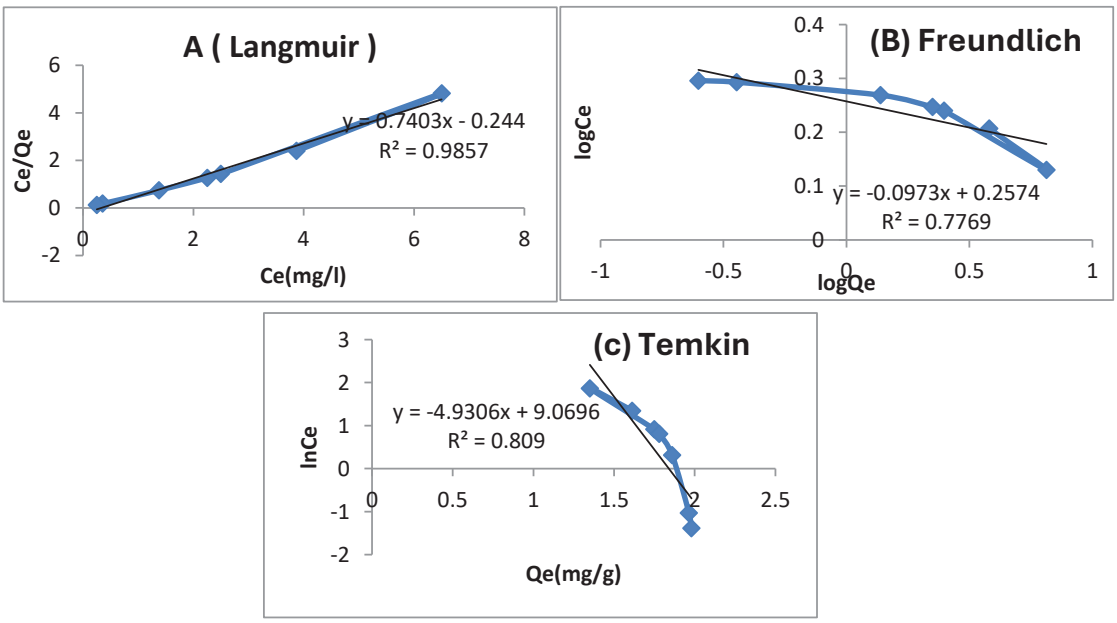

Fig. 6. Langmuir isotherm (A) , Freundlich (B) and Temkin isothermal(c) at 298 K.

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Table 2. Thermodynamic parameter.

ΔH (KJ/mol^{-1})	ΔG (KJ/mol^{-1})	ΔS (J/mol*K)
30.487	9.345	64.97

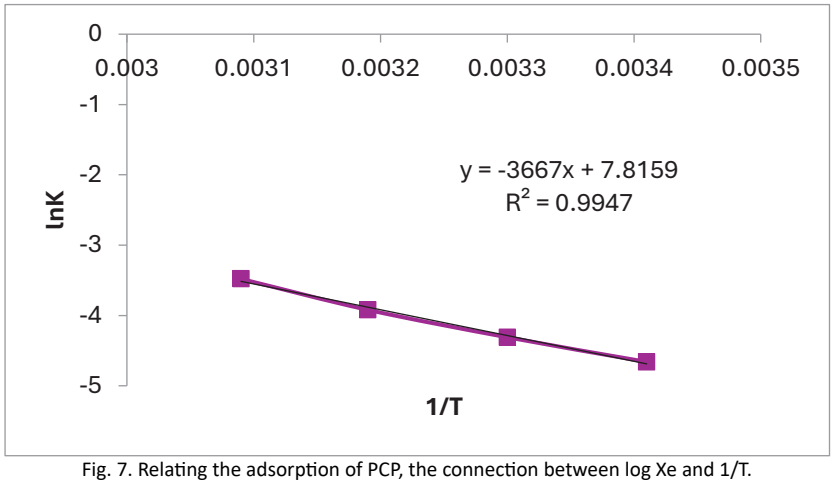

Fig. 7. Relating the adsorption of PCP, the connection between log Xe and 1/T.

van't Hoff plots of log (Xm) vs 1/T and (ΔS) was calculated using the y intercept.

ΔH was equivalent to 30.487 kJ/mol derived from the slope, and ΔS was equivalent to 64.97 J/mol K derived from the y-intercept. This may be attributed to both absorption and adsorption, since ΔH shows that the molecules that have been adsorbed are still moving about in a steady state on the surface [28]. The ΔG for the adsorption was calculated to be 9.345 kJ/mol at 298 K, indicating that the adsorption was not spontaneous. (Table 2).

CONCLUSION

In this research, we examined the removal of PCP from an aqueous solution using a polymer, and the majority of the findings indicated that it is a promising and efficient technique. PCP absorption increases with increasing initial PCP concentration until a certain limit is reached. Increasing the duration of contact increases the removal rate by 81%.Reduce PCP by up to 90% in any case.balance data It is most accurately represented by the Langmuir isothermal model. The model's outcomes show that intraparticle diffusion was ubiquitous. The concentration of polymers in PCP elimination increases with time. The polymers utilized in this study are non-hazardous to the environment, easily available, and offer more possibilities for wastewater treatment to eliminate chlorine pollution such as PCP.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this manuscript.

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