Using Nano Composites to Purify Water from Phenol Pollutants

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Abstract: Nano industry is applicable to refinery of water. This study presents the theoretical model in order to separating the phenol pollution with polymer Nano composite. Relation shown that the bending the particles is a method to identification of this particles. Increasing the size of phenol lead to suitable performance of polymer nano composite to refinery of water. Magnet property helps to high performance in absorbing the phenol nanoparticles. Performance of this method is higher than 60%. This result is suitable to resume the separating the nanoparticles. But size of particle has no relation with performance of this method.

Keywords: boron nanotube, composite, phenol nanoparticle, polymer nanoparticle.

1. Introduction

Water is one of the most vital bases for the living system and is used in daily life activities. Due to rapid industrial growth, natural water resources are affected by several water pollutants [1]. The World Health Organization (WHO) 2014 report on water supply and sanitation estimated that 748 million people still lack safe drinking water, 2.5 billion peoples without access sanitation and 3900 children die every day due to poor quality water and communicable diseases [2]. These statistics indicated that water pollution by numerous pollutants becomes an alarming issue worldwide. Consequently, competent water treatment technologies have been established to raise the potential of water resources and to decline the challenges and concerns associated with water pollution [3]. In this regard, nanocomposite has to play a significant role in the water purification technology including potable water treatment, wastewater desalination, and treatment in order to deliver the real technology to clean water at a lower price using less energy by decreasing further ecological impacts [4]. Nanomaterials are materials which have the structural components sized from 1 to 100 nm [5]. They have unique properties when compared with other conventional materials, such as mechanical, electrical, optical, and magnetic properties due to their the small size and higher specific surface area, nanomaterials [6]. In recent years, nanomaterials have been effectively applied to numerous perspectives as catalysis [7], medicine [7], sensing, and biology [7]. They have extensive applications to prevent several environmental problems like water and wastewater treatment. Because, nanomaterials have the potential to eliminate different toxins, for instance, heavy metals, organic pollutants, inorganic anions, and pathogens [8]. Zero-valent metal nanoparticles (nZVI), metal oxides nanoparticles, carbon nanotubes (CNTs) and nanocomposites are the most recent appropriate nanomaterials for water and wastewater treatment [8]. The nZVI is one of
the most useful nanomaterials for water purification [9-10]. The nZVI has a role in water purification as an electron subscriber which encourages the conversion toxic metals to safe forms (the reduction of chromium from hexavalent into trivalent form), adsorption, co-precipitation processes and strong reducing ability [10]. The nZVI has discovered real application for eliminating various organic and inorganic pollutants such as polychlorinated compounds, Nitrates, phosphates and perchlorates, nitro aromatic compounds, organic dyes, phenols, heavy metals, metalloids, and radio elements. Application of polymer composite to removing the pollution of water be done with beyene and ambaye in 2019 [1]. Then polymer Nano composite be applied to purification of water with pandey et al [2]. Economic model to production of water refinery on basis the nano polymer de done and stated that is has no economic reason to line production of this device. This result be present with hutton (2013) [3]. But stated that it can improve with a new version of Nano composite. Another model about the water refinery in medical application show that health system need to nano particle magnet to removing microbes from water that entered to patient’s body. This issue stated with heijnon et al in 2014 [4]. To first time mechanical model to nanoparticle in polluted water be present that can be control the separating the nanoparticle from liquid. This model shows the importance of strength property of nanoparticles in refinery process. Tortajada and Biswas (2018) present the theoretical model to water refinery with nanocomposite [5]. Silver nanocomposit to water refinery be present with beyene et al [6]. Silver nanocomposite has no economic reason to production this system and its property to synthesis is low. But removing the phenol be used in medical applications to separating this particle to production of drug. This issue shows with liang et al in 2012 [7]. This issue shown in proposals of research in sanino et al (2017) [8]. Then this issue be applied in fu et al (2014) with introduction of iron nanocomposite [9]. Ghasemzadeh et al (2014) present the theoretical model to separating of phenol from water [10]. In this research, refinery the phenol pollutants in water be studied and theoretical model be present about this model. Mechanical property of nanoparticle be modeled and principle governed on this problem be model to finding the way of removing the phenol with Nano composite.

2. Numerical Method

In this section theoretical model about nano particle phenol in water present that with this relation, methods of separating the nano particle be done. Selection of a suitable numerical solution has a significant effect on the accuracy and quality of the produced responses. Also, choosing an appropriate method can dramatically decrease the time of problem solving. In the meantime, the numerical method has many advantages, because despite the fact that the number of discrete points is considerably less than the finite element method, the results are much more accurate than the finite difference method. Therefore, choosing this method as a quick method, which is also highly accurate, seems to be a logical decision.

Like any other numerical method, GDQ decomposes geometry of a problem and defines unknown cases as functions of unknown values at discrete points. This method defines its function and its derivatives as linear summation of the function values at all discrete points. This makes method more precise than similar methods.

As stated above, the fundamental problem in the generalized differential squares method is to define the derivatives of a function at any point as the sum of the weight of the function values in all points. In this method, with the suggestion of Cowan and Chang [10], the Lagrange interpolation function is used to overcome the problems in the DQ method. Therefore, for function derivatives we have at each point:

\[
 f^{(n)}_x(x_i) = \sum_{i=1}^{N} C^{(n)}_{ij} f(x_i) \quad n = 1, ..., N - 1
\]

F is the function from x

\[
 f^{(n)}_x(x_i, y_j) = \sum_{k=1}^{N_x} A^{(n)}_{ik} f(x_k, y_j) \quad n = 1, ..., N_x - 1
\]

F is the function from x and y
\[ f_y^{(m)}(x_i, y_j) = \sum_{l=1}^{N_y} b_{jl}^{(m)} f(x_i, y_l) \quad m = 1, ..., N_y - 1 \quad (3) \]

\[ f_{xy}^{(n+m)}(x_i, y_j) = \sum_{k=1}^{N_x} \sum_{l=1}^{N_y} A_{lk}^{(n)} b_{jl}^{(m)} f(x_k, y_l) \quad \{i = 1, ..., N_x - 1 \} \quad \{j = 1, ..., N_y - 1 \} \quad (4) \]

If a network \(N \times 1\) in physical region be considered that \(N\) is the points in X direction, Quadrature differential rules for differential of an assumption function as \(f(x)\) present as below:

\[ \frac{\partial^n f(x_i)}{\partial x^n} = \sum_{k=1}^{N} c_{ik}^{(n)} f(x_k) \quad , i = 1, ..., N \quad , n = 1, ..., N \quad (5) \]

In this relation, \(c_{ik}^{(n)}\) is the weights coefficient in “n” order and X direction. The improved method, weights coefficient first order be present [11]:

\[ c_{ij}^{(1)} = \frac{M^{(1)}(x_i) - M^{(1)}(x_j)}{(x_i - x_j)} \quad i, j = 1, 2, ..., N / i \neq j \]

\[ c_{ii}^{(1)} = - \sum_{j=1 \atop j \neq i}^{N} c_{ij}^{(1)} \quad i = 1, 2, ..., N \quad (6) \]

Then

\[ M^{(1)}(x_i) = \prod_{j=1 \atop j \neq i}^{N} (x_i - x_j) \quad i = 1, 2, ..., N \quad (7) \]

And the weight coefficients of the order are higher than the following recurrence relation:

\[ c_{ij}^{(n)} = n \left( c_{n}^{(n-1)} c_{ij}^{(1)} - c_{y}^{(n-1)} c_{y}^{(1)} \right) \quad i, j = 1, 2, ..., N / i \neq j \quad n = 2, 3, ..., N - 1 \quad (8) \]

\[ c_{ii}^{(n)} = - \sum_{j=1 \atop j \neq i}^{N} c_{ij}^{(n)} \quad i = 1, 2, ..., N \quad n = 1, 2, ..., N - 1 \]

The distribution of network points commonly used in articles to normalized in the interval [1,0] and as follows [12]:

- Uniform distribution

\[ i = 1, 2, ..., N \times \frac{i - 1}{N - 1} \quad (9) \]
\[ i = 1,2, ..., N \]

The root of the polynomial Chbi Shaf type 2 (C II):

\[ i = 1,2, ..., N \]

The Lagrangian polynomial root (Leg):

\[ i = 1,2, ..., N \]

Chebie-Chef-Gauss-Louboutin (C-G-L):

\[ i = 1,2, ..., N \]

N is the total point in sampling in each direction. If the selected period is not \([0,1]\) selecting the network points in each period be done.

3. Investigation of Strength

To modeling the dynamic and static of phenol nanoparticle s, there are the different theories. There present several famous theories about phenol nanoparticle investigation. And then be modeled with real data to investigation of results.

3.1 Bernoulli’s principle

This theory can be generalized by Euler Bernoulli theory in phenol nanoparticle modeling. In this theory, it is assumed that each section of the phenol nanoparticle after the application of force remains flat and perpendicular to the neutral plate or the middle plate and is excluded from the tensions and shear sections. In this theory, the displacement field is defined as follows:

\[ u = u_0 + z \frac{\partial w_0}{\partial x} \]
\[ w = w_0 \]

u, w are the displacement factors in x and z direction. U0, w0 are the displacement of a point in middle plane in x and z direction.

Fig 1. Displacement field in Bernoulli phenol nanoparticle
3.2 Timoshenko Phenol Nanoparticle Theory

The Timoshenko phenol nanoparticle theory was developed by Stephen Timoshenko early in the 20th century. The model takes into account shear deformation and rotational bending effects, making it suitable for describing the behavior of thick phenol nanoparticle s, sandwich composite phenol nanoparticle s, or phenol nanoparticle s subject to high-frequency excitation when the wavelength approaches the thickness of the phenol nanoparticle. The resulting equation is of 4th order but, unlike Euler–Bernoulli phenol nanoparticle theory, there is also a second-order partial derivative present. Physically, taking into account the added mechanisms of deformation effectively lowers the stiffness of the phenol nanoparticle, while the result is a larger deflection under a static load and lower predicted Eigen frequencies for a given set of boundary conditions. The latter effect is more noticeable for higher frequencies as the wavelength becomes shorter (in principle comparable to the height of the phenol nanoparticle or shorter), and thus the distance between opposing shear forces decreases.

Displacement field be present as below:

\[ u = u_0 + z\Psi(x), \]  
\[ w = w_0 \]

\( \Psi(x) \) is the angle of turning in middle plane about y axis.  

![Fig 2. displacement field in Timoshenko phenol nanoparticle.](image)

Elongation and wide displacement \( U(x,z,t) \) \( W(x,z,t) \) in each point in phenol nanoparticle be present as:

\[ U(x,z,t) = u_0(x,t) + z\Psi(x,t), \]  

\[ W(x,z,t) = w_0 + \frac{d\Psi}{dz}(x,t) \]
W(x, z, t) = w_0(x, t)

Strain-linear displacement relation is present as below:

\[ \varepsilon_x = \frac{d u_0}{d x} + 2 \frac{d \psi}{d x}, \quad \gamma_{xz} = \frac{d w_0}{d x} + \psi \]  \hspace{1cm} (17)

3.3 Moving Equations

Equation is extract with Principle of virtual work. This equation is present as below:

\[ \delta \int_0^t (T - U + V) dt = 0 \]  \hspace{1cm} (18)

T is kinetic and U is potential energy. V is the done work. Loading the external force, the equation be present as below [14]:

\[ T = \frac{b}{2} \int_0^h \int_{-h/2}^{h/2} \rho(z) u_i dz dx \]  \hspace{1cm} (19)

\[ U = \frac{b}{2} \int_0^h \int_{-h/2}^{h/2} \sigma_{ij} e_{ij} dz dx + \frac{b}{2} \int_0^l (k_w w^2 - k_s \left( \frac{\partial w}{\partial x} \right)^2) dz dx \]

\[ V = 0 \]

\( \rho(z) \) is density of phenol nano particle .

Placing of relations and integration from it, the relation be present as [13]:

\[ \int_0^{t_L} \int_0^l \left[ - \left( \frac{\partial N_x}{\partial x} - l_1 \frac{\partial^2 u_0}{\partial t^2} - l_2 \frac{\partial^2 \psi}{\partial t^2} \right) \right] \delta u - \left( \frac{\partial Q_x}{\partial x} + k_w w - k_s \frac{\partial^2 w}{\partial x^2} - l_1 \frac{\partial^2 w_0}{\partial t^2} \right) \delta w - \left( \frac{\partial M_x}{\partial x} - Q_x - l_2 \frac{\partial^2 u_0}{\partial t^2} - l_3 \frac{\partial^2 \psi}{\partial t^2} \right) \delta \psi \] \[ dx \] \[ dt = 0 \]  \hspace{1cm} (20)

With assumption the \( \delta u \), \( \delta w \), and \( \delta \psi \) are zero the movement equations present below:

\[ \delta u : \quad \frac{\partial N_x}{\partial x} = l_1 \frac{\partial^2 u_0}{\partial t^2} + l_2 \frac{\partial^2 \psi}{\partial t^2} \]  \hspace{1cm} (21)

\[ \delta w : \quad \frac{\partial Q_x}{\partial x} - k_w w + k_s \frac{\partial^2 w}{\partial x^2} + \frac{d}{d x} \left( N_x \frac{d w_0}{d x} \right) = l_1 \frac{\partial^2 w_0}{\partial t^2} \]

\[ \delta \psi : \quad \frac{\partial M_x}{\partial x} - Q_x = l_2 \frac{\partial^2 u_0}{\partial t^2} + l_3 \frac{\partial^2 \psi}{\partial t^2} \]

Variation the time is zero in bending problem, then eq (22) be present:

\[ \delta u = \frac{\partial N_x}{\partial x} = 0 \]

\[ \delta w = \frac{\partial Q_x}{\partial x} + \frac{d}{d x} \left( N_x \frac{d w_0}{d x} \right) = 0 \]  \hspace{1cm} (22)
\( \delta \psi = \frac{\partial M_x}{\partial x} - Q_x = 0 \)

Replacing the relation 15 in balance equation the movement equation is obtained:

\[
A_{11} \frac{\partial^2 u_0}{\partial x^2} + B_{11} \frac{\partial^2 \psi}{\partial x^2} = 0 \tag{23}
\]

\[
\kappa A_{55} \left( \frac{\partial^2 w_0}{\partial x^2} + \frac{\partial \psi}{\partial x} \right) + \frac{d}{dx} \left( N_x \frac{dw_0}{dx} \right) = 0
\]

\[
B_{11} \frac{\partial^2 u_0}{\partial x^2} + D_{11} \frac{\partial^2 \psi}{\partial x^2} - \kappa A_{55} \left( \frac{\partial w_0}{\partial x} + \psi \right) = 0
\]

There are 4 boundary condition in phenol nano particle analysis \((X=0, L)\)

**Hinged supported:**

\[
u = 0 \\
w = 0 \\
M_x = B_{11} \frac{\partial u_0}{\partial x} + D_{11} \frac{\partial \psi}{\partial x} - M_x^t h = 0
\]

**Movable simply supported:**

\[
w = 0 \\
N_x = A_{11} \frac{\partial u_0}{\partial x} + B_{11} \frac{\partial \psi}{\partial x} - N_x^t h = 0 \\
M_x = B_{11} \frac{\partial u_0}{\partial x} + D_{11} \frac{\partial \psi}{\partial x} - M_x^t h = 0
\]

**Clamped supported:**

\[
u = 0 \\
w = 0 \\
\psi = 0
\]

**Free:**

\[
N_x = A_{11} \frac{\partial u_0}{\partial x} + B_{11} \frac{\partial \psi}{\partial x} - N_x^t h = 0 \\
M_x = B_{11} \frac{\partial u_0}{\partial x} + D_{11} \frac{\partial \psi}{\partial x} - M_x^t h = 0 \\
Q_x = \kappa A_{55} \left( \frac{\partial w_0}{\partial x} + \psi \right)
\]

**Dimensionless Equation**

\[
\xi = \frac{x}{L}, \quad U^* = \frac{u_0}{L}, \quad \delta = \frac{h}{L}, \quad W^* = \frac{w}{h}, \quad \psi = \psi
\]

\[
N_x^* = \frac{N_x L^2}{E_c^{ref} * I_0}, M_x^* = \frac{M_x L}{E_c^{ref} * I_0}
\]

\[
N_x^T^* = \frac{N_x^T L^2}{E_c^{ref} * I_0}, M_x^T^* = \frac{M_x^T L}{E_c^{ref} * I_0}, Q_x^* = \frac{Q_x L^2}{E_c^{ref} * I_0}
\]

(25)
\[(a_{11}, a_{55}, b_{11}, d_{11}) = \left( \frac{A_{11}}{\varepsilon_{c}^{\text{eff}} \varepsilon_{s}^{\text{eff}} h}, \frac{A_{55}}{\varepsilon_{c}^{\text{eff}} \varepsilon_{s}^{\text{eff}} h^2}, \frac{B_{11}}{\varepsilon_{c}^{\text{eff}} h^3}, \frac{d_{11}}{\varepsilon_{c}^{\text{eff}} h^3} \right) \]

Eq 25 be simple to eq 26:

\[a_{11} \frac{\partial^2 U^*}{\partial \xi^2} + b_{11} \delta \frac{\partial^2 \psi}{\partial \xi^2} = 0\]

\[\kappa a_{55} \left( \delta \frac{\partial^2 W^*}{\partial \xi^2} + \frac{\partial \psi}{\partial \xi} \right) + \left[ \frac{N_x T^*}{12} \right] \left( \delta \frac{\partial^2 W^*}{\partial \xi^2} \right) = 0\]

\[b_{11} \delta \frac{\partial^2 U^*}{\partial \xi^2} + d_{11} \delta \frac{\partial^2 \psi}{\partial \xi^2} - \kappa a_{55} \left( \frac{\partial W^*}{\partial \xi} + \psi \right) = 0\]

Boundary condition in dimensionless state be present as below (\(\xi=0,1\))

\[H(\text{hinged supported}) : \quad U^* = W^* = M_x^* = 0\]

\[C(\text{clamped}) : \quad U^* = W^* = \psi = 0\]

\[F(\text{free}) : \quad N_x^* = M_x^* = Q_x^* = 0\]

\[R(\text{roller}) : \quad U^* = \psi = Q_x^* + (N_x^*) \delta \frac{\partial W^*}{\partial \xi} = 0\]

Then

\[N_x^* = \frac{12}{\delta^2} a_{11} \left( \frac{\partial U^*}{\partial \xi} \right) + \frac{12}{\delta} b_{11} \left( \frac{\partial \psi}{\partial \xi} \right) - N_x T^*\]

\[M_x^* = \frac{12}{\delta^2} b_{11} \left( \frac{\partial U^*}{\partial \xi} \right) + 12 d_{11} \left( \frac{\partial \psi}{\partial \xi} \right) - M_x T^*\]

\[Q_x^* = \frac{12}{\delta^2} \kappa a_{55} \left( \delta \frac{\partial W^*}{\partial \xi} + \psi \right)\]

3.4 Applying the QUADRATURE Method

\[a_{11} \sum_{j=1}^{N} B_{ij} (2) U_j = b_{11} \delta \sum_{j=1}^{N} B_{ij} (2) \psi_j = 0\]

\[\kappa a_{55} \left( \delta \sum_{j=1}^{N} B_{ij} (2) W_j + \sum_{j=1}^{N} B_{ij} (1) \psi_j \right) + \left[ - \frac{1}{12} \delta^2 \sum_{j=1}^{N} B_{ij} (0) N_x T^* \right] \left( \sum_{j=1}^{N} B_{ij} (2) W_j \right) \]

\[= 0\]

\[\kappa a_{55} \left( \sum_{j=1}^{N} B_{ij} (0) \psi_j + \delta \sum_{j=1}^{N} B_{ij} (1) W_j \right) - b_{11} \delta \sum_{j=1}^{N} B_{ij} (2) U_j - d_{11} \delta^2 \sum_{j=1}^{N} B_{ij} (2) \psi_j = 0\]

Improved quadrature method:
\[ H : U^*_i = W^*_i = 0, M_x^* = b_{11} \sum_{j=1}^{N} B_{ij} (1) U^*_j + \delta d_{11} \sum_{j=1}^{N} B_{ij} (1) \psi_j - \frac{\delta}{12} \sum_{j=1}^{N} B_{ij} (0) M_x^{*} T^*_j = 0 (i = 1 \text{ at } \xi = 0, i = N \text{ at } \xi = 1) \]

\[ C : U^*_i = W^*_i = \psi_i = 0 \]

\[ F : N_x^* = a_{11} \sum_{j=1}^{N} B_{ij} (1) U^*_j + \delta b_{11} \sum_{j=1}^{N} B_{ij} (1) \psi_j - \frac{\delta^2}{12} \sum_{j=1}^{N} B_{ij} (0) N_x^{*} T^*_j = 0, \]

\[ M_x^* = \alpha_{55} \left( \sum_{j=1}^{N} B_{ij} (0) \psi_j + \frac{\delta^2}{12} \sum_{j=1}^{N} B_{ij} (0) N_x^{*} T^*_j \right) = 0 \]

\[ Q_x = \kappa \alpha_{55} \left( \sum_{j=1}^{N} B_{ij} (0) \psi_j + \frac{\delta^2}{12} \sum_{j=1}^{N} B_{ij} (0) N_x^{*} T^*_j \right) = 0 \]

\[ R : U^*_i = \psi_i = 0 \]

\[ = \kappa \alpha_{55} \left( \sum_{j=1}^{N} B_{ij} (0) \psi_j + \delta \sum_{j=1}^{N} B_{ij} (1) W^*_j \right) + \left[ -\frac{\delta^3}{12} \sum_{j=1}^{N} B_{ij} (0) N_x^{*} T^*_j \left( \sum_{j=1}^{N} B_{ij} (1) W^*_j \right) = 0 \right] (i = 1 \text{ at } \xi = 0, i = N \text{ at } \xi = 1) \]

4. Result

By examining the conditional state based on the presented relationships it is clear that increasing the phenol size increases the efficiency of the nanocomposite in identifying and separating the phenol and generally the performance of the nanocomposite is evaluated in this respect but it is worth noting that the relationship is quite It is not linear. These relationships can vary in different parts. It seems that there is another factor in the water purification performance of phenol contaminated water so measuring it can partly improve the performance of nanocomposites even at very low nanocomposite yields. Not less than 60% and This is a good result, which makes the use of nanocomposites suitable for fan separation.
Fig 3. Performance the separation of phenol on basis the size.

Fig 4. Performance the separation of phenol on basis the magnet ability.

The next important factor in the nanocomposite separation performance is the magnetic property of phenol nanoparticles. It is therefore possible to conclude that by increasing the magnetic properties of the particles the absorption power will be improved.

5. Conclusion
Numerical results showed that:

- Polymer nanocomposite due to its magnet property has high ability to absorbing the phenol nanoparticles.
- Magnet ability of phenol nanoparticle has direct relation with performance of absorbing the particles.
- Performance of polymer nanocomposite is more than 60% in all stage in investigation.
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