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## Simulation of Phenol Adsorption in a Packed Bed Column

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**Abstract:** Water pollution is a very persistent problem. The intensive throwing up of different toxic substances without control constitutes a real danger for humanity. Phenolic compounds are common contaminants in wastewater, generated by petroleum and petrochemical, coal conversion and phenol producing industries. The phenols are considered as priority pollutants since they are harmful to organisms at low concentrations because of their potential harm to human health. United State Environmental Protection Agency (EPA) regulations call for lowering phenol content in wastewater to less than 1 mg L<sup>-1</sup> before discharging. This study focuses on the feasibility of using activated carbon to remove phenol from waste water in industry. Simulation by Aspen Adsorption is conducted to investigate the feasibility. Several sensitivity analyses such as changing the parameters which affected the rate of adsorption are discussed. Besides that, it is found that the scaling up of the column is not practicable in industry.

**Key words:** Adsorption, phenol, activated carbon, simulation, wastewater

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### INTRODUCTION

Phenol is generally considered as the main organic pollutants which cause unpleasant taste and odor of drinking water. The major sources of phenol contaminants are wastewater from paint, pesticide, coal conversion, polymeric resin and petroleum and petrochemicals industries. It is very soluble in water, oils and numerous organic solvents. Moreover, phenol is flammable and catches fire easily (Ahmaruzzaman, 2008). These phenolic compounds are harmful and toxic to organisms at low concentration and can be carcinogenic when present in high amounts (Kumar *et al.*, 2011). In addition, phenol has been classified as one of the primary pollutants as enacted by Department of Environment (DOE), Malaysia in Environmental Quality Act 1979 (Sewage and Industrial Effluent) which should be treated to be less than 1 ppm for inland water discharge. In view of the high toxicity, wide prevalence and poor biodegradability of phenols, a prior treatment is required before discharging the effluents to the environment. Therefore, phenolic compound has been selected in the study area due to the objectionable taste of water and its nauseous odour. Furthermore, they are considered to be very toxic compounds, carcinogenic and their adverse effects have also been found on some useful bacteria such as nitrification bacteria and bacteria in sediment, etc. (Namane and Hellal, 2006).

Currently, the available technologies for the abatement of phenol from water and gaseous streams are briefly reviewed and the recent advancements summarized. Separation technologies such as distillation, liquid-liquid extraction with different solvents, adsorption over Activated Carbons (AC) and polymeric and inorganic adsorbents, membrane pervaporation and membrane-solvent extraction, have been discussed. Destruction technologies such as non-catalytic, supercritical and catalytic wet air oxidation, ozonation, non-catalytic, catalytic and enzymatic peroxide wet oxidation, electrochemical and photocatalytic oxidation, supercritical wet gasification, destruction with electron discharges as well as biochemical treatments have been considered. As for the abatement of phenol from gases, condensation, absorption in liquids, adsorption on solids, membrane separation, thermal, catalytic, photocatalytic and biological oxidation have also been considered. The experimental conditions and the performances of the different techniques have been compared (Busca *et al.*, 2008).

The objective of the current study was to determine the suitable bed column size required to remove phenol content from wastewater by using Aspen Adsorption simulation program (Aspen Tech, 2008; Anisuzzaman *et al.*, 2014). It also aims to determine the feasibility of the scale up for industrial wastewater application.

**THEORETICAL MODELING**

**Activated Carbon (AC):** AC also known as activated charcoal, is a form of carbon that processed to be riddled with small, low volume pores that increases the surface area available for adsorption or chemical reaction. It is a solid, porous, black carbonaceous material. Any carbon source can be processed and converted into AC via a number of methods. In addition, the AC is produced in various forms, such as powders, cylindrical extrudates, spherical beads, granular and fibers. The pores structure determines its usage as the most important property of AC.

Nevskaia *et al.* (2004) have studied the removal of phenol from water by the AC with high surface area graphite with oxygen (HSAGox), AC with oxygen (ACox) and without oxygen (HSAGT, ACT) surface groups. Microporous carbons (called APET) of similar surface area (1200-1500 m<sup>2</sup> g<sup>-1</sup>) and porosity but different surface compositions were prepared from poly (ethyleneterephthalate) (PET) based AC by chemical (HNO<sub>3</sub>) and thermal (700°C) post-treatment (Laszlo, 2005). The waste removal capacity was studied by adsorption from buffered aqueous phenol and aniline solutions. Adsorption isotherms were satisfactorily fitted by both the Langmuir and Freundlich models. Moreover, TiO<sub>2</sub>-mounted AC was prepared through hydrolytic precipitation of TiO<sub>2</sub> from teraisopropyl orthotitanate and followed heat treatment at 650-900 °C for 1 h under a flow of N<sub>2</sub> gas (Tryba *et al.*, 2003). The removal of phenol from aqueous solutions under UV irradiation was measured on the prepared TiO<sub>2</sub>-mounted AC.

Consequently, AC remains extensively used in practice because of the high capacity of phenol adsorption, mechanic stability and fast adsorption rate. The capacity is mainly due to their structural characteristics and their porous texture which provides them a large surface area and their chemical nature can be modified by chemical treatment in order to increase their properties (Liu *et al.*, 2010).

**Adsorption isotherm:** In single component adsorption, dynamic phase equilibrium is established in between adsorbate and adsorbent surface. An adsorption equilibrium isotherm relates the adsorbate loading on the adsorbent (q<sub>e</sub>) and liquid phase concentration of adsorbate (C<sub>e</sub>) at equilibrium condition keeping temperature constant. Thus, adsorption isotherm describes the interaction between adsorbate and adsorbent which is critical in optimizing the use of adsorbent amount. Out of several isotherm models available in the literature, two isotherm models have been chosen for the present study to correlate the data, namely

Langmuir model and Freundlich model (Kumar *et al.*, 2011). The model equations are as follows:

Langmuir model:

$$q_e = \frac{Q_s b C_e}{1 + b C_e} \tag{1}$$

Freundlich model:

$$q_e = K_f C_e^{1/n} \tag{2}$$

**Mathematical modeling:** The mathematical models are based on the following assumptions:

- Process is isothermal
- Mass and velocity gradient are negligible in radial direction of the bed
- Fluid phase behaves as the ideal condition
- Particles are spherical and packed uniformly into fixed bed column

**Material balance:** The differential mass balance equations for an element of the adsorption column and for an adsorbent particle within such an element provide the starting point for development of a mathematical model to describe the dynamic behaviour of the system. If the flow pattern can be represented as axially dispersed plug flow the differential fluid phase mass balance is:

$$-D_L \frac{\partial^2 c}{\partial z^2} + \frac{\partial}{\partial z}(vc) + \frac{\partial c}{\partial t} + \left( \frac{1-\epsilon}{\epsilon} \right) \frac{\partial \bar{q}}{\partial t} = 0 \tag{3}$$

where, D<sub>L</sub> is axial dispersion coefficient, c is fluid concentration, z is column height, v is interstitial velocity of fluid, t is time, ε is voidage of adsorbent bed,  $\bar{q}$  is average concentration.

**Linear lumped resistance:** With linear lumped resistance selected, the mass transfer driving force for component i is expressed as a linear function of the liquid phase concentration or solid phase loading:

$$\rho_s \frac{\partial w_i}{\partial t} = MTC_{li} (c_i - c_i') \text{ (fluid)} \tag{4}$$

$$\frac{\partial w_i}{\partial t} = MTC_{si} (w_i' - w_i) \text{ (solid)} \tag{5}$$

where, ρ<sub>s</sub> is adsorbent bulk density (kg m<sup>-3</sup>), w<sub>i</sub> is loading of component I (kmol kg<sup>-1</sup>), w<sub>i</sub>' is loading at equilibrium with the actual liquid phase composition (kmol kg<sup>-1</sup>), t is time (sec), MTC<sub>li</sub> is liquid film mass transfer coefficient (1/sec), MTC<sub>si</sub> is solid film mass transfer coefficient

(1/sec),  $c'_i$  is bulk liquid phase concentration of component I ( $\text{kmol m}^{-3}$ ),  $c_i$  is liquid phase composition at equilibrium with the actual loading ( $\text{kmol m}^{-3}$ ).

**Micro and macropore model:** The two concentration gradients that greatly affect the diffusion rate:

- Within the pores of the solid
- Within the void spaces between the particles, that is, within the crystallizes
- Under practical conditions in gas separation, pore diffusion limits the overall mass transfer rate between the bulk flow and the internal surface of a particle, so it is an important factor in the dynamics of adsorbers

**Micropore effect:** Fluid film model as follows:

$$(1 - \varepsilon_p) \rho_s \frac{\partial w_k}{\partial t} = K_{mic} (c_{msk} - c_k^*) \quad (6)$$

Accumulation = Rate of mass transfer from micropore

Solid film model as follows:

$$(1 - \varepsilon_p) \rho_s \frac{\partial w_k}{\partial t} = (1 - \varepsilon_p) \rho_s K_{mic} (w_{sk}^* - w_k) \quad (7)$$

Accumulation = Rate of mass transfer from macropore

where,  $\varepsilon_s$  is intraparticle voidage ( $\text{m}^3 \text{ void/m}^3 \text{ bead}$ ),  $\rho_s$  is adsorbent bulk density ( $\text{kg m}^{-3}$ ),  $w_k$  is loading on adsorbent surface ( $\text{kmol kg}^{-1}$ ),  $w_{sk}^*$  is equilibrium loading on adsorbent surface ( $\text{kmol m}^{-3}$ ),  $c_{msk}$  is concentration of adsorbate in macropore ( $\text{kmol m}^{-3}$ ),  $c_k^*$  is equilibrium concentration on adsorbent surface ( $\text{kmol m}^{-3}$ ),  $t$  is time (sec),  $K_{mic}$  is micropore resistance constant.

**Macropore effect:** Fluid film model as follows:

$$(1 - \varepsilon_i) \varepsilon_p \frac{\partial c_{msk}}{\partial t} + (1 - \varepsilon_p) \rho_s \frac{\partial w_k}{\partial t} = K_{mac} (c_{bk} - c_{msk}) \quad (8)$$

Accumulation+Mass transfer to micropore = Rate of mass transfer from bulk gas

Solid film model as follows:

$$(1 - \varepsilon_i) \varepsilon_p \frac{\partial c_{msk}}{\partial t} + (1 - \varepsilon_p) \rho_s \frac{\partial w_k}{\partial t} = (1 - \varepsilon_p) \rho_s K_{mac} (w_{bk}^* - w_{msk}^*) \quad (9)$$

Accumulation+Mass transfer to micropore = Rate of mass transfer from bulk gas

where,  $\varepsilon_i$  is interparticle voidage ( $\text{m}^3 \text{ void/m}^3 \text{ bed}$ ),  $\varepsilon_p$  is intraparticle voidage ( $\text{m}^3 \text{ void/m}^3 \text{ bed}$ ),  $c_{bk}$  is bulk

concentration of adsorbate in macropore ( $\text{kmol m}^{-3}$ ),  $c_{msk}$  is concentration of adsorbate in macropore ( $\text{kmol m}^{-3}$ ),  $w_{bk}^*$  is bulk loading of adsorbate ( $\text{kmol kg}^{-1}$ ),  $w_{msk}^*$  is loading of adsorbate in macropore ( $\text{kmol kg}^{-1}$ ),  $K_{mac}$  is macropore resistance constant.

**Quadratic lumped resistance:** With quadratic lumped resistance selected, the mass transfer driving force is expressed as a quadratic function of the liquid phase concentration or solid phase loading, as shown in the following:

$$\rho_s \frac{\partial w_i}{\partial t} = \frac{MTC_{li} (c_i^2 - (c_i^*)^2)}{2c_i} \quad (\text{fluid}) \quad (10)$$

$$\frac{\partial w_i}{\partial t} = MTC_{si} \frac{((w_i^*)^2 - w_i^2)}{2w_i} \quad (\text{solid}) \quad (11)$$

where,  $\rho_s$  is adsorbent bulk density ( $\text{kg m}^{-3}$ ),  $c_i$  is bulk liquid phase concentration of component i ( $\text{kmol m}^{-3}$ ),  $c_i^*$  is liquid phase composition at equilibrium with the actual loading ( $\text{kmol m}^{-3}$ ),  $w_i$  is loading of component i ( $\text{kmol kg}^{-1}$ ),  $w_i^*$  is loading at equilibrium with the actual liquid phase composition ( $\text{kmol kg}^{-1}$ ),  $t$  is time (sec),  $MTC_{li}$  is liquid film mass transfer coefficient (1/sec),  $MTC_{si}$  is solid film mass transfer coefficient (1/sec).

**Kinetic fitting:** The kinetics is fitted with the pseudo-first-order and pseudo second-order models which are extensively used in kinetic studies (Liu *et al.*, 2010).

The pseudo-first-order model can be expressed as:

$$\frac{dq_t}{dt} = k_1 (q_e - q_t) \quad (12)$$

After integration and applying boundary conditions  $t = 0$  to  $t$  and  $q_t$ , the integrated form of the equation becomes as follows:

$$\ln(q_e - q_t) = \ln q_e - k_1 t \quad (13)$$

where,  $k_1$  is the first-order rate constant. The value of  $\ln(q_e - q_t)$  are calculated from the experimental data and plotted against  $t$ ,  $k_1$  is calculated from the slope of the plot.

According to Ho and MicKay (1998), in order to fit the equation, the equilibrium sorption capacity ( $q_e$ ) must be known from experimental data. Based on literature, the pseudo order kinetics model usually does not fit well for the whole range of contact time and is normally applicable over initial 20-30 min of the adsorption process.

The pseudo-second-order model can be expressed as:

$$\frac{dq_t}{dt} = k_2(q_e - q_t)^2 \quad (14)$$

Equation 14 is not the linear form of the kinetic model. The linearized form of pseudo second order kinetic models is express as:

$$\frac{t}{q_t} = \frac{1}{k_2 q_e} + \frac{t}{q_e} \quad (15)$$

where,  $k_2$  is the second-order rate constant. The values of  $t/q_e$  are plotted against  $t$ ,  $q_e$  and  $k_2$  are calculated from the slope and intercept of the plot.

### METHODOLOGY

**Adsorption process data:** For the equilibrium adsorption isotherm, from the study of Dursun *et al.* (2005) and Hameed and Rahman (2008), common isotherm models have been proposed which include Langmuir isotherm and Freundlich isotherms. The following data is used for simulation purpose (Table 1-3).

**Configuration of Aspen Adsorption v7.1** (Aspen Tech, 2008)

- Firstly, configure the component list in the Aspen Adsorption menu
- Select ‘use Aspen property system’ and click on ‘edit using Aspen properties’
- From the Aspen property menu, click ‘find’ to search for the component to be adsorb in the search bar such as phenol
- Double click the selected component and return to the main configuration menu
- After that, click ‘next’ to enter the global tab
- From the global tab, change the process type to ‘all’ and select ‘PENG-ROB’ for the property method
- After finish configure the properties, click next until the end and save the file as PropsPlus and then close the Aspen properties
- In the process flow sheet window, construct the diagram by adding the liquid feed, liquid product and the also liquid bed. All these three components are connected using the connection
- Next, configure the liquid feed by double click the button and specify. From there, insert the flow rate, temperature and the pressure
- After that, click on the bed column and configure

Table 1: Isotherm constants for phenol adsorbed onto AC (Hameed and Rahman, 2008)

Temperature (°C)	Langmuir model			Freundlich model		
	$q_b$ (mg g <sup>-1</sup> )	$K_L$ (L mg <sup>-1</sup> )	$R^2$	$K_F$ (mg g <sup>-1</sup> (L mg <sup>-1</sup> ) <sup>1/n</sup> )	$n$	$R^2$
25	149.25	0.16	0.98	29.37	2.48	0.98

Table 2: Isotherm constants for phenol adsorbed onto zeolite (Yousef *et al.*, 2011)

Temperature (°C)	Langmuir model			Freundlich model		
	$q_b$ (mg g <sup>-1</sup> )	$K_L$ (L mg <sup>-1</sup> )	$R^2$	$K_F$ (mg g <sup>-1</sup> (L mg <sup>-1</sup> ) <sup>1/n</sup> )	$n$	$R^2$
25	34.5	0.45	0.979	10.8	2.87	0.999

Table 3: Various adsorbent properties (Hameed and Rahman, 2008; Yousef *et al.*, 2011)

Adsorbent and their property	Value
<b>AC</b>	
Inter-particle voidage (m <sup>3</sup> void/m <sup>3</sup> bed)	0.500
Intra-particle voidage (m <sup>3</sup> void/m <sup>3</sup> bead)	0.600
Solid density (kg m <sup>-3</sup> )	400.000
<b>Natural zeolite</b>	
Inter-particle voidage (m <sup>3</sup> void/m <sup>3</sup> bed)	0.500
Intra-particle voidage (m <sup>3</sup> void/m <sup>3</sup> bead)	0.300
Solid density (kg m <sup>-3</sup> )	600.000
Adsorbent particle radius (mm)	0.375

- Specify the height of adsorbent layer, internal diameter of adsorbent layer and the specified flow direction
- After finish configuring the properties of the adsorbent, close the box and can start the simulation
- From the top of the menu, add in the new form and name it as ‘trial1’
- Then open the new form that created from the left side of the menu and edit the y-axis of the graph by dragging the outlet concentration from the liquid product
- Start the simulation and let it run until the components adsorbed reach saturated state. Then stop the simulation
- Right click the graph and select ‘show as history’. Copy all the data into Microsoft Excel to perform the data analysis and breakthrough curves
- Repeat step 10 for different isotherm and step 11 for the properties of different adsorbent used

### RESULTS AND DISCUSSION

In order to determine the equilibrium data from the literature the adsorption isotherms such as Langmuir and Freundlich model are selected. The parameters obtained from these experiments are at the same conditions. After that, simulation is done based on the parameters to observe the degree of deviation of the breakthrough curve.

Firstly, adsorption of phenol is simulated onto different adsorbents which are AC and Zeolite with the

Langmuir isotherm. The result is shown in Fig. 1; it indicates that each adsorbent gives different equilibrium concentration curve. The leading adsorbent that shows towards ideal adsorption equilibrium is zeolite followed by AC. Since most complete saturation of adsorption occurs in zeolite, the adsorption rate also tends to be faster than activated carbon. This is due to each adsorbent possess difference in adsorption kinetic, isotherm parameter and adsorbent properties. The zeolite used in the simulation is smaller in adsorption kinetic constant than the activated carbon enabling it to adsorb faster and reach equilibrium. However, the focus this project is on the feasibility of adsorption onto AC. Hence, the AC will be used for the following simulation for comparison.

For this set of simulation, using the same properties of adsorbent characteristics that is activated carbon, the same size of adsorption bed, flow condition but different in isotherm model shows the result as in Fig. 2. This simulation uses the AC adsorption model with Langmuir isotherm,  $Q_{max} = 34.5 \text{ mg g}^{-1}$ ,  $K_L = 0.45 \text{ L mg}^{-1}$ , Freundlich isotherm,  $K_F = 10.8 \text{ mg g}^{-1}(\text{L mg}^{-1})^{1/n}$ ,  $n = 2.87$ . It can be seen that both Langmuir and Freundlich models shows no significant between each other. Both of the isotherm parameters of Langmuir and Freundlich show the same breakthrough curve and also reach the equilibrium state at the same time which is shown in the Fig. 2 as they overlap each other. Thus, it can be conclude that these two models perfectly fit the data for both models. Therefore, we assume the Langmuir isotherm as the reference isotherm for the subsequent comparison.

Using Langmuir isotherm, we compared breakthrough curve simulated with linear lumped resistance as the reference, the constant of the linear lumped resistance kinetics model is altered in 20% increase and 20% decrease on the reference value. The adsorbent used in the simulation with a kinetic constant of 0.013 (1/h) as the reference value. Reduce 20% of this reference value is 0.0104 (1/h) and increase 20% of this value is 0.0156 (1/h). As shown in Fig. 3, the effect of linear lumped resistance kinetic constant in decrease and increase 20% do not affect the rate of the adsorption process. This might be due to the reference value is too small and the changes of variation is not detected. However, if the reference value is high enough, increase of the reference value causes the breakthrough curve lagging behind the reference breakthrough curve which means it will take more time to reach breakthrough time and vice versa.

In this simulation, the comparison is done between the material balance assumption of phenol adsorption and the result of the breakthrough curve is showed in Fig. 4. In Aspen Adsorption software, the assumptions available are convection, convection with constant dispersion and

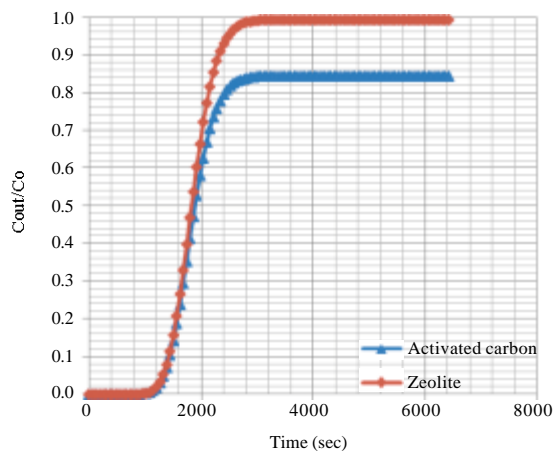


Fig. 1: Comparison of adsorbents for phenol adsorption

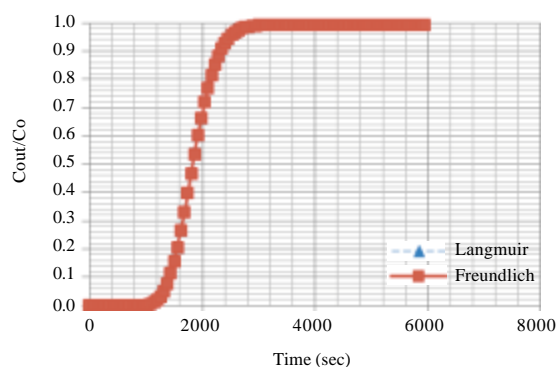


Fig. 2: Comparison of isotherms for phenol adsorption

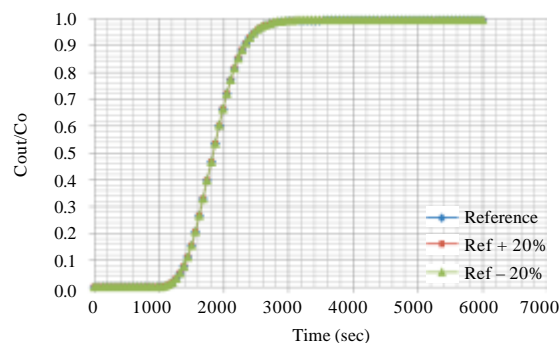


Fig. 3: Comparison of variation of kinetic constant

convection with estimated dispersion. Due to the limitation of the data applicability, therefore only comparison between convection and convection with estimated dispersion are run in this attempt. As a result,

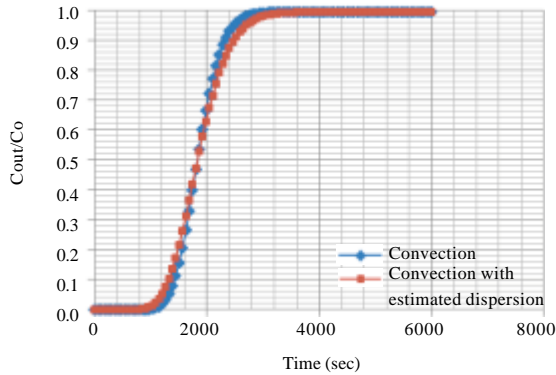


Fig. 4: Comparison of material balance for phenol adsorption

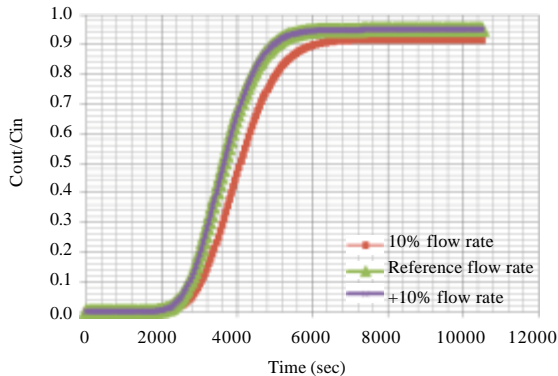


Fig. 5: Effect of feed flow rate affects the rate of adsorption

the convection with estimate dispersion breakthrough time is shown faster than the model of the convection only. It was indicated that the convection with estimated dispersion model is faster to achieve the equilibrium. Hence the convection with estimated dispersion will give better accuracy. The different of simulation data might be due to the presence of the adsorbent pellet radius. Convection with estimated dispersion in the Aspen Adsorption software requires the specification of the adsorbent radius; meanwhile convection is not required. The provided pellet radius should improve the adsorption simulation precision. In order to see if the fluctuation of feed flow rate affects the simulation result, we simulated a feed flow rate of -10 and +10% of the original feed flow rate and determined the affect own result.

From the simulation result, as indicated in Fig. 5, at the lower flow rate, relatively higher uptake values were observed. At higher flow rates, the breakthrough occurred

faster and the breakpoint time and total adsorbed quantity decreased. This behaviour can be explained by insufficient residence time of the solute in the column. The residence time decrease with the increase of the flow that leads to insufficient time for diffusion of the phenol into the pores of activated carbon and limits the number of the available active sites for adsorption, thus reducing the volume of the aqueous solution being treated and the solute left the column before equilibrium occurred.

The increase in the flow causes a reduction of the resistance of film in the external transfer which causes an improvement in the kinetics of adsorptions. But we should mention that this increase is favourable only until one value of the flow beyond which this external resistance is not any more limited.

**Scale up calculation:** The exhaustion time is found to be 95% of the fully saturated bed. In this case, the exhaustion time is found to be 3420 sec at an outlet concentration of  $2.64 \times 10^{-4} \text{ mol L}^{-1}$ . From the breakthrough time and exhaustion time, this column can be scaled up the adsorption bed to a bed which has more than 1 week breakthrough time.

$$C_o = 2.66 \times 10^{-4} \text{ mol L}^{-1}$$

$$C_b = 1.82 \times 10^{-6} \text{ mol L}^{-1}$$

Breakthrough time:

$$t_u = \int_0^{t_b} \left(1 - \frac{c}{c_o}\right) dt = 1200 \text{ sec}$$

The time required for fully saturated:

$$t_u = \int_0^{\infty} \left(1 - \frac{c}{c_o}\right) dt = 3420 \text{ sec}$$

Bed length used at break point:

$$H_B = \frac{t_u}{t_i} H_T = \frac{0.3333}{0.95} (1/m) = 0.351 \text{ m}$$

Unused bed length:

$$H_{UNB} = H_T - H_B = (1 - 0.351) \text{ m} = 0.649 \text{ m}$$

To find out the new used bed length for scale up bed, with 2 m as the new diameter of the bed:

$$\frac{t_u}{t_{ud}} = \frac{H_B \times [D_b]^2}{H_{Ba} \times [D_{ba}]^2}$$

$$H_{Bd} = \frac{168 \text{ h} \times 0.351 \text{ m} \times 1^2}{0.3333 \text{ h} \times 2^2} = 44 \text{ m}$$

New total bed length:

$$\frac{t_u}{t_{ud}} = \frac{H_B \times [D_b]^2}{H_{Bd} \times [D_{bd}]^2}$$

$$H_{Td} = \frac{168 \text{ h} \times 0.649 \text{ m} \times 1^2}{0.3333 \text{ h} \times 2^2} = 82 \text{ m}$$

Total time required for the bed to fully saturated:

$$t_{td} = \frac{H_{Td}}{H_{Bd}} t_{ud} = \frac{82 \text{ m}}{44 \text{ m}} \times 168 \text{ h} = 313 \text{ h}$$

### CONCLUSION

The scale up dimension of the adsorption bed for one week was found out that it is too large for the adsorption process with the flow rate  $2 \times 10^4 \text{ m}^3 \text{ sec}^{-1}$ . The total bed length required is 82 m, with the diameter of 2 m. Hence, it is concluded that the adsorption column is not feasible in large scale in the treatment of the industry wastewater. Before the adsorption process takes place, the wastewater should undergo pre-treatment or chemically treated until certain low concentration of phenol achieved. Adsorption process always the last treatment of the phenol concentration in the wastewater until  $1 \text{ mg L}^{-1}$  before discharging to the environment. Some of the simulated data such as the adsorbent properties and adsorption kinetic constant need to be computed exactly same as the laboratory based experiments. With only assumption and guessing of adsorbent characteristic based on the literature provided may not give enough information for this simulation software. More trials on the adsorption simulation with complete set of parameter available especially adsorbent properties are recommended to obtain before running any simulation model.

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