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ORIGINAL ARTICLE

A study on dynamic simulation of phenol adsorption in activated carbon packed bed column

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Abstract This study is mainly concerned about the dynamic simulation of phenol adsorption within the packed bed column filled with activated carbon derived from dates' stones. The process parameters such as column length, inlet liquid flow rate, initial phenol concentration of feed liquid and characteristics of activated carbon for the small scale packed bed adsorption column are investigated based on the dynamic simulation results using Aspen Adsorption V7.1 simulation program. The relationship between inlet liquid feed flow rate, breakthrough time and saturation time, relationship between initial phenol concentration, breakthrough time and saturation time, and relationship between packed bed column height, breakthrough time, saturation time, and C/Co ratio were studied. Based on the optimized simulation results, the ideal proposed small scale adsorption column suitable for a single household to treat drinking water which is contaminated with 2.0189×10^{-7} mol/l phenol concentration on annual usage should have a column diameter, column height, and activated carbon particle diameter magnitudes 1.0 m, 10.0 m and 1.5 mm, respectively with 240 m^3/year inlet feed liquid flow rate. However, based on the simulation, the adsorption column is not feasible for conventional water treatment plant.
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1. Introduction

Phenol is a pollutant that can be found in the effluents of various industries such as chemical plants, oil refineries, paper and pulp mills, gasification, phenolic resin manufacturing, paint stripping etc. (Chan and Lim, 2007; Busca et al., 2008; Ahmaruzzaman, 2008; Wang et al., 2012). It could pose a threat to living organisms even at low concentration and it had received great concern especially when polluted water body served as drinkable water for human beings (Kumar et al., 2011). Although many treatment alternatives had been implemented to remove phenolic compounds, adsorption is still regarded as the best alternative based on its performance

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(Dąbrowski et al. 2005). However, most researchers reported the removal of phenolic compounds within single packed-bed column in lab-scale model.

Adsorption is a physical technique which involves the adherence of particular molecules onto the surfaces of adsorbent. Adsorption techniques employing solid adsorbent have been widely used to remove certain classes of chemical pollutants from waste-water, such as phenolic compounds (Ahmaruzzaman, 2008; Ahmaruzzaman and Sharma, 2005). Richard et al. (2010) demonstrated that various adsorbents are available as the choices of adsorbent used to remove phenolic compounds from effluents via adsorption process, such as bark (Vazquez et al., 2006), activated sludge (Aksu and Gönen, 2004), resins (Otero et al., 2005; Pan et al., 2005), modified alumina (Adak and Pal, 2006) and activated carbon (Ahmaruzzaman, 2008; Lua and Jia, 2009; Canizares et al., 2006; Girods et al., 2009; Mukherjee et al., 2007; Nevskaia et al., 1999). Among all those adsorbent materials aforementioned, activated carbon is the most popular absorbent that was used due to its adsorption ability for relatively low-molecular-weight organic compounds (Dąbrowski et al. 2005).

Packed-bed systems are widely used in adsorption of water vapor, organic solvent and some toxic gases. A simple packed-bed system consists of a single column loaded with a particular type of adsorbent. In a single packed-bed system, suitable type of adsorbent is selected for specific adsorbate in order to obtain high removal efficiency for particular adsorbate. For example, activated carbon is usually used for adsorption of oil and organic solvent, meanwhile silica gel and molecular sieves are commonly used for adsorption of water vapor (San et al. 1998).

In this study, dynamic simulation of the adsorption process was carried out by using Aspen Adsorption V7.1 program (Aspen One, 2009). Material Safety Data Sheet of Occupational Safety and Health Administration (OSHA) Permissible Exposure Limit (PEL) for phenol was 19 mg/l, which is equivalent to 2.0189×10^{-7} mol/l (Crowl and Louvar, 2002). Thus, few important factors such as column height, particle diameter of adsorbent, and inlet feed water flow rate of contaminated water were varied and studied by simulating the estimated mechanism of phenol adsorption in single packed bed column filled with specified activated carbon particles by reasonable theoretical assumptions such as kinetic model, material balance, isotherm, and heat assumption within the simulation program in order to propose a small-scale adsorption column for single household usage. The feasibility of adsorption column application in conventional water treatment plant was evaluated.

2. Materials and methods

All the data of current research were obtained by carrying out the dynamic simulation of phenol adsorption by using both Aspen Properties V7.1 and Aspen Adsorption V7.1 simulation program (Aspen One, 2009). Besides that, optimization program such as Design Expert V8.0.7.1 was needed in this study to determine the optimum value for the adsorbent particle diameter and column height for household adsorption column for phenol removal (Bono et al., 2008). Meanwhile, the experimental data that was used as reference to feed into the simulation program interface was obtained from the literature (Alhamed (2009)) on adsorption kinetics and performance of packed bed adsorber for phenol removal using activated carbon from dates' stones.

2.1. Research chronology

The chronology of current research project can be summarized in a single flow chart as shown in Fig 1:

2.2. Theoretical assumptions of phenol adsorption simulation

The following statements show the summary of theoretical assumptions that were prepared for Aspen Adsorption V7.1 program for current dynamic simulation of phenol adsorption in activated carbon packed bed column:

(a) Discretization Method: Upwind Differencing Scheme 1
(b) Mass/momentum Balance: Convection with Estimated Dispersion
(c) Pressure Drop Assumption: None
(d) Velocity Assumption: None
(e) Kinetic Model: Linear Lumped Resistance
(f) Film Model: Fluid
(g) Isotherm: Freundlich
(h) Energy Balance: Isothermal

2.3. Mathematical model

Theoretical assumptions suitable to describe the phenol adsorption within the packed bed column are identified and

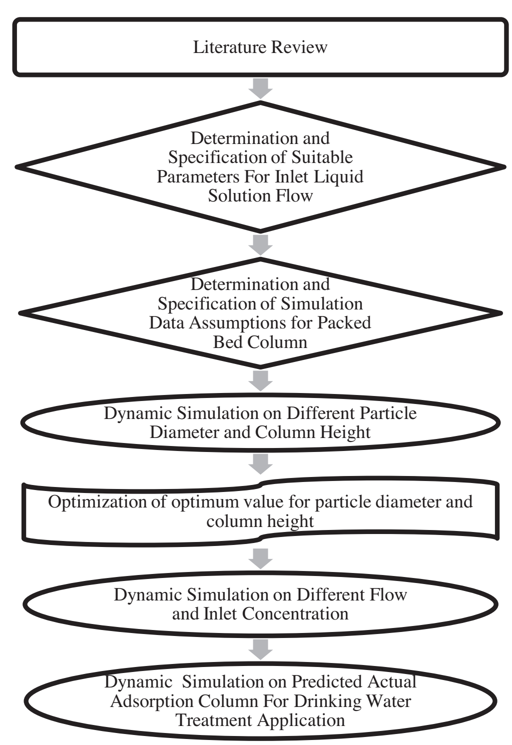

Figure 1 Chronology of dynamic simulation of phenol adsorption using aspen adsorption.

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determined before feeding the experimental parameters that are obtained from the research literature narrated by Alhamed (2009). After the suitable experimental parameters data and inlet feed water conditions are determined, these data are fed into the simulation program to begin the dynamic simulation of phenol adsorption. The relationship between the different adsorbent particle diameters and different column heights with the breakthrough time and saturation time of the activated carbon packed bed column was determined. Then, simulation data are done by manipulating adsorbent particle diameter and column height which are fed into the optimization program, Design Expert V8.0.7.1 to determine the optimum adsorbent particle diameter and column height that is able to obtain the highest C/Co ratio and longest breakthrough time and saturation time. Based on the result of optimization, the simple design of household adsorption column for phenol removal is determined.

The dynamic simulation of phenol adsorption is conducted by using different initial phenol concentrations and inlet flow rates in order to determine the feasibility of activated carbon packed bed adsorption column in conventional water treatment plant by using the highest column height, which is near to 20.0 m and optimum particle diameter that was determined from the optimization program. Eventually, dynamic simulation of phenol adsorption within packed bed column was done based on various column heights again for the purpose to identify the suitable column height that can be achieved with the saturation time of the adsorbent bed which is equivalent to 7 days.

2.4. Concentration of inlet liquid flow

Inlet concentration of phenol fed into packed bed column which was applied in most simulations was assumed at 2.0189 × 10–7 mol/l for current simulation (Crowl and Louvar, 2002). On the other hand, the effect of inlet phenol concentration on the total breakthrough time and total time needed for saturation of adsorbent (indicated the necessity to replace new set of activated carbon adsorbent) was also observed. The relationship between inlet concentration, breakthrough time and saturation time of packed bed was studied by varying the inlet liquid concentration to 2×10^{-5} mol/l, 2×10^{-6} mol/l, 2.0189×10^{-7} mol/l, 2×10^{-8} mol/l, and 2×10^{-9} mol/l. Meanwhile, the inlet liquid flow rate was varied from 24 m^3/year to 240,000 m^3/year to study the effect of flow rate on phenol adsorption within packed bed column.

2.5. Mass transfer coefficient

Alhamed (2009) reported that the experimental data with mass transfer coefficient of phenol in packed bed column varied with different activated carbon particle diameters and column heights. The equations that were related to these three parameters are given as:

$$\frac{C}{Co} = \exp\left[\frac{Pe}{2} - \sqrt{\frac{Pe^2}{4} + \frac{(1-\varepsilon)k_f a L^2}{\varepsilon D_L}}\right] \quad (1)$$

$$A = \frac{6(1-\varepsilon)}{d_p} \quad (2)$$

$$Pe = \frac{vL}{D_L} \quad (3)$$

Thus, Eqs. (1)–(3) can be used to calculate the mass transfer coefficient based on the particle diameter and assumed column height of the packed bed column. Table 1 shows experimental and calculated data obtained from the literature by Alhamed (2009).

The calculated values of mass transfer coefficient for different adsorbent particle diameters and column heights are summarized in Table 2.

The effect of different particle diameters and column heights on the breakthrough curve of the phenol adsorption in activated carbon packed bed column was also simulated by using Aspen Adsorption simulation program. Based on the simulation result, a simple central composite optimization by using Design-Expert V8.0.7.1 optimization program with two manipulated variables particle diameter and column height and with two output responses total saturation time (seconds) and ratio of C/Co was obtained from Aspen Adsorption simulation.

2.6. Properties of packed bed column

Table 3 shows the properties of activated carbon produced from dates' stones which referred to the experimental data obtained from Alhamed (2009). This was the source for the input for some of the parameters that were fed into the simulation program as to characterize the packed-bed column that is used in the current simulation.

2.7. Optimization of small scale adsorption column

In this study, the method that was chosen to conduct optimization was the center point surface response analysis to optimize the optimum value for particle diameter and column height suitable as household small scale adsorption column to treat contaminated drinkable water. Table 4 shows the experimental configuration for simulation to be conducted to obtain a perfect optimization for the current research study.

3. Results and discussion

3.1. Simulation data in different types of activated carbon packed bed column

Table 5 shows the summary simulation result that was conducted based on different particle diameters and column heights with inlet liquid condition fixed at $T = 30\,°C$, $P = 1.0$ atm, inlet flow rate of 240 m^3/year and initial phenol concentration of 2.0189×10^{-7} mol/l. Fig. 2 shows comparison of breakthrough curves for various particle diameters with 1.0 m (a), 1.5 m (b), and 2.0 m (c). Meanwhile, Fig. 3 shows comparison of breakthrough curves for various heights with 0.45 mm (a), 0.80 mm (b) and 1.50 mm (c).

As the column height and particle diameters of activated carbon increased, it will prolong the breakthrough time and saturation time of the activated carbon packed bed column. Thus, the result shows that the breakthrough time and saturation time of the adsorbent packed bed are greatly affected by column height, but not really significant for particle diameter

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Table 1 Experimental and calculated data for mass transfer area per unit bed volume (a), estimated dispersion coefficient (D_L) and Peclet number (Pe) adapted from research literature (With permission, Alhamed, 2009).

Particle diameter, d_p (mm)	a (m^{-1})	Estimated dispersion coefficient, D_L (m^2/min)	Peclet number, Pe
0.45	7640.0	0.0171	6.309
0.80	4297.5	0.1214	0.888
1.50	2292.0	1.9867	0.026

Table 2 Values of mass transfer coefficient based on different particle diameters and column heights.

D_p (mm)	Height (m)	K_f value (m/min)	K_f value (1/min)
1.50	2.0	5.85088×10^{-8}	2.92544×10^{-8}
1.50	1.5	1.04016×10^{-7}	6.93437×10^{-8}
1.50	1.0	2.34035×10^{-7}	2.34035×10^{-7}
0.80	2.0	4.75004×10^{-8}	2.37502×10^{-8}
0.80	1.5	8.44452×10^{-8}	5.62968×10^{-8}
0.80	1.0	1.90002×10^{-7}	1.90002×10^{-7}
0.45	2.0	2.64819×10^{-8}	1.32409×10^{-8}
0.45	1.5	4.70789×10^{-8}	3.13859×10^{-8}
0.45	1.0	1.05927×10^{-7}	1.05927×10^{-7}

Table 3 Properties of activated carbon produced from dates' stones.

Characteristic	Value	Units
Bulk density	0.74	g/cm^3
Total pore volume	0.456	cm^3/g
Micropore volume	0.355	cm^3/g
Bed porosity	0.427	Dimensionless
Average diameter	1.29	Nm
BET surface area	951	m^2 g
Freundlich equation parameters	$k = 24.6$	(mg/g) $(l/mg)^{1/n}$
	$n = 2.74$	

Table 4 Proposed simulation experiment configuration for optimization of particle diameter and column height of activated carbon packed bed column.

Run	Particle diameter (mm)	Column height (m)
1	0.80	1.50
2	0.45	2.00
3	1.50	2.00
4	0.80	1.50
5	0.45	1.00
6	0.45	1.50
7	1.50	1.50
8	0.80	1.50
9	0.80	1.50
10	0.80	1.00
11	0.80	1.50
12	0.80	2.00
13	1.50	1.00

of adsorbent as referred to the simulation data shown in Table 5.

Fig 3(a–c) shows the trend of simulation result for three different particle sizes of activated carbon derived from dates' stone with the column height varied from 1.0 m to 2.0 m. Fig. 3(a–c) also shows that column height has the effect on the breakthrough time and saturation time of the activated carbon packed bed column significantly as the whole breakthrough of phenol adsorption could shift to right as the column height is increased and vice versa. For example, the saturation time for activated carbon with same particle diameter of 1.5 mm is 252,000 s at column height of 2.0 m while the saturation time is 208,800 s when column height is 1.0 m. In the nutshell, as the column height is increased, it will also prolong the breakthrough time and saturation time of the activated carbon packed bed column significantly.

3.2. Optimization of small scale adsorption column

The ideal solution that was obtained in the current simulation and predicted response of the saturation time and C/Co ratio is shown in Table 6.

Table 7 shows the detailed data and simulation configuration that were implemented to conduct a simple optimization in order to identify the optimum particle diameter and column height and to obtain the optimum saturation time period for current proposed potable adsorption column to treat drinking water contaminated with 2.0189×10^{-7} mol/l of phenol.

The result of current optimization is shown in Fig. 4 based on the criteria set as maximum particle diameter, minimum column height, maximum saturation time and maximum C/Co ratio (ratio of outlet over inlet phenol concentration).

On the other hand, the mathematical model that can be synthesized based on the simulation data is shown in Table 5 from the phenol adsorption within the different particle sizes and various column heights by using Design Expert V8.0.7.1 optimization program. The breakthrough time dependence on the particle diameter and height of column is:

$$\text{Breakthrough time} = -14,387.15 + 4915.98 * d_p + 38,480.00 * h \quad (4)$$

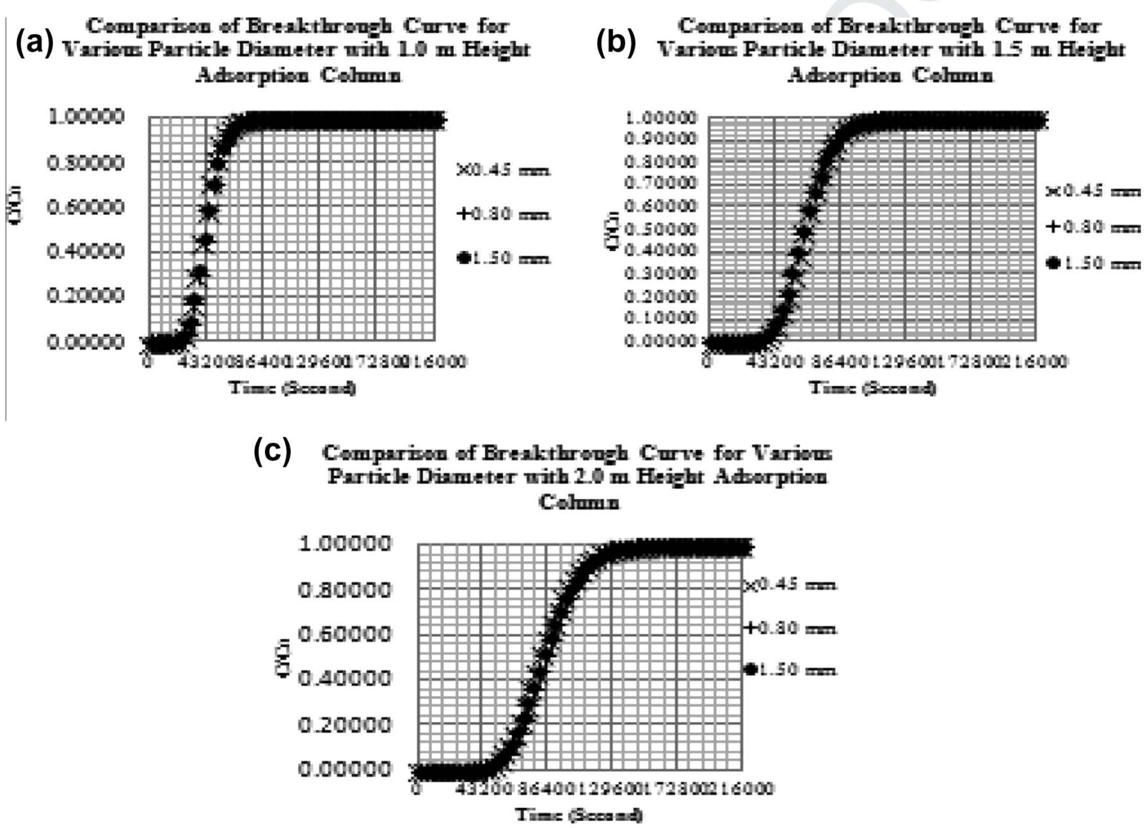
Eq. (4) is a linear equation that was synthesized based on the simulated data obtained in Table 5 to describe the relationship between breakthrough time of the phenol adsorption, activated carbon particle diameter and column height within the activated carbon column.

3.3. Application of simulation results of phenol adsorption

Table 8 and Fig. 5 show the simulation results to compare the adsorption column performance with different column heights. From the simulation data, it can be observed that if adsorption column height is increased to a value of 10.0 m, a more feasible adsorption column is created.

Table 5 Summary of simulation result of phenol adsorption in different types of activated carbon packed bed column.

Particle diameter (mm)	Column height (m)	Breakthrough time (s)	Breakthrough C/Co ratio	Saturation time (s)	Saturation C/Co ratio
0.45	1.00	14,400	0.00008	104,400	0.99990
	1.50	18,000	0.00001	158,400	0.99996
	2.00	25,200	0.00001	208,800	0.99998
0.80	1.00	14,400	0.00010	158,400	0.99983
	1.50	18,000	0.00001	154,800	0.99992
	2.00	25,200	0.00001	208,800	0.99996
1.50	1.00	14,400	0.00015	111,600	0.99978
	1.50	18,000	0.00001	158,400	0.99990
	2.00	25,200	0.00001	216,000	0.99995



Q9 **Figure 2** Breakthrough curves for adsorption of phenol for various activated carbon particle diameters of activated carbon filled in 1.0 m (a), 1.5 m (b), 2.0 m (c) adsorption column.

Q8 If the user interested to build current proposed adsorption column, instead of building a 10.0 m column height, it can be changed into two adsorption columns that are connected in series configuration, with the column height equivalent to 2.0 m with the column diameter of 1.0 m as shown in Table 8. This simulation is based on the mass transfer coefficient which is calculated for packed bed column height of 2.0 m filled with activated carbon derived from dates' stones with the particle diameter of 1.50 mm. In this series configuration, a dual-directional valve has to be set up in the inlet pipeline of the feed water stream so that the user just needs to interchange the direction of the inlet feed water either to first adsorption column or second adsorption column after 49 h or 2 days usage.

3.4. Simulation result of phenol adsorption for various inlet liquid conditions

Figs. 6 and 7 show the effect of inlet liquid conditions on the breakthrough time and saturation time of the packed bed adsorption column. Fig. 6 shows simulation results for

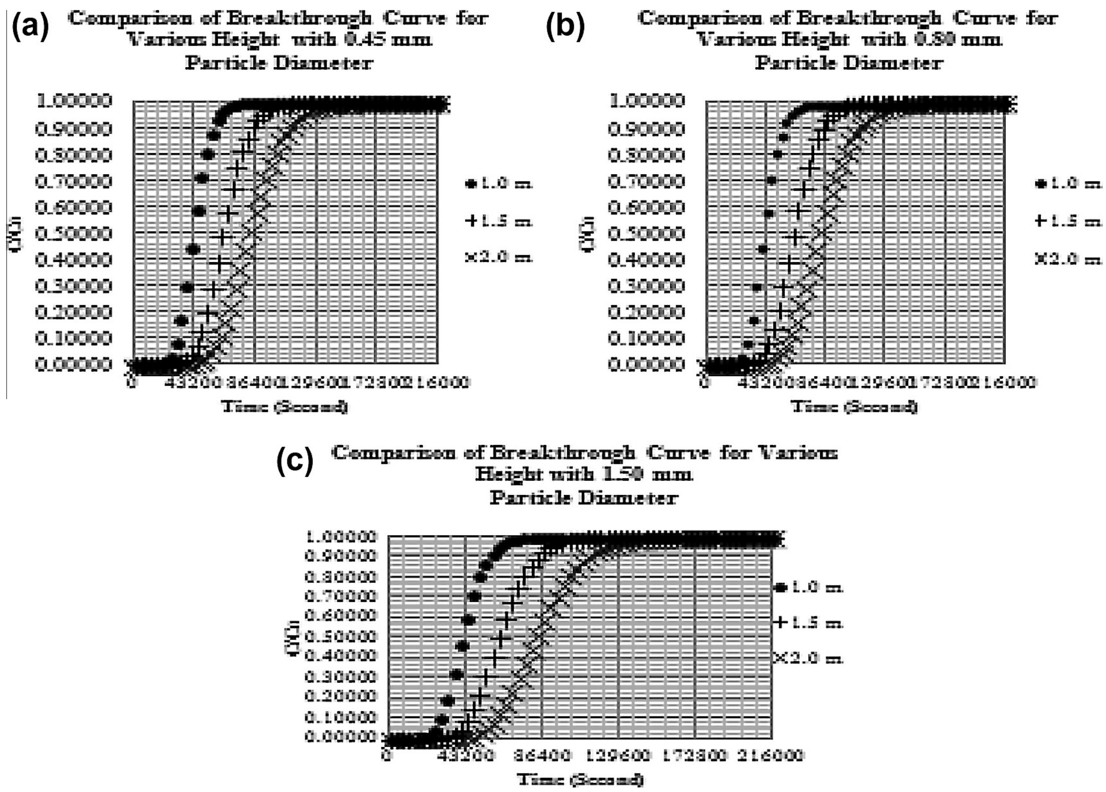


Figure 3 Breakthrough curves for adsorption of phenol for various column heights of activated carbon filled with 0.45 (a), 0.80 mm (b), 1.50 mm (c) diameter of activated carbon particle.

Table 6 Optimum parameters of small scale adsorption column.

Parameter	Optimum value
Column height	1.6 m
Particle diameter	1.50 mm
Saturation time	176,451 s
C/Co ratio	0.999911
Desirability	0.643

different inlet liquid flow rates of activated carbon packed bed column with a height of 19.2 m. It shows that when the inlet liquid flow rate is increased by 10 times from one parameter to another, it does affect the breakthrough time and saturation time of adsorption column.

Based on the simulation data as shown in Table 9, it can be observed that it was not feasible for current small scale potable adsorption column to be used in conventional water treatment plant to treat the contaminated water with the initial phenol concentration of 2.0189×10^{-7} mol/l as the inlet flow rate is increased up to 240,000 m^3/year. The saturation time of current

Table 7 Simulation data implemented for determining optimum values for particle diameter and column height optimization of small scale adsorption column.

Run	Particle diameter (mm)	Column height (m)	Absorbent saturation time (s)	C/Co
1	0.80	1.50	163,560	0.999921
2	0.45	2.00	206,760	0.999975
3	1.50	2.00	215,520	0.999946
4	0.80	1.50	163,560	0.999921
5	0.45	1.00	106,860	0.999901
6	0.45	1.50	156,240	0.999955
7	1.50	1.50	163,020	0.999901
8	0.80	1.50	163,560	0.999921
9	0.80	1.50	163,560	0.999921
10	0.80	1.00	158,340	0.999827
11	0.80	1.50	163,560	0.999921
12	0.80	2.00	208,620	0.999955
13	1.50	1.00	115,740	0.999782

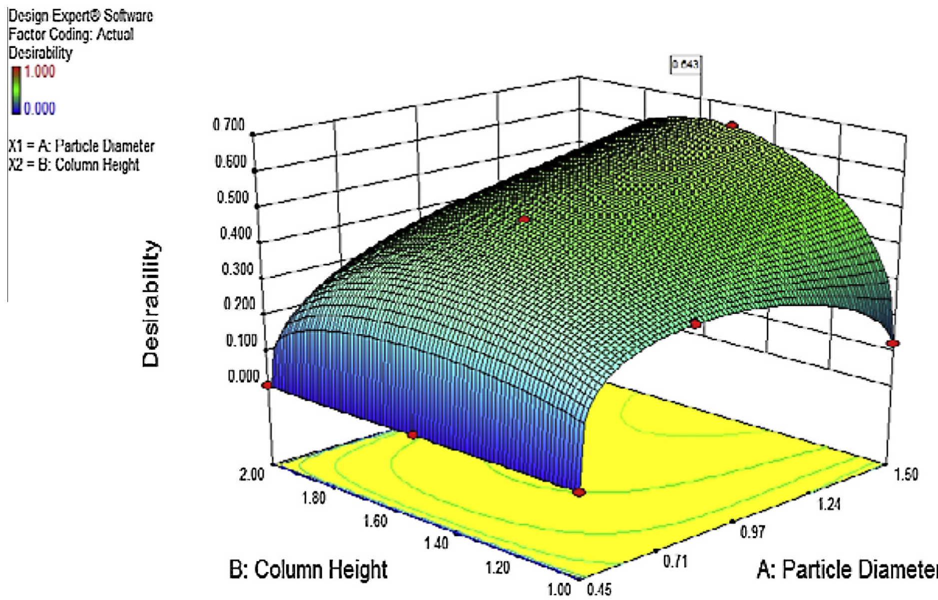


Figure 4 Desirability graph of optimization done by using Design-Expert V8.0.7.1 program for determination of optimum value for particle diameter and column height.

Table 8 Summary of simulation result of phenol adsorption in different heights of activated carbon packed bed column for real life application.

Column height (m)	Breakthrough time (s)	Breakthrough C/Co ratio	C/Co Ratio after 1 week
6.4	79,200	0.00001	0.96625
10.0	126,000	0.00001	0.96296
12.8	154,800	0.00001	0.72901
15.0	180,000	0.00001	0.46641
19.2	234,000	0.00001	0.13573

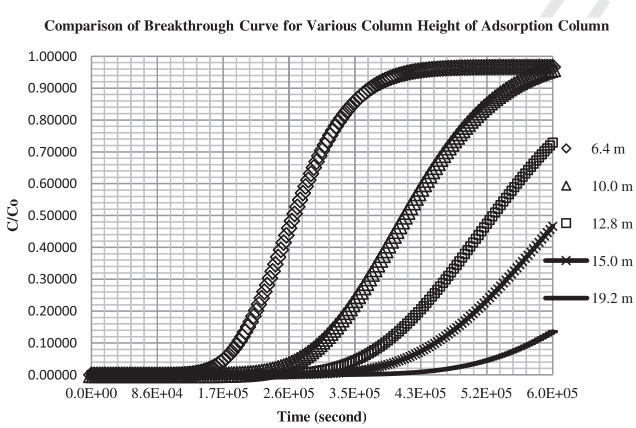


Figure 5 Breakthrough curves for adsorption of phenol for various proposed column heights for real life application in water treatment plant.

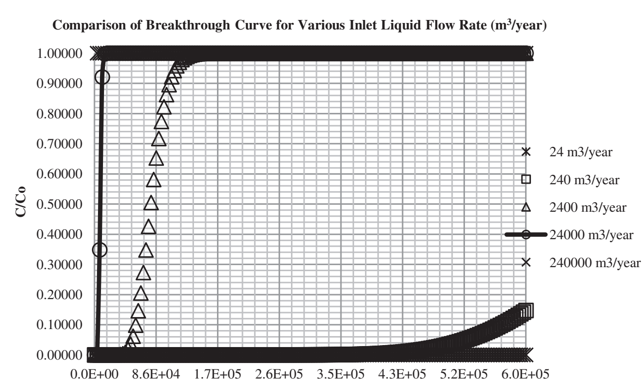


Figure 6 Breakthrough curves for adsorption of phenol for various inlet liquid flow rates within 19.2 m height of activated carbon packed bed column with fixed initial phenol concentration of 2.0189×10^{-7} mol/l.

proposed activated carbon adsorption column is less than or equivalent to 1 h. Thus, this level of saturation time period has proven that it was not feasible for its application in conventional water treatment plant.

In this study the results show that due to the technical assumptions that are made, there was no relationship between initial phenol concentration with breakthrough time and saturation time of the proposed packed bed column. Fig. 7 shows that all the simulation data overlapped one and other. It indicates that there is no relationship between initial phenol concentration with breakthrough time or saturation time.

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Table 9 Summary of simulation results of phenol adsorption in different inlet liquid flow rates.

Inlet liquid flow rate (m3/year)	Breakthrough time (s)	Breakthrough *C*/*C*o ratio	Saturation time (s)	Saturation *C*/*C*o ratio
24	0	0.00000	N/A*	N/A*
240	230,400	0.00001	N/A*	N/A*
2400	25,200	0.00002	198,000	0.99995
24,000	3600	0.00146	21,600	1.00000
240,000	N/A*	N/A*	3600	1.00000

Note: N/A*, not determined.

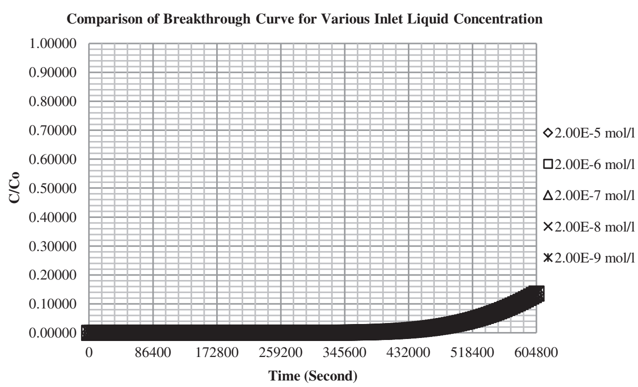

Figure 7 Breakthrough curves for adsorption of phenol for various initial phenol concentrations within 19.2 m height of activated carbon packed bed column with fixed flow rate of 240 m^3/year.

However, this is not the actual phenomenon as reported Alhamed (2009). Another possibility is that the assumption of linear lumped resistance in the kinetic model does not fully characterize the whole mechanism of adsorption of phenol onto the activated carbon particles.

4. Conclusion

Based on the dynamic simulation results on adsorption of phenol within the packed bed column filled with activated carbon derived from dates' stones, a small-scale adsorption column, which is suitable to remove phenol from contaminated drinking water for single household usage was proposed. Based on the optimized simulation results, the ideal proposed small scale adsorption column suitable for a single household to treat drinking water which is contaminated with 2.0189×10^{-7} mol/l phenol concentration on annual usage should have a column diameter, column height, and activated carbon particle diameter magnitudes 1.0 m, 10.0 m and 1.5 mm, respectively with 240 m^3/year inlet feed liquid flow rate. This column is able to feed the packed bed column so that the user just needs to replace the whole packed bed column once a week as the activated carbon bed could be saturated up to 0.96296 level of *C*/*C*o ratio. However, instead of building a 10.0 m height of column, the design can be changed into two adsorption columns that can be connected in series, with each column height of 2.0 m and with the column diameter of 1.0 m and the particle diameter is equivalent to 1.50 mm filled with activated carbon derived from dates' stones.

On the other hand, based on the simulation data, as the inlet flow rate of the feed water increased, the breakthrough time and saturation time of the activated carbon packed bed column become shorten because the adsorbent bed will be saturated with phenol faster than it is in low inlet feed water flow rate. In the nutshell, the simulation data shows that activated carbon packed bed column is only feasible to use for single household water treatment application.

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