

## Short Original Communications

# Kinetics of Benzene Adsorption onto Activated Carbon

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**Abstract.** An activated carbon bed adsorption process is influenced by the adsorbents' characteristics, volatile organic compound (VOC) characteristics, and process conditions. In the literatures, the adsorption processes of the adsorbents and VOCs were usually considered to be in equilibrium. In this study, the VOC adsorption processes by activated carbon were considered to be a kinetic process, i.e. they are not in equilibrium. Then, isothermal adsorption curves and a small column experiment were simulated.

**Keywords:** Activated carbon; adsorption; benzene; desorption; kinetics

## Introduction

Activated carbon (AC) has been used extensively by industries as an adsorbate for the removal of hazardous air pollutants among other applications. Major parameters that may affect the adsorption process include the surface property of the AC, characteristics and concentration of VOC, and temperature. As far as the modeling of adsorption isotherm is concerned, three types of model can be recognized: the kinetic model, i.e. the Langmuir model [1], the thermodynamic model, i.e. the Gibbs adsorption isotherm equation [2], and the statistical thermodynamic model, i.e. the Dubinin equation [3]. In the AC bed adsorption study, the usual models involve an isothermal plug-flow trace-component system with a linear equilibrium isotherm equation [4,5], a homogeneous surface diffusion model (HSDM) [6], and an ideal adsorbed solution theory (IAST) [7]. They consider adsorption to be an irreversible reaction or each solute to be in equilibrium.

In the actual adsorption process, the adsorption is not at an equilibrium condition and both adsorption and desorption processes occur at the same time. The objective of this investigation is intended to develop a thermodynamic model with a non-linear driving force in conjunction with the Langmuir model for predicting the effect of temperature and gaseous concentration on activated carbon adsorption.

## 1 Model Development

### 1.1 Kinetic adsorption/desorption model

In 1916, Langmuir [1] developed an isotherm equation, according to the Langmuir hypothesis and considering the following adsorption/desorption reaction condition of VOC

(C<sub>6</sub>H<sub>6</sub>) on AC. Initially, time = 0, the adsorption ratio on AC is 0; after reaction time t, the adsorption ratio is X; finally, the equilibrium adsorption ratio is X<sub>e</sub>, and the VOC concentration is always maintained at C.

From the adsorption reaction rate and desorption reaction rate equilibrium, it can thus be integrated to

$$k_a \times C \times t = X_e \times \ln [X_e / (X_e - X)] \quad (1)$$

$$(k_a \times C + k_d) \times t = \ln [X_e / (X_e - X)] \quad (2)$$

Subsequently, the k<sub>a</sub>, k<sub>d</sub>, and K can be solved, where K is the reaction constant equal to k<sub>a</sub>/k<sub>d</sub>.

### 1.2 Activated carbon bed adsorption simulation

Based on the above hypothesis, the physicochemical parameters including k<sub>a</sub>, k<sub>d</sub>, and K, determined from the kinetic adsorption/desorption studies, can be used for the AC bed adsorption process. Assuming the adsorption process is a series of continuous-flow stirred tank reactors (CFSTRs), it can be simulated by the numerical method as:

$$\Delta X_{s,t,i} / \Delta t = k_a \times (1 - X_{s,t,i}) \times C_{g,t,i} - k_d \times X_{s,t,i} \quad (3)$$

$$\Delta C_{g,t,i} / \Delta t = (\Delta X_{s,t,i} / \Delta t \times q_0 \times M/n) / [(L \times A - M/d)/n] \quad (4)$$

where X<sub>s,t,i</sub> is the adsorption ratio on AC in the i-th unit CSTR at time, t, in the solid phase, q<sub>0</sub> is the unit-layer adsorption weight per AC, M is the weight of AC, L is the length of the column, A is the cross-sectional area, and d is the density of AC.

## 2 Experimental Method

### 2.1 Kinetic adsorption/desorption studies

In each reaction, about 25 to 40 mg of treated AC was measured and placed in a small scale that was 0.8 cm in diameter. Then, the scale was placed in a reaction chamber and the treated benzene vapor, which was controlled at the same temperature and concentration, passed through the reaction chamber. The measured weight change every 10 seconds was collected by a personal computer.

### 2.2 Activated carbon bed tests

A small column about 6 cm in length and 1 cm in diameter was used in this test. The reaction temperature was controlled by a thermostat at 303°K, the weight of packed AC

**Table 1:** Adsorption conditions and results of kinetic tests performed at different temperatures

Parameter	Unit	Run 1	Run 2	Run 3	Run 4	Run 5
Temperature, T	K	283	303	323	343	363
Concentration, C	mole/L	7.11E-05	1.01E-04	6.94E-05	7.21E-05	6.58E-05
Weight of AC, M	mg	32.60	35.01	35.97	36.45	36.17
Equilibrium adsorption weight, $W_e$	mg	19.7	19.8	10.0	8.2	5.3
Ideal adsorption weight, $W_o$	mg	21.7	23.3	23.9	24.2	24.1
Adsorption capacity, $X_e$	%	91.0	85.0	42.0	34.0	22.2
Slope of model <sup>a</sup>	-	0.0056	0.0100	0.0160	0.0237	0.0413
R	-	0.99	0.99	0.98	0.99	0.95
Adsorption rate constant, $k_a$	Lmin <sup>-1</sup> mole <sup>-1</sup>	71.5	83.7	96.8	111.7	139.4
Desorption rate constant, $k_d$	min <sup>-1</sup>	5.03E-04	1.50E-03	9.28E-03	1.56E-02	3.21E-02
Equilibrium constant, K	Lmole <sup>-1</sup>	142100	55900	10400	7100	4300
Arrhenius equation <sup>b</sup>		$\ln(k_a) = -740/T + 6.87, R^2 = 0.98$				
		$\ln(k_d) = -4894/T + 9.84, R^2 = 0.96$				

a: Model:  $\ln [X_e/(X_e - X)] = k_a \times C \times t / X_e = (k_a \times C + k_d) \times t = \text{slope} \times t$

b:  $\ln(k) = \ln(A) - E/RT$

was about 2,500 mg, and the outflow gas concentration was measured every 15 min by GC-FID.

### 3 Results and Discussion

#### 3.1 Determinations of adsorption reaction rate ( $k_a$ ) and Desorption reaction rate ( $k_d$ )

Table 1 shows the adsorption conditions and calculated parameters of  $C_6H_6$  by AC at different temperatures in the kinetic adsorption/desorption studies. It illustrates when the temperature rose from 283°K to 363°K and the benzene concentrations were almost the same,  $X_e$  declined from 91% to 22%, indicating that adsorption was influenced by temperature, and when the temperature increases,  $k_a$  and  $k_d$  also increase, but the reaction equilibrium constant (K) decreases. Based on Arrhenius' equation, physicochemical parameters can be calculated. Since, the slope of  $\ln(k_a)$  is -740, the adsorption activated energy,  $E_a$ , is equal to 1470 cal mole<sup>-1</sup>. A similar observation shows that the desorption activated energy,  $E_d$ , is 9725 cal mole<sup>-1</sup>. Therefore, the heat of adsorption of  $C_6H_6$  can be determined as  $\Delta H = E_a - E_d$ , i.e., -8255 cal mole<sup>-1</sup>.

#### 3.2 Influence of physicochemical parameters

In this study, we can obtain the physicochemical parameters ( $E_a$ ,  $E_d$ ,  $A_a$ ,  $A_d$ , and K) of  $C_6H_6$  adsorption on AC from kinetic adsorption/desorption studies, and these parameters can be used to predict the results under different conditions. Fig. 1 presents the effect of the temperature on adsorption isotherm, and that has about 5–10% error between predict data and experimental data in this study. The above simulations and kinetic parameters indicate that the adsorption efficiency has a high relationship with temperature. With increasing temperature, the adsorption rate and desorption rate rise, but the adsorption weight decreases. At high benzene concentrations, the temperature effect is not significant

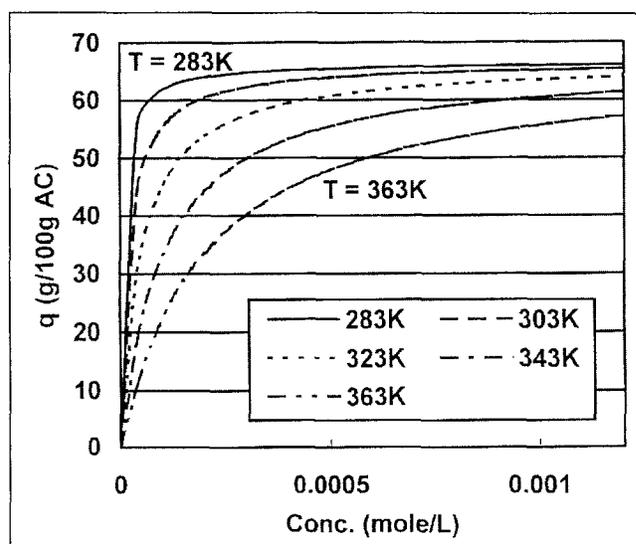


Fig. 1: Effect of temperature on the adsorption isotherm curve

for the equilibrium adsorption weight. That is, during treatment of high benzene concentrations, raising the reaction temperature can increase the reaction rate and reduce the treatment time. On the other hand, if the benzene concentration is low, raising the reaction temperature will decrease the efficiency of AC adsorption.

#### 3.3 Simulation of adsorption breakthrough curve

Fig. 2 illustrates the simulation results of a breakthrough curve of the AC bed adsorption process. The results show that the adsorption process can be simulated. The simulation breakthrough curve did not fit very well with experimental data, and may be caused by the simulation parameters ( $k_a$ ,  $k_d$ ,  $A_a$ , and  $A_d$ ) error between kinetic study and real column reaction. That is, because all of the simulation

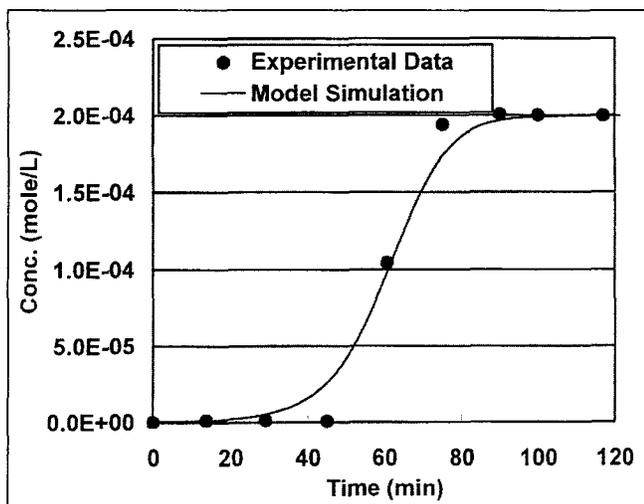


Fig. 2: Result of breakthrough curve of experimental data and model simulation

parameters were derived from the kinetic adsorption/desorption studies, there may be other reasons that were not completely considered in this model, but it could be a preliminary predictor of AC bed adsorption.

#### 4 Conclusion

An AC bed adsorption process is influenced by the surface characteristics of adsorbent, characteristics and concentration of VOC, humidity and flow rate. Temperature is a very important parameter. In this study, a new adsorption/desorption model is developed, it can be used to simulation the

adsorption isotherm and the column adsorption process, and model simulation shows that a high reaction temperature will cause both the adsorption reaction rate and desorption reaction rate to rise, and the adsorption efficiency to decrease. But at high VOC concentrations, a high temperature effect of adsorption efficiency is evidently less.

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