

# Determination of gas phase adsorption isotherms—a simple constant volume method

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## Abstract

Single and ternary solute gas phase adsorption isotherms were conducted in this study to evaluate the effectiveness of a simple constant volume method, which was utilized by using Tedlar gas sampling bags as a constant volume batch reactor. For this purpose, gas phase adsorption of toluene, methyl ethyl ketone (MEK), and methyl isobutyl ketone (MIBK) on two types of activated carbons, BPL—bituminous base and OVC—coconut base, were investigated. For the single solute adsorption, the experimental adsorption data were found to be well correlated with Freundlich and Myers adsorption equations. The pore size distribution of adsorbents was found to affect their adsorption capacities; its effect was dependant on the solute concentration. The ternary adsorption experimental isotherms were accurately predicted by using the well-known model, i.e., ideal adsorbed solution theory (IAST).

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*Keywords:* Gas adsorption isotherm; Granular activated carbon; Volatile organic compounds; Constant volume; Ideal adsorbed solution theory (IAST); Pore size distribution

## 1. Introduction

Adsorbents have been widely used for removing organic contaminants from the environment—air, water, and wastewater (Chiang et al., 2001; Monneyron et al., 2003; Lordgooei and Kim, 2004). Activated carbon has long been recognized as one of the most versatile adsorbents due to its high porosity and the resulting high surface area (Prakash et al., 1994; Yang, 2003). The performance of the adsorption process is strongly affected by both the adsorbent and adsorbate characteristics. Fundamental studies of adsorption have long been the objectives of many researchers (Prakash et al., 1994; Chiang et al., 2001; Yang, 2003; Lordgooei and Kim, 2004).

The design and efficient operation of an adsorption process require beforehand the adsorption capacity, which is

often obtained from experimental isotherm data (Nirmalakhandan and Speece, 1993; Chiang et al., 2001; Allen et al., 2004). Experimental methods for obtaining the gas phase equilibrium isotherm data can be divided into three categories: dynamic adsorption column method (Lin et al., 1996); gravimetric method (Cal et al., 1997; Paulsen and Cannon, 1999; Ramirez et al., 2004); and constant volume method (Golden and Sircar, 1994; Brosillon et al., 2001; Monneyron et al., 2003). By using the dynamic adsorption column, one can obtain adsorption equilibrium derived fundamentally from mass balances around the adsorption bed. However, its prediction is complicated because kinetics concepts (e.g., film diffusion, surface diffusion, and pore diffusion) should be also incorporated into the mass balances (Sontheimer et al., 1988). In an adsorption fixed column test, Lin et al. (1996) predicted adsorption isotherms from kinetic adsorption/desorption experiments. They then compared the adsorption isotherm predictions to experimental data based on a micro gravimetric balance and column experiments. Higher predictive

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errors (5% on average with a maximum of 13%) were obtained for adsorption capacity measured in the column experiments while excellent agreement (less than 4%) was obtained from the gravimetric method. It is worthwhile noting that the gravimetric method using an electrobalance is typically designed only for single solute adsorption. Given the above limitation, further measurements are required for multi-component adsorption. Cal et al. (1997) tested mixture–component adsorption by using the gravimetric balance to measure the total mass adsorbed and a multi-ported hang-down tube for gas sampling at the inlet and the outlet. One expects relatively accurate adsorption isotherm data by the gravimetric method. However, this method requires complicated experimental equipment which is rather expensive. The third adsorption isotherm determination is the constant volume method. This method is commonly used for obtaining adsorption isotherms for single solute and multi-component solute (Monneyron et al., 2003). A batch reactor is employed and calculations procedures are relatively simple.

The adsorption isotherm approach presented in this paper is a simple constant volume method utilized by using Tedlar gas sampling bags as a constant volume batch reactor. Gas phase adsorption isotherms for both the single solute and multi-component solute were used to evaluate the effectiveness of the current adsorption isotherm approach. For this purpose, two different activated carbons, i.e., bituminous based BPL and coconut based OVC, were tested for three single solutes, namely, toluene, methyl ethyl ketone (MEK), and methyl isobutyl ketone (MIBK) and their ternary mixture. The ternary adsorption experimental isotherm data were verified against the well-known model in predicting the multi-component adsorption, i.e., ideal adsorbed solution theory (IAST) that was originally developed by Myers and Prausnitz (1965). Furthermore, the pore size distribution of the adsorbents was evaluated to assess its effects on the adsorption capacities for the solutes of concern.

## 2. Materials and methods

### 2.1. Adsorbate

Three commercially available volatile organic compounds, toluene, MEK, and MIBK (Fisher Scientific, Fair Lawn, NJ) were used as single solutes and as three-component mixtures. These contaminants are common solvents employed in the industry. The properties of these adsorbates are summarized in Table 1.

### 2.2. Adsorbent

Two kinds of activated carbon, bituminous based BPL and coconut based OVC (Calgon Carbon Corporation, Pittsburgh, PA), were used for this study. These adsorbents will be referred to as BPL and OVC in this manuscript.

Table 1  
Adsorbates main characteristics (Poling et al., 2001)

	Toluene	MEK <sup>a</sup>	MIBK <sup>b</sup>
Formula	C <sub>7</sub> H <sub>8</sub>	C <sub>4</sub> H <sub>8</sub> O	C <sub>6</sub> H <sub>12</sub> O
Molecular weight (g mol <sup>-1</sup> )	92.14	72.11	100.16
Vapor molar volume (cm <sup>3</sup> mol <sup>-1</sup> )	316	267	340
Kinetic diameter (Å)	5.8	5.2	7.35
Vapor pressure (kPa)	3.79	12.6	2.0
Dipolar moment, 3.162 × 10 <sup>-25</sup> (J m <sup>3</sup> ) <sup>1/2</sup>	0.4	3.3	2.8

<sup>a</sup> Methyl ethyl ketone.

<sup>b</sup> Methyl isobutyl ketone.

Prior to use in the study, the adsorbents were dried in an oven at 110 °C for 2 days to remove any moisture present and then stored in a desiccator until use.

### 2.3. Isotherm procedure

The adsorption isotherms that relate the concentration of volatile organic compounds (VOCs) in the adsorbed state versus its gas phase concentrations were determined by using the constant volume method. Each isotherm point was obtained by using a “Gas Sampling Bag”, which is a 10 l Tedlar gas sample bag (SKC inc., Eighty Four, PA). Each bag has two ports. One is used for pumping air/gas and the other port, which has a threaded cap with septa, is used to insert the adsorbent and later for sampling purposes. Different masses of the adsorbents were carefully weighed to the nearest 0.1 mg and placed inside each bag through the port provided. Masses of the adsorbents ranged from 4 to 50 mg per bag for the single-solute isotherms and the ternary systems. Each bag was then filled accurately with six liters of hydrocarbon-free and moisture-free compressed air by using a calibrated six-liter canister, which can withstand pressure up to 10 atm. At a pressure of one atmosphere, this canister contains an air volume of 6 l. When more air was allowed into the canister until a two atmospheres pressure was reached at the same temperature, the canister would hold an air volume of 12 l. The pressure inside the canister was recorded by a digital pressure gauge (Cole parmer, Vernon Hills, IL). When the outlet valve of the canister, which was connected to the exhaust port of the bag, was opened, it allowed the air to expand until a final pressure of 1 atmosphere was reached. Therefore, an air volume of 6 l was embodied in each isotherm bag. To obtain the desired initial concentration in the bag, a known volume of gaseous VOC was injected into the bag (through the septum) by using a gas-tight syringe (VICI Precision Sampling, Inc.) with a side-port needle, which lead to an initial concentration of 3.0–15.0 mmol m<sup>-3</sup> for each set of the single solute isotherm and 0.8–5.5 mmol m<sup>-3</sup> for the ternary adsorption. The quantity of VOC injected depended on the initial gas-phase concentration desired in the bag. The gaseous VOC was prepared by injecting pre-calculated volume of liquid VOC (0.3–1.5 ml) into a 6 l air inside another bag.

For each set of single solute isotherm, three different initial concentrations were considered in order to ensure true equilibration had been attained. For ternary adsorption, two different compositions of multi-component VOC were considered. One was defined from US Environmental Protection Agency (EPA) Toxic Release Inventories (TRIs) (1998–2001). The approximate molar ratio of the mixture was assumed to be 6:3:1 (toluene:MEK:MIBK). The other was equal-molar ratio of each component.

Each set of bags under study was accompanied by blank bags (without any adsorbent) that contained the same initial VOC concentration that was used in the isotherm bags. These procedural blanks served to quantify adsorption of VOC due to the bag alone. All of the bags were equilibrated in a room that has a constant temperature of  $20 \pm 1$  °C. After a 1-h equilibration period, the blank bags were sampled and analyzed. The measured values were recognized as the initial concentration for each set of bags. Through initial testing, it was found that 6 days were enough for attaining equilibrium. Gas samples were taken and analyzed to determine the equilibrium gas phase concentrations of VOCs on day 7. The bags were turned over every day to ensure proper contact of the adsorbent with the VOC. The percent loss of VOCs in the blank bags after an equilibration period of 6 days were  $23.1 \pm 1.6$ ,  $13.0 \pm 1.6$ , and  $8.4 \pm 1.8$  for toluene, MEK, and MIBK, respectively. In an evaluation test of Tedlar bags conducted by Wang et al. (1996), it was demonstrated that the losses of the VOCs were mostly due to sorption losses to the bag alone. Therefore, the obtained isotherm data were compensated for the loss of VOCs due to adsorption on the bags surface. In this study, the percentage VOC loss was independent on the initial concentration of VOC and the type of adsorbent.

#### 2.4. Analytical procedure

The determination of the adsorbate concentrations was made by a gas chromatograph (HP 5890, Series II, Hewlett–Packard, Palo Alto, CA) with a flame ionization detector (FID), and 30-m length, 0.25-mm I.D., 0.25- $\mu$ m Film thickness narrow bore column (DB 624, J&W Scientific, Folsom, CA). The GC oven temperature was programmed from 40 to 120 °C at rate of 10 °C  $\text{min}^{-1}$  with a 2-min hold at 40 °C and a 2-min hold at 120 °C. The carrier gas ( $\text{N}_2$ ) flow rate was set at 2.3  $\text{ml min}^{-1}$ . The FID detector was used with  $\text{N}_2$  make-up gas at a flow rate of 20  $\text{ml min}^{-1}$ , a fuel gas flow ( $\text{H}_2$ ) of 30  $\text{ml min}^{-1}$ , and an oxidizing gas flow (air) of 300  $\text{ml min}^{-1}$ . The detector temperature was 250 °C. Retention times of 1.8 min for MEK, 3.1 min for MIBK, 3.4 min for toluene were obtained under the conditions used.

Tristar 3000 (Micromeritics, Norcross, GA) was used to investigate the pore size distribution, using liquid nitrogen adsorption and desorption isotherms. The samples were purged with nitrogen gas for 2 h at 150 °C using Flow prep 060 (Micromeritics, Norcross, GA).

#### 2.5. Theoretical models

##### 2.5.1. Single solute adsorption isotherm

The Freundlich equation and Myers isotherm equation (Sorial et al., 1993) were used for correlating the experimental isotherm data. The Freundlich isotherm equation is represented by

$$q_{e,i} = k_i \cdot C_{e,i}^{1/n_i} \quad (1)$$

where,  $k_i$  and  $1/n_i$  are regression parameters;  $C_{e,i}$  is equilibrium adsorbate concentration in the gas phase;  $q_{e,i}$  is adsorbate concentration adsorbed on the adsorbent.

The gas phase concentration,  $C_{e,i}$ , was determined by gas chromatograph and the loading,  $q_{e,i}$ , was calculated from a mass balance on each isotherm bag by using the following equation:

$$q_{e,i} = \frac{(C_{0,i} - C_{e,i}) \cdot V}{m} \quad (2)$$

where,  $C_{0,i}$  is initial gas phase concentration of solute  $i$ ;  $m$  is the mass of adsorbent; The adsorbate volume represented by  $V$  is 6 l.

The drawback of using the Freundlich equation is that it does not follow Henry's law equation at low coverage. This criterion is very important when predicting the multi-component adsorption data by IAST because the model utilizes the Gibbs adsorption equation that requires isotherm data at low coverage.

The experimental adsorption isotherm data were plotted on logarithmic plots (see Fig. 1, e.g., MEK adsorption on OVC), the regressed adsorption isotherm was then developed and the experimental data were validated by using the 99% confidence interval (SigmaPlot 9.0, Systat Software, Inc., 2004). The validated isotherm data were also correlated by the Myers isotherm equation which is presented by

$$C_{e,i} = \frac{q_{e,i}}{H_i} \cdot \exp(K_i q_{e,i}^{P_i}) \quad (3)$$

where,  $H_i$ ,  $K_i$ , and  $P_i$  are regression parameters.

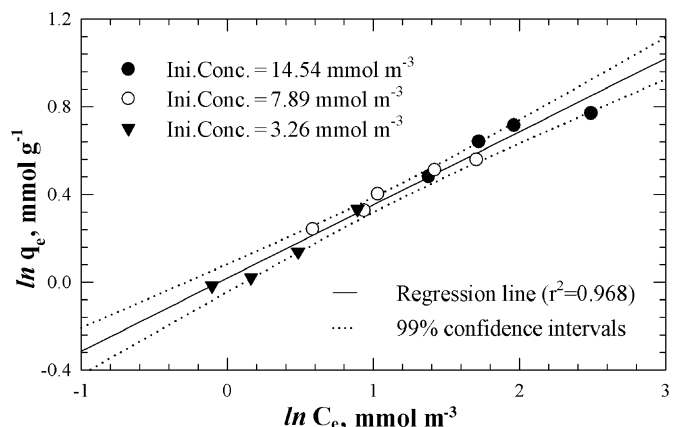


Fig. 1. MEK adsorption on OVC.

The Myers isotherm equation has the property of satisfying Henry's law at low concentration. Thus, it is more suitable for multi-component computations than the Freundlich-type isotherm equation. Details about Myers isotherm equation can be found elsewhere (Sorial et al., 1993; Lu and Sorial, 2004).

### 2.5.2. Ternary adsorption isotherm

If the adsorbed phase is thermodynamically ideal, the equilibrium relationship for an adsorbed mixture can be driven from the pure component isotherms. Based on this hypothesis, Myers and Prausnitz developed the IAST, to describe competitive adsorption for gas mixtures (Myers and Prausnitz, 1965). The IAST basically utilizes three equations. One is the Raoult's law equivalence equation for an adsorption system, the other is the Gibbs adsorption equation, and the third is based on the assumption of an ideal adsorbed solution. A detailed description of the IAST equations can be found elsewhere (Sorial et al., 1993; Lu and Sorial, 2004).

## 3. Results and discussion

### 3.1. Single solute isotherm

Single solute gas phase adsorption isotherms for toluene, MEK, and MIBK, on two adsorbents, i.e., BPL and OVC, were investigated at the room temperature ( $20 \pm 1$  °C). Three sets of different initial concentration for each isotherm were incorporated for checking the reliability of adsorption isotherm. Fig. 1 represents the single solute adsorption of MEK on OVC adsorbent. Analysis of the data in Fig. 1 reveals that the accuracy of adsorption isotherm was confirmed by using the three sets of initial concentration. The three sets of the experimental were within the 99% confidence interval of the linear regression performed in a log–log scale. Similar results were obtained for the other solutes studied on the two adsorbents (data are not shown). The R square values for the linear regression (logarithmic Freundlich equation) are presented in Table 2.

For all the compounds studied, the isotherm curves obtained on BPL and OVC were typically type 1 according

to International Union of Pure and Applied Chemistry (IUPAC) classification (1985). The single solute adsorption isotherms for the three adsorbates are given in Fig. 2 together with the correlated isotherm models, i.e., Freundlich isotherm and Myers isotherm. The correlation of the experimental data to the two isotherm equations was done by using non-linear least square regression algorithm for minimizing the total relative error (Ramirez et al., 2004). The total relative error is defined by

Total relative error (%)

$$= \frac{1}{N_I} \sum_{i=1}^{N_I} \left( \frac{1}{N_{T,i}} \sum_{j=1}^{N_{T,i}} \left[ \frac{|q_m - q_e|}{q_e} \times 100 \right] \right) \quad (4)$$

where  $q_m$  = modeled adsorbate concentration adsorbed on the adsorbent;  $q_e$  = experimental adsorbate concentration adsorbed on the adsorbent;  $N_T$  = number of data points;  $N_I$  = number of adsorption isotherms.

The obtained results for both isotherm equations are presented in Table 2. It is seen from Table 2 that the total relative error was less than 10% for all cases, implying good agreement between the model and the experimental data. The adsorption capacities of the two adsorbents increased with an increase in molecular weight, molar volume, and kinetic diameter of the adsorbates studied, but decreased with an increase in their vapor pressures (see Table 1).

Fig. 3 shows the ratio of the adsorption capacities of the two adsorbents, (BPL/OVC), for the three adsorbates. The adsorbents capacities were compared by using the Freundlich predicted adsorbed phase concentration,  $q_e$ . It is seen from Fig. 3 that as the equilibrium solute concentration was increased, BPL provided much higher adsorption capacity for MIBK, while it provided lower adsorption capacity for MEK. In case of toluene, BPL gave a slightly higher adsorption capacity. It is also interesting to observe that, at MIBK concentration of about  $0.1 \text{ mmol m}^{-3}$  or below, the adsorption capacity of OVC was higher than BPL.

The process of gas phase adsorption is influenced by both the adsorbate properties and the adsorbents properties. The pore size distribution of the adsorbent strongly affects adsorption (Chiang et al., 2001; Lu and Sorial,

Table 2  
Freundlich and Myers isotherm equations parameters for the single solute system

		Number of isotherm data	Freundlich isotherm				Myers isotherm			
			$K \text{ (mmol g}^{-1}) \cdot \text{(mmol m}^{-3})^{-n^{-1}}$	$n^{-1}$	$R^{2a}$	TRE <sup>b</sup> (%)	$H \text{ (m}^3 \text{ g}^{-1})$	$K \text{ (mmol g}^{-1})^{-p}$	$P$	TRE (%)
Toluene	BPL	11	1.742	0.314	0.976	3.7	$2.474 \times 10^5$	10.722	0.181	3.8
	OVC	11	1.542	0.272	0.961	2.8	$1.549 \times 10^4$	8.201	0.272	2.9
MEK	BPL	11	0.756	0.298	0.971	3.1	$6.737 \times 10^1$	5.149	0.441	3.4
	OVC	13	1.018	0.334	0.968	3.4	$4.483 \times 10^3$	8.379	0.219	3.3
MIBK	BPL	10	2.824	0.241	0.927	9.2	$5.839 \times 10^3$	5.248	0.356	9.4
	OVC	12	2.136	0.094	0.958	2.7	$2.583 \times 10^5$	6.504	0.775	2.8

BPL: bituminous base activated carbon; OVC: coconut base activated carbon.

<sup>a</sup> R-square value in the linear regression.

<sup>b</sup> Total relative error.

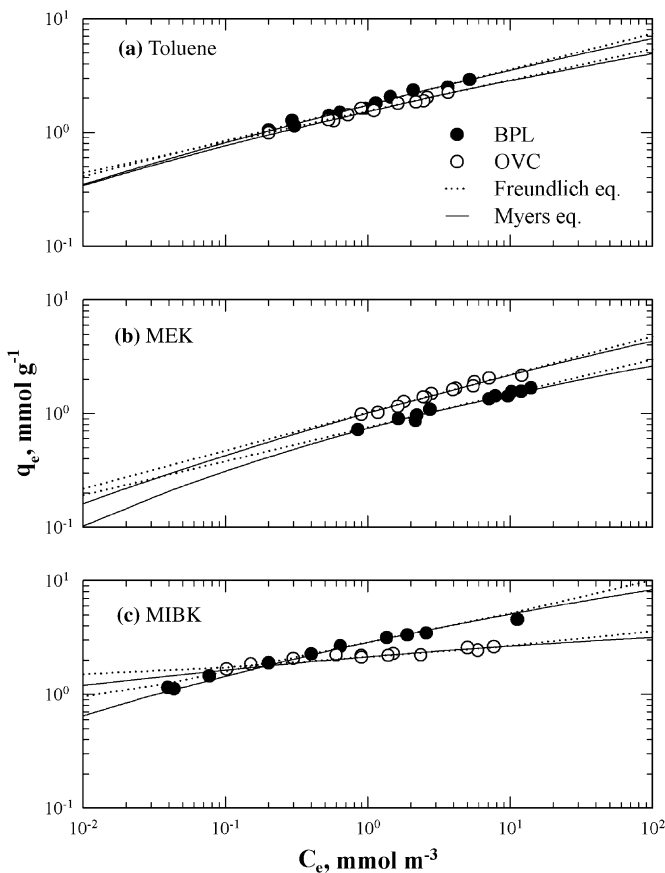


Fig. 2. Adsorption isotherms for the single solute system.

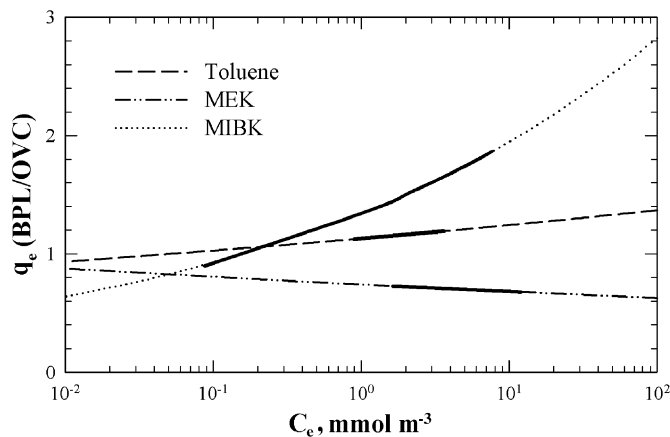


Fig. 3. Comparison of activated carbon adsorption capacities for the three VOCs (solid curves indicate the experimental observation for each solute).

2004). At high solute concentration, the activated carbon in which large pores predominate has higher capacity than those with predominant small pores. However, at low concentration, the large pore activated carbon has a lower capacity (Cheremisinoff and Ellerbusch, 1978). Fig. 4 clearly indicates that BPL has higher pore volume for the pore size diameters (2–200 nm) as compared to OVC. This property is in accordance with the experimental data for

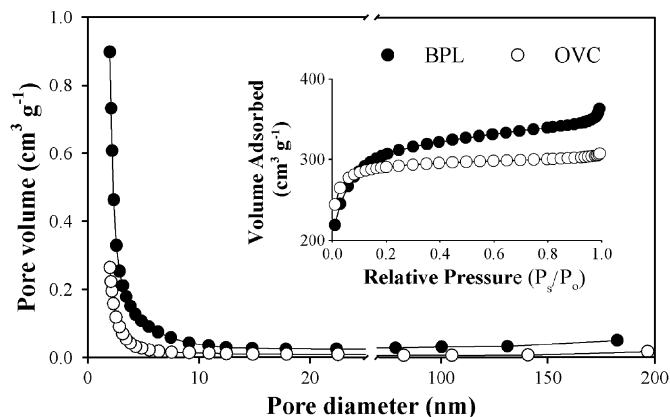


Fig. 4. Pore size distribution of BPL and OVC.

toluene and MIBK. However, this result contradicted the observation of MEK adsorption. It is speculated that the abnormal phenomenon was caused by a strong dipolar moment as compared to the other adsorbates. In physical adsorption, adsorption of gas molecules on activated carbon is also dominated by interaction potentials of adsorbate on the adsorbent surface: the van der Waals forces interaction; electrostatic interactions comprising polarization; dipole moment and quadrupole moment interaction (Ruthven, 1984). For a gas molecule that has strong dipole moment, the adsorption of this gas molecule increases because the field dipole interaction term becomes significant (Yang, 2003). This property could play a role in the adsorption potential of MEK within the smaller pore volume of OVC.

### 3.2. Ternary isotherm

In this study, since toluene was the major component among VOCs of concern in the US EPA TRIs (1998–2001) and since in the single solute isotherms BPL gave higher adsorption capacity for toluene than OVC in the range of concentration considered, BPL was hence chosen for the ternary adsorption. Sorial et al. (1993) demonstrated that the Freundlich equation represents well typical single solute adsorption data over a restricted range of concentration, but the IAST using the Freundlich equation showed high deviations from the experimental data. It is worthwhile noting that, at extremely low concentration the Freundlich equation does not satisfy Henry's law. Consequently, this will strongly influence the integration of the Gibbs adsorption equation in the IAST.

The IAST, using the Myers isotherm equation for correlating the single solute data, predicted reasonably well the two concentration combinations for the ternary system (see Fig. 5). The TRE values for the ternary system are shown in the legend of Fig. 5. It is worthwhile noting that, Smith (1991) observed that the predictive ability of the IAST was dependant on the solute concentration. However, in previous studies in our laboratory by Sorial et al. (1993) and Lu and Sorial (2004), high predictive ability

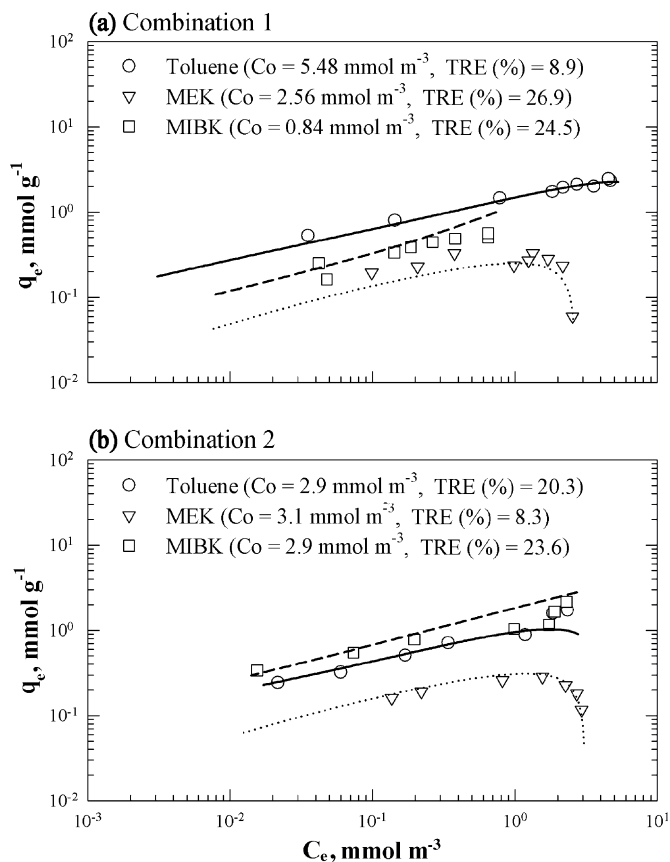


Fig. 5. Ternary adsorption of toluene, MEK, and MIBK on BPL. (IAST simulation curve: (—) toluene, (···) MEK, MIBK, (---) TRE: total relative error (%)).

of the IAST was revealed in the solute concentration range of  $10^{-2}$ – $10^4$   $\text{mmol m}^{-3}$ . Considering the range of solute concentration ( $10^{-2}$ – $10$   $\text{mmol m}^{-3}$ ) used in this study, Fig. 5 together with the reported TRE values reveals the effectiveness of IAST predictions.

For single-solute isotherms, BPL activated carbon gave the lowest adsorption capacity for MEK as compared to toluene and MIBK. Fig. 5 shows that MEK was outcompeted more at high concentrations by toluene and MIBK than at low concentration. This behavior is usually observed for the least competitive adsorbate in multi-component adsorption which is also well predicted by IAST. Factors that affect overall adsorption of multi-component adsorption include the relative molecular size and configuration, the relative adsorptive affinities, and the relative concentrations of the solute (Ruthven, 1984). Hence, competitive adsorption is most likely to occur since the available surface area of the activated carbon will be occupied, to varying degrees, by all the adsorbate components.

#### 4. Conclusion

Single and ternary solute gas phase adsorption isotherms were conducted in this study to evaluate the effectiveness of a simple constant volume method, which was

utilized by using Tedlar gas sampling bags as a constant volume batch reactor. Three initial concentrations of the single solutes and two different combinations of the ternary system were evaluated in this study. The single solute adsorption isotherms based on the three initial concentrations of the adsorbates were adequately represented by both the Freundlich and the Myers isotherm equations. The total relative errors between the observed and the modeled data were less than 10%. The adsorption capacity of bituminous base (BPL) and coconut base (OVC) activated carbons for the solutes studied was strongly dependent on the physical properties of the adsorbent and the adsorbate. The pore size distribution of the adsorbents was found to affect their adsorption capacities. Its effect was dependant on the solute concentration. The experimental results of the ternary systems for the two combinations studied were further confirmed by using the IAST. Accurate predictions of the IAST were achieved by using the Myers equation for correlating the single solute data.

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