

Determination by Modeling of the Interactions during the Adsorption Equilibrium of N-Propanol and Ortho Xylene on Activated Carbon Surface

Abdouliliah Hachimi*

Research Institute of Catalysis and Environment of Lyon (IRCELYON), UMR 5256 CNRS, Claude University, Bernard Lyon I, Villeurbanne, France

Abstract

Temperature Programmed Adsorption Equilibrium (TPAE) procedure was used to determine the heats of adsorption of ortho xylene and 1-propanol on activated carbon at 300 K. The evolutions of the surface coverage with the adsorption temperature ($\theta_s=f(T_a)$) were compared to the Temkin model in order to determine the heats of adsorption and reveal the affinity to the surface of activated carbon regarding the polarity of each adsorbate. It has been shown that the heats of adsorption of ortho xylene were $E_{s0}=100$ kJ/mol and $E_{s1}=62$ kJ/mol at 185 Pa, respectively, at low and high surface coverage. Whereas the heats of adsorption of 1-propanol at the adsorption equilibrium was found to be dependent to the surface coverage with $E_{s0}=67$ kJ/mol and $E_{s1}=58$ kJ/mol at 475 Pa. It was shown that ortho-xylene molecules have more affinity to the activated carbon surface than 1-propanol regarding the difference in the heats of adsorption.

Keywords: Adsorption equilibrium; Heat of adsorption; Temkin model; Langmuir Model; VOCs removal; Adsorption modeling

Introduction

Alcohol and benzene derived compounds among others volatile organic compounds (VOCs) are known to participate to the air quality alteration. These compounds are generally emitted from petrochemical process industries, vehicles and building/construction materials. Their abatement constitutes a priority to anticipate their effects on human health [1]. The adsorption-desorption/destruction constitutes the most processes currently used to prevent the VOCs emission in the atmosphere [2-5]. Their severe reduction to lowest level needs sorbents with large surface area and pore volume. Zeolites [2], metal-organic framework (MOF) [4] and activated carbons [3,6-8], are the most frequently utilized adsorbents, having great adsorption capacity for VOCs.

Activated carbon has been the subject of several studies for the removal of VOCs from air [9] and water [10]. The gas adsorption on activated carbon is dominated by the forces of dispersion and repulsion of Van Der Waals [11]. The electrical charges on the activated carbon are low, which leads to a low potential gradient on surface [12]. The existence of small pore sizes plays an important role in the adsorption capacity of gases on activated carbons [13]. Furthermore, the surface groups have a significant effect in the adsorption of gas polar. Thus, the adsorbed amount increases with the existence of oxidic sites on surface such as carboxyl, lactone, carbonyl, quinone, phenol, ether, carboxylic anhydride, lactol...etc [11-13].

Activated carbon has hydrophilic and hydrophobic adsorption sites that promote adsorption of non-polar and polar molecules in the micropores [14]. However, condensation can occur in the micropores and the mesopores in the adsorption pressure once approaches the critical pressure [15]. Dobruskin [16] modeled the adsorption of benzene on a microporous activated carbon ($BET=805$ m²/g, $V_{micr}=0.42$ cm³/g), he concluded that the inflection point after the saturation of the monolayer is obtained at a relative pressure of 0.17. For alcohols, Salame and Badosz [17] studied the adsorption of methanol on several microporous activated carbons; they noticed that the methanol begins to condense at the relative pressure of 0.3. Pre et al. [11] conducted a quantitative study to predict the heat of adsorption and activation energy of desorption of VOCs on activated carbon using micro-calorimetry

technique. They studied several parameters having a relationship with charcoal-VOCs interactions, including dipole moment, ionization potential, the dielectric constant, polarizability and surface tension. They showed linear regression between these variables and that the adsorption/desorption varies inversely with the potential of ionization and linearly with the polarizability. The heats of adsorption found in the range 40-80 kJ/mol.

The goal of the present investigation was to study the kinetic parameters (heats of adsorption and surface coverage) involved in the adsorption equilibrium of 1-propanol and ortho-xylene on activated carbon using temperature programmed adsorption equilibrium method (TPAE). Therefore, it is of great scientific and practical interest to study the adsorption properties of a commercial activated carbon with respect to different adsorbates (polar and/or non-polar). Such investigations could provide evidence for the importance of some adsorbent parameters including the surface heterogeneity and polarity of adsorbate and leading to measure by modeling the interactions in the adsorbate/adsorbent system. In addition, discussions about the determination the heats of adsorption of alcohol and benzene-derived compounds on activated carbon are limited in the open literature.

Experimental

Materials

Activated carbon (denoted AC) from Prolabo has been selected for two main interests: (a) it is a micro-porous solid and (b) it has non-reactivity with OX or PrOH excepted the adsorption. The AC samples were pretreated before each adsorption in order to remove eventual trace of adsorbates, as follow:

*Corresponding author: Abdouliliah Hachimi, Research Institute of Catalysis and Environment of Lyon (IRCELYON), UMR 5256 CNRS, Claude University, Bernard Lyon I, Villeurbanne, France, Tel: +33782676957; E-mail: hachimi@outlook.fr

Received July 16, 2014; Accepted August 28, 2014; Published September 01, 2014

Citation: Hachimi A (2014) Determination by Modeling of the Interactions during the Adsorption Equilibrium of N-Propanol and Ortho Xylene on Activated Carbon Surface. J Chem Eng Process Technol 5: 206. doi: [10.4172/2157-7048.1000206](https://doi.org/10.4172/2157-7048.1000206)

Copyright: © 2014 Hachimi A. This is an open-access article distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

He, 300 K → He, 723 K (2 h) → He, 300 K.

For the adsorption experiments, ortho di-methyl benzene (Alfa Aesar, 99%) and 1-Propanol (VWR BDH Prolabo, 99%) were used as adsorbates. Dry helium was used as carrier gas with purity greater than 99.999%.

Sorbent characterization

The textural properties (specific surface area and pores volume) of AC were determined by exploiting the isotherm data of the nitrogen physisorption at 77 K. The adsorption of nitrogen was performed on an automated Micrometrics ASAP 2010 V5.02H analyzer after out degassing the samples at 873 K in a vacuum of a relative pressure $<10^{-7}$ to ensure a dry clean surface and free sites of adspecies.

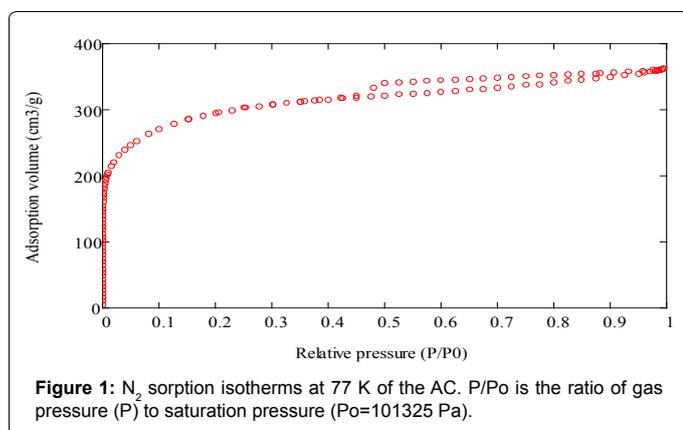
Figure 1 shows the nitrogen adsorption and desorption isotherms of the AC sample. It is obvious that the adsorption isotherm of N_2 on the AC is of typical type-I profile with secondary uptakes, which implies the presence of micro and mesopores. The BET and Langmuir surface areas and pores volume are given in the table 1.

Analytical procedures

The temperature programmed adsorption equilibrium (TPAE), previously developed for hydrogen chemisorption on Pt/ Al_2O_3 catalysts [18], was used in the present work in order to determine the kinetic parameters (heats of adsorption and surface coverage) involved in the adsorption equilibrium of heavy molecules such as PrOH and OX on AC, and to evaluate its efficiency of VOCs removing from bulk stream. TPAE experiments were performed in dynamic conditions using a purpose-built device described above. In brief, it consisted of a gas chromatography (GC) with flame ionization detector (FID) for transient experiments. The assembly permitted (i) to prepare gas mixture in the reactor inlet and to control feeding flow rate, (ii) to perform in-situ pre-treatment, adsorption and desorption steps in quartz micro reactor (1 cm^3) and (iii) to monitor OX and PrOH molar fractions in the reactor outlet by mean of GC-FID system.

TPAE experiments

The principle of the TPAE experiments was reported elsewhere [5,19]. Briefly, around 0.100 g of AC was treated as described above and



cooled down under helium to 300 K in order to remove moisture and adspecies from the surface. Afterward, under atmospheric pressure, a switch He x% PrOH/He or y% OX/He (x and y fixed by saturator/condenser system using the well-known coefficient table of Antoine Equation) was performed to start the adsorption step and the mixture in the reactor outlet was analyzed by GC-FID at the frequency of 1/180 Hz. Once molar fractions at the reactor inlet and outlet are equal, the adsorption equilibrium was considered established. The adsorption temperature (T_a) was slightly increased (0.5-1 K/min) under quasi-constant partial pressure of the adsorbate (PrOH or OX) leading to desorption of the adspecies associated to positive peaks. An isothermal desorption is carried out under helium to verify the total desorption of adspecies once the molar fractions are again equal at high temperature. Finally, the AC was cooled down to the room temperature. The experimental data was presented as breakthrough curves showing the evolution of molar fractions with time.

Results and Discussion

Mathematic models

Surface coverage (θ) variation with temperature (T_a) and pressure (P_a) of adsorption allows measuring the interaction strengths implied in the adsorbate/adsorbent systems. The heats of adsorption (denoted by E_θ) of the adspecies and their evolutions with the surface coverage θ (with $0 \leq \theta \leq 1$) constitute a fundamental characterization of the adsorbate/adsorbent systems. Temkin model [20] among numerous mathematical models describes the curve of $\theta = f(T_a)$ using statistical thermodynamics. This model assumes that (i) the adspecies are localized, (ii) the heat of adsorption linearly decreases with increase in surface coverage, (iii) heterogeneous surface sites and (iv) indirect interactions between adspecies. The Temkin model is given by the following equation:

$$\theta_e = \frac{RT_a}{\Delta E} \ln \left(\frac{1 + K_{\theta_0} P_a}{1 + K_{\theta_1} P_a} \right) \quad (1)$$

Where R is the gas constant, K_{θ_0} and K_{θ_1} are the coefficient of adsorption respectively at low ($\theta = 0$) and high coverage ($\theta = 1$) with:

$$K_{\theta_0} = \frac{h^3}{(2\pi M)^{3/2} (kT_a)^{5/2}} \exp\left(\frac{E_{\theta_0}}{RT_a}\right), \quad K_{\theta_1} = \frac{h^3}{(2\pi M)^{3/2} (kT_a)^{5/2}} \exp\left(\frac{E_{\theta_1}}{RT_a}\right)$$

and $\Delta E = E_{\theta_0} - E_{\theta_1}$ Where E_{θ_0} and E_{θ_1} are the heats of adsorption respectively at low ($\theta = 0$) and high ($\theta = 1$) coverage. The heats of adsorption ($E_\theta = E_a - E_d$) are the difference between the activation energy of adsorption (E_a) and desorption (E_d) at the adsorption equilibrium.

The theoretical curve obtained from Eq. 1 provides the evolution of the surface coverage with the adsorption temperature (T_a) by supposing E_{θ_0} and E_{θ_1} , and its comparison with the experimental surface coverage variation permits the determination of the adsorption heats (E_{θ_0} and E_{θ_1}). It could be noted that during TPAE step, the slight perturbation of the equilibrium by increasing the temperature of adsorption leads to a slight variation of adsorption pressure of about 20% that conducts to the variation of heat of adsorption of around 3 kJ/mol. This value was considered as the measurement error of the heat of adsorption determined by TPAE.

Reference of AC	Particles Size (mm)	S_{BET} (m^2/g)	S_{ext} (m^2/g)	S_{meso} (m^2/g)	S_{micr} (m^2/g)	V_{micr} (cm^3/g)	V_{meso} (cm^3/g)	V_p (cm^3/g)	D_p (\AA)
N° 89067	1 to 5	1055	125	250	680	0.36	0.13	0.56	10.6

Table 1: Measured Textural parameters of activated carbon with particle diameter (D_p), volumes: total pore (V_p), mesopores (V_{meso}), micropores (V_{micr}), surfaces: BET (S_{BET}), external (S_{ext}), microporous (S_{micr}) and mesoporous (S_{meso}).

At the equilibrium, the surface coverage ($\theta_e(T_a, P_a)$) can be determined by the ratio of the adsorbed amount (Q_a) at T_a and P_a and the amount forming the monolayer (Q_{ML}):

$$\theta_e(T_a) = \frac{Q_a}{Q_{ML}} \quad (2)$$

The Q_{ML} can be calculated considering surface area of the solid ($S = 1055 \text{ m}^2/\text{g}$) and the cross-section area σ ($\text{m}^2/\text{molecule}$) of an adsorbed molecule (Eq. 3):

$$Q_{ML} = \frac{S \cdot 10^{20} \cdot 10^6}{\sigma \cdot N_A} (\mu\text{mol/g}) \quad (3)$$

Where N_A is the Avogadro number ($N_A = 6.02210^{23} \text{ molecule} \cdot \text{mol}^{-1}$), S is the surface area (m^2/g) and σ (m^2) is the cross-section between a molecule and an adsorbent. This later has been determined experimentally by McClellan and Harnsberger [21]. They found that the cross-section of PrOH and OX is around 31 and 48 ($\text{\AA}^2/\text{molecule}$), respectively. Considering Eq. 3 the Q_{ML} was determined to around 5650 and 3650 $\mu\text{mol/g}$, respectively, for PrOH and OX. The adsorption pressures were chosen to be significantly less than those obtained by the vapor at the saturation at the temperature of adsorption ($T_a = 300 \text{ K}$), 0.75% and 2.3%, respectively, for OX and PrOH. Those values were calculated considering the molar fractions at the peaks of TPAE, which are linked to the adsorbate partial pressure that increases with

20% during the TPAE step. At the equilibrium, the surface coverage evolution, during TPAE step, can be determined using the following equations:

$$\theta(T_a) = \frac{Q_a - \frac{F}{W} \int_{t_0}^{t_{eq}} (C_t - C_{t_{eq}}) dt}{Q_{ML}} \quad (4)$$

$$\text{With } Q_a(T_a, P_a) = \frac{F}{W} \int_{t_0}^{t_{eq}} (C_{t_{eq}} - C_{t_0}) dt \quad (5)$$

Where: Q_a is the amount (mol/g) of an adsorbate at T_a and P_a . F is the flow rate (cm^3/min) of adsorbate/He. W is the weight (g) of the adsorbent. C_{t_0} , $C_{t_{eq}}$ and C_t are the adsorbate's molar fraction at the reactor outlet, respectively, at the start time of the adsorption (t_0), at the time at which equilibrium is established (t_{eq}) and at any time during TPAE experiment ($t > t_{eq}$). Q_{ML} is the amount (mol/g) of an adsorbate forming monolayer.

Characterization of the OX adsorption equilibrium on AC

The breakthrough curve permitted the monitoring of adsorbate loading on adsorbent as function of time. Figure 2 shows the evolution of molar fractions of the 0.183%OX/He mixture at the reactor outlet in presence (curve (b)) and absence of 0.100 g of AC (curve (a)) during the TPAE experiment steps. The adsorption step of OX on AC was carried out using an isobaric ($P_a = 185 \text{ Pa}$) of OX at $T_a = 300 \text{ K}$. The equilibrium was established after 100 minutes with AC in the reactor whereas the breakthrough time for the empty reactor is less than minute. The amount of adsorbed OX was determined using Eq. 5. The subtraction of the area of (curve (b)) from the area of the empty reactor (curve (a)) permitted to assess the adsorbed amount of OX. This later was found to be 4160 $\mu\text{mol/g}$ corresponding to $\theta_e = 114\%$ of the AC surface coverage. This result can be explained by the fact that, at 185 Pa and 300 K, the pores were partially filled with OX molecules because of the formation of multilayers on the surface of AC [22]. This assumption could be verified with comparing the adsorbed volume with the total pores volume. Indeed, such result is consistent since the total pores volume of the AC is 0.56 cm^3/g which is close to the corresponding adsorbed volume of OX (0.51 cm^3/g) even though the adsorption pressure (185 Pa) is lower than the OX saturation pressure at 300 K (970 Pa) with a relative adsorption pressure of 0.19. This result is consistent with the work of Dobruskin [16]. The author [16] has modeled the adsorption of benzene on a microporous activated carbon ($\text{BET} = 805 \text{ m}^2/\text{g}$, $V_{\text{micr}} = 0.42 \text{ cm}^3/\text{g}$), he concluded that the inflection point after the saturation of the monolayer is obtained at a relative pressure of 0.17.

Once the equilibrium established (OX molar fractions are equal at reactor inlet and outlet), the temperature programmed (1 K/min) was performed under 0.183%OX/He mixture resulting a positive and asymmetric peak of desorbed OX adspecies. The amount of the OX adspecies desorbed during TPAE was determined using the Eq. 5 by subtracting areas of the curve (b) from the curve (a) in the temperature range 300-550 K and found to be 4130 $\mu\text{mol/g}$. While the amount of OX desorbed during the isotherm at high temperature, was 30 $\mu\text{mol/g}$.

Similar results were obtained by applying high adsorption pressure (680 Pa) until equilibrium using 0.100 g of AC and under 0.68% OX/He mixture at 300 K. The amount of OX adsorbed was around 4655 $\mu\text{mol/g}$ which corresponds to the adsorbed OX volume of 0.56 cm^3/g that matches with the total pores volume of AC and then the saturation of AC. However, the adsorption potential depends not only on the characteristics of the adsorbent but also on those of the adsorbate. Materials having narrow micropores adsorb more than those with

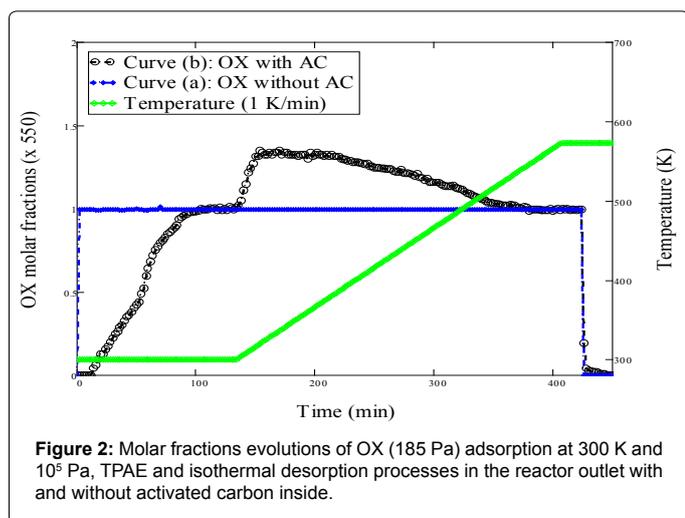


Figure 2: Molar fractions evolutions of OX (185 Pa) adsorption at 300 K and 10^5 Pa , TPAE and isothermal desorption processes in the reactor outlet with and without activated carbon inside.

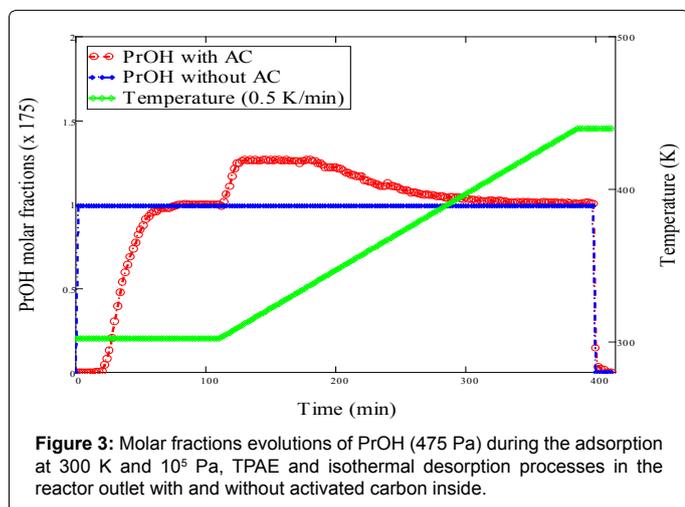


Figure 3: Molar fractions evolutions of PrOH (475 Pa) during the adsorption at 300 K and 10^5 Pa , TPAE and isothermal desorption processes in the reactor outlet with and without activated carbon inside.

wide or non-porous. The adsorption capacity of AC for OX could be compared with those given for the adsorption of xylene on activated carbon AC40 (1300 m²/g) [23] and much higher than those obtained for non-porous silica (220 m²/g) [5].

Characterization of the PrOH adsorption equilibrium on AC

Similar experiments to the adsorption of OX were carried out on the adsorption of PrOH on AC (Figure 3). The adsorption equilibrium was obtained during 70 min using 0.147 g of AC and 0.46% PrOH/He at 300 K. Same methods were used for determination of the PrOH adsorbed amounts as for OX on AC. The amounts of the PrOH uptake during the adsorption, TPAE and desorption under helium steps were, 6050, 5950 and 100 μmol/g, respectively. The adsorbed amount corresponds to 0.45 cm³/g which represents 80 vol. % of pores filling and $\theta_c=112\%$ of the surface coverage at the relative pressure of 0.16 at 300 K. The effect of the adsorption pressure was studied in order to reveal the saturation limit of the AC. The experiment revealed that the amount of PrOH adsorbed on AC increases with the adsorption pressure. In fact, at the saturation pressure and $T_a=300$ K, the uptake amount was found to be 7550 μmol/g which corresponds to the volume of 0.56 cm³/g of PrOH adsorbed. These results can be explained by formation of multilayers on the surface and condensation of PrOH molecules in the pores of AC. However, These results are unlike to those found by Salame and Bandosz [17]. They noticed in similar studies that the adsorption of methanol on several microporous activated carbons leads to the interparticulate and the pores capillary condensation that starts with applying relative pressure from 0.3. The difference, in the condensation at relative pressure, could be linked to the chemical properties of the adsorbents used in both studies. On the other hand, the AC was completely regenerated at 420 K and 550 K for PrOH and OX, respectively; unlikely to that found in a previous work performing similar studies on non-porous silica sorbent [5]. This later was found readily regenerated at around 400 K for both adsorbates.

Heats of adsorption of OX and PrOH on AC under adsorption equilibrium

The experimental curves in Figure 4, show the plot of $\theta_c=f(T_a)$ obtained from the data in Figure 2 by using (Eq. 4) and (Eq. 5) and provides the evolution of OX surface coverage on AC for $T_a > 300$ K and $P_a=185$ Pa (OX) during TPAE experiment. The equilibrium surface

coverage was obtained using the ratio of the amount of desorbed molecules at a given T_a and P_a during TPAE step to the amount of OX necessary for the formation of monolayer on the AC surface (Eq. 4). At 300 K and 185 Pa, the equilibrium surface coverage was $\theta_c=1.14$ and its variation $\theta_c=f(T_a)$ (experimental curve, Figure 4) was modeled using Temkin model (Eq. 1) taking into account that the heats of adsorption depend to the surface coverage with $E_{00} = 100$ kJ/mol, $E_{01} = 62$ kJ/mol and $P_a=185$ Pa.

It could be noticed that the experimental data deviates of the theoretical model in the temperature range 300-360 °C. In fact, at this temperature range the surface coverage drops from 1.14 to 0.73 because of desorption of the OX adspecies forming multilayers and/or probably from the evaporation of condensed OX molecules into AC pores [24]. However, at $T_a>360$ °C, the model Temkin fitted perfectly the experimental data curve. This result can be explained by desorption of the OX adspecies forming the monolayer of AC surface; in agreement with Hill [24] work in which the author reported that the multilayer formation occurred at surface coverage $\theta>0.70$. On the other hand, the heats of adsorption of OX on AC determined using Temkin model parameters at high and low surface coverage under adsorption equilibrium found to be close to those found by Pre et al. [11] for the adsorption of toluene on activated carbon (63 to 71 kJ/mol), and to those found by Dollimore et al. [25] using micro-calorimetric technique and isosteric heats of adsorption for meta-xylene on non-porous graphite (60 kJ/mol). The authors [25] showed that at low surface coverage the heats of adsorption were much higher than at high surface coverage; they explained their results by the fact that the graphite surface was heterogeneous and the high values of the heats of adsorption at low surface coverage were associated to the oxygen chemisorbed on the surface. Hockey and Pethica [26] studied the adsorption of benzene on silica in various forms, and they have shown that micro porosity and lateral interactions increases the heats of adsorption at low surface coverage of silica. If their theory is correct, the high values of the heats of adsorption found at low surface coverage ($E_{00}=100$ kJ/mol) are due to the presence of micropores in AC, and at high surface coverage ($E_{01}=62$ kJ/mol) are due to the hydrogen physisorption on sites with low energy. The very first molecules adsorbed will be onto highly energetic sites and the molecules will remain fixed. Molecules arriving at high surface coverage will release less energy upon adsorption and may form a dilute mobile film due to the condensation.

On the other hand, similar results were obtained during the adsorption of PrOH on AC. Figure 5 depicts the variation of the surface coverage of PrOH on AC at 475 Pa with the adsorption temperature ($T_a>300$ K). The fitting of the Temkin model on the experimental curve permitted determination of the heats of adsorption. These later were found to be $E_{00}=67$ kJ/mol, $E_{01}=58$ kJ/mol at low and high surface coverage, respectively. Same remark could be noted on deviation of the experimental curve at high coverage. This could be related to the PrOH desorption that adsorbed physically on sites with low energy. However, it could be noticed that the heats of adsorption for polar molecules (PrOH) were found to be lower than those for non-polar molecules (OX), and the large difference in the heats of adsorption between low and high surface coverage for OX (100 kJ/mol) against that for PrOH (67 kJ/mol) let's assume that the heats of adsorption of OX could not be associated in major part to the microporosity of AC but to the chemisorption phenomena on specific sites in contrast to the PrOH adsorbate. The difference in the interactions between both adsorbates and AC can be associated to the difference in their dipolar moments. Indeed, the OX and PrOH molecules are characterized by different dipole moment 0.64 D and 1.68 D, respectively [27,28]. This

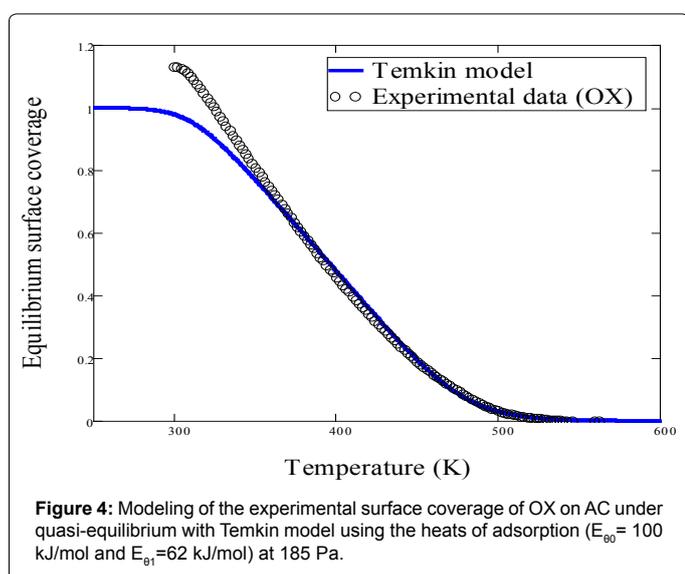
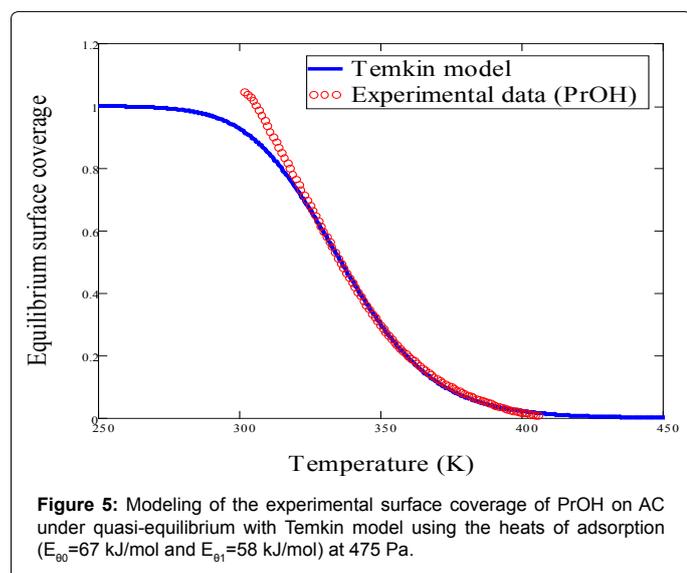


Figure 4: Modeling of the experimental surface coverage of OX on AC under quasi-equilibrium with Temkin model using the heats of adsorption ($E_{00}=100$ kJ/mol and $E_{01}=62$ kJ/mol) at 185 Pa.



characteristic may lead to different affinities to the AC surface sites and subsequently promotes their adsorption.

The heats of adsorption of PrOH on activated carbon obtained by using the Temkin model and adsorption equilibrium that were found to be consistent with the isosteric heats obtained for the adsorption of alcohol compounds on AC. Herry et al. [29] have found similar heats of adsorption for ethanol (54.78 kJ/mol), 1-propanol (59.47 kJ/mol) and butanol (76.87 kJ/mol), while Nastaj et al. [30] and Salame Badosz [17] have found, 60.08 kJ/mol for the adsorption of 2-propanol and 55 kJ/mol for ethanol on AC. However, the heats of adsorption determined by microcalorimetric analysis which is an accurate tool were found to be close to those found by TPAE method. Pre et al. [11] have found, in similar investigation on AC, that of the adsorption of ethanol (54.7 kJ/mol) and isopropanol (55 kJ/mol) whereas Popescu et al. [31] found similar results for butanol (63 kJ/mol).

Note that heats of adsorption given in literature seem to be an average values and did not take into account the surface coverage factor; in contrast, TPAE method gives variation of the heats of adsorption of PrOH with the surface coverage of AC.

In the present investigation, the heat of adsorption obtained indicates that weak interactions between PrOH and AC surface that may be due to the nonspecific interactions (Van Der Waals forces, London forces) and present good agreement with the fact that the PrOH adsorption is reversible.

Conclusions

The main objective of the present work was to demonstrate the interest of an easy and efficient method to determine the heats of adsorption. Polar (Propanol) and non-polar (ortho xylene) molecules were selected for the adsorption on a microporous adsorbent (activated carbon). The adsorption capacities for OX and PrOH showed that both adsorbates were condensed into the micropores of AC at 300 K at relative adsorption pressures of 0.16 and 0.19, respectively, of PrOH and OX. The evolutions of the surface coverage (θ_e) at the equilibrium of adspecies with the temperature of adsorption (T_a) have been determined by using temperature programmed adsorption equilibrium (TPAE) method. The heats of adsorption have been determined by modeling the experimental curves ($\theta_e=f(T_a)$) with the theoretical

model of Temkin considering that PrOH and OX adspecies were localized and the heats of adsorption found to depend to the surface coverage. The heats of adsorption of OX on AC found to be $E_{00}=100$ kJ/mol at low coverage and $E_{01}=62$ kJ/mol at high coverage. Whereas, the heats of adsorption of PrOH on AC were found to be lower than for OX with $E_{00}=67$ kJ/mol, $E_{01}=58$ kJ/mol at low and high surface coverage, respectively. It was concluded that OX molecules have more affinity to the AC surface than PrOH regarding the difference in the heats of adsorption. It could be concluded that TPAE experiment could be used into the characterization of the interactions involved in the adsorption of polar or non-polar molecules on microporous adsorbents.

Acknowledgment

I gratefully acknowledge the funding of the Institute of Research on Catalysis and Environment of Lyon (IRCELYon), France, for this study.

References

- Larson RA, Weber EJ (1994) Reaction mechanisms in environmental organic chemistry. Boca Raton ed., Lewis Publishers.
- Takeuchi Y, Iwamoto H, Miyata N, Asano S, Harada M (1995) Adsorption of 1-butanol and p-xylene vapor and their mixtures with high silica zeolites. Separations Technology 5: 23-34.
- Lillo-Rodenas MA, Fletcher AJ, Thomas KM, Cazorla-Amorós D, Linares-Solano A (2006) Competitive adsorption of a benzene-toluene mixture on activated carbons at low concentration. Carbon 44: 1455-1463.
- Yang K, Xue F, Sun Q, Yue R, Lin D (2013) Adsorption of volatile organic compounds by metal-organic frameworks MOF-177. Journal of Environmental Chemical Engineering 1: 713-718.
- Hachimi A (2014) Adsorption models and heat of adsorption of adsorbed ortho di-methyl benzene and 1-propanol species in competitive adsorption on silica by using temperature programmed adsorption equilibrium methods. Journal of Environmental Chemical Engineering, 2 377-385.
- Fuertes AB, Marbán G, Nevskaja DM (2003) Adsorption of volatile organic compounds by means of activated carbon fibre-based monoliths. Carbon 41: 87-96.
- Mirzaei A, Ebadi A, Khajavi P (2013) Kinetic and equilibrium modeling of single and binary adsorption of methyl tert-butyl ether (MTBE) and tert-butyl alcohol (TBA) onto nano-perfluorooctyl alumina. Chemical Engineering Journal 231: 550-560.
- Sing KSW (2014) 10-Adsorption by Active Carbons. In: F. Rouquerol, J. Rouquerol, K.S.W. Sing, P. Llewellyn, G. Maurin (Eds.) Adsorption by Powders and Porous Solids (Second Edition). Academic Press, Oxford 321-391.
- Gallego E, Roca FJ, Perales JF, Guardino X (2013) Experimental evaluation of VOC removal efficiency of a coconut shell activated carbon filter for indoor air quality enhancement. Building and Environment 67: 14-25.
- Marbán G, Fuertes AB (2004) Co-adsorption of n-butane/water vapour mixtures on activated carbon fibre-based monoliths. Carbon 42: 71-81.
- Pré P, Delage F, Faur-Brasquet C, Le Cloirec P (2002) Quantitative structure-activity relationships for the prediction of VOCs adsorption and desorption energies onto activated carbon. Fuel Processing Technology 77-78: 345-351.
- Tanada S, Nakamura T, Kawasaki N, Torii Y, Kitayama S (1999) Removal of Aromatic Hydrocarbon Compounds by Hydroxypropyl-cyclodextrin. See comment in PubMed Commons below J Colloid Interface Sci 217: 417-419.
- Daifullah AAM, Girgis BS (2003) Impact of surface characteristics of activated carbon on adsorption of BTEX. Colloids and Surfaces A: Physicochemical and Engineering Aspects 214: 181-193.
- Bae JS, Do DD (2006) On the equilibrium and dynamic behavior of alcohol vapors in activated carbon. Chemical Engineering Science 61: 6468-6477.
- Dobruskin VK (2001) Correlation between two- and three-dimensional condensations in cylindrical mesopores of active carbons. Carbon 39: 583-591.
- Dobruskin VKh (2002) Micropore structure of activated carbons and predictions of adsorption equilibrium. Carbon 40: 1003-1010.
- Salame II, Badosz TJ (2000) Adsorption of Water and Methanol on Micro- and Mesoporous Wood-Based Activated Carbons. Langmuir 16: 5435-5440.

18. Derrouiche S, Bianchi D (2004) Heats of adsorption using temperature programmed adsorption equilibrium: application to the adsorption of CO on Cu/Al₂O₃ and H₂ on Pt/Al₂O₃. See comment in PubMed Commons below *Langmuir* 20: 4489-4497.
19. Hachimi A, Chafik T, Bianchi D (2008) Adsorption models and heat of adsorption of adsorbed ortho di-methyl benzene species on silica by using Temperature Programmed Adsorption Equilibrium methods. *Applied Catalysis A: General* 335: 220-229.
20. Tompkins FC, Gundry PM (1960) *Chemisorption of Gases on Metals*. Harcourt Brace Jovanovich.
21. McClellan AL, Harnsberger HF (1967) Cross-sectional Areas of Molecules Adsorbed on Solid Surfaces. *Journal of Colloid and Interface Science* 23: 577-599.
22. Rouquerol J, Llewellyn P, Rouquerol F (2007) *Studies in Surface Science and Catalysis*. Elsevier 49-56.
23. Benkhedda J, Jaubert JN, Barth D, Perrin L, Bailly M (2000) Adsorption isotherms of m-xylene on activated carbon: measurements and correlation with different models. *The Journal of Chemical Thermodynamics* 32: 401-411.
24. Hill TL (1946) Theory of Multimolecular Adsorption from a Mixture of Gases. *Journal of Chemical Physics* 14: 441.
25. Dollimore D, Heal GR, Martin DR (1972) Thermodynamics of adsorption of a series of related organic molecules on graphite and a carbon black. Part 1.- Heat of adsorption. *J Chem Soc Faraday Trans* 68: 832-838.
26. Hockey JA, Pethica BA (1962) Thermodynamic studies of adsorption on characterized silicas. Part 1.-Benzene. *Transactions of the Faraday Society* 58: 2017-2026.
27. Wilson RD, Barton DG, Baertsch CD, Iglesia E (2000) Reaction and Deactivation Pathways in Xylene Isomerization on Zirconia Modified by Tungsten Oxide. *Journal of Catalysis* 194: 175-187.
28. Zheng S, Jentys A, Lercher JA (2006) Xylene isomerization with surface-modified HZSM-5 zeolite catalysts: An in situ IR study. *Journal of Catalysis* 241: 304-311.
29. Herry C, Baudu M, Raveau D (2001) Estimation of the influence of structural elements of activated carbons on the energetic components of adsorption. *Carbon* 39: 1879-1889.
30. Nastaj JF, Ambrozek B, Rudnicka J (2006) Simulation studies of a vacuum and temperature swing adsorption process for the removal of VOC from waste air streams. *International Communications in Heat and Mass Transfer* 33: 80-86.
31. Popescu M, Joly JP, Carré J, Danatou C (2003) Dynamical adsorption and temperature-programmed desorption of VOCs (toluene, butyl acetate and butanol) on activated carbons. *Carbon* 41: 739-748.

Citation: Hachimi A (2014) Determination by Modeling of the Interactions during the Adsorption Equilibrium of N-Propanol and Ortho Xylene on Activated Carbon Surface. *J Chem Eng Process Technol* 5: 206. doi: [10.4172/2157-7048.1000206](https://doi.org/10.4172/2157-7048.1000206)