



# Adsorbed solution theory based modeling of binary adsorption of nitrobenzene, aniline and phenol onto granulated activated carbon



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## HIGHLIGHTS

- Simultaneous adsorptive removal of three binary systems by granular activated carbon.
- Binary system studied: nitrobenzene–aniline, nitrobenzene–phenol and phenol–aniline.
- Single component isotherm modeling by Langmuir, Freundlich and Redlich–Peterson models.
- Binary adsorption data modeled by ideal and real adsorbed solution theory (IAST and RAST) models.
- Calculation of activity coefficients.

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## ABSTRACT

The modeling study on simultaneous adsorption of three binary systems (nitrobenzene–aniline (NI–AN), nitrobenzene–phenol (NI–PH) and phenol–aniline (PH–AN)) onto granular activated carbon (GAC) in aqueous solution were performed at 30 °C by conducting batch experiments. The single solute equilibrium adsorption data of nitrobenzene (NI), aniline (AN) and phenol (PH) were fitted with Langmuir, Freundlich and Redlich–Peterson model. The Redlich–Peterson and Freundlich model gave better fitting as compared to Langmuir model for individual adsorption. The binary adsorption data were examined and compared by using ideal adsorbed solution theory (IAST) and real adsorbed solution theory (RAST) models. IAST model didn't provide an acceptable prediction of binary data except for low liquid concentration levels, as it undervalued AN and PH adsorption capacity and overvalued NI adsorption capacity. This is due to the non-ideality of binary mixtures at high concentration levels in the solution. The RAST model gave an excellent prediction of binary adsorption experimental data, thus it can be used as a reliable model for the design of industrial adsorption equipment.

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## 1. Introduction

Benzene derivatives such as nitrobenzene, aniline and phenol are considered as toxic, carcinogenic and/or mutagenic agents. These compounds are frequently used in chemical processes as raw materials in the industries like plastic, paint, pharmaceuticals, pesticides, dyes, gasoline, rubber proofing, disinfectant, steel industries, lubricating oils refinement, soaps or shoe polishes; and as intermediates in the chemical synthesis industries [1–4]. They are introduced into the surface water from industrial effluents and their existence in wastewater even in very small concentrations is harmful to animals and human beings.

A number of technologies are available for removal of these chemical from wastewater such as adsorption [5–9], photochemical reduction [10], oxidation by O<sub>3</sub>/UV processes [11,12] and biodegradation [13]. Adsorption is one of the most frequently used

methods for the removal of these chemicals from wastewater [9,14–15]. A considerable amount of work on the adsorption of organic chemicals has dedicated on the uptake of single solute by various kinds of adsorbents such as granular activated carbons (GACs), and polymeric adsorbents. However, it is necessary from industrial point of view to study the interactive effect of the adsorption of one compound on another during simultaneous adsorption of toxic compounds.

The design of adsorption units essentially depends on adsorbent adsorption capacity at equilibrium condition; and their performance is influenced by the competitive interactions of the compounds present in mixture. Hence, the assessment of the adsorption capacity of a compound in the presence of other solutes by suitable theoretical models is necessary for proper design of a cost effective adsorption system [16]. Various multicomponent adsorption models such as the modified competitive Langmuir model [17], extended Langmuir model [18], extended Freundlich model [19] and Sheindorf–Rebuhn–Sheintuch model [20] can be used to describe the equilibrium characteristics of multicomponent

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**Table 1**

Comparison of individual adsorption equilibrium uptakes and yields of nitrobenzene, aniline and phenol adsorption onto GAC.

$C_o$ (mmol/L)	$C_e$ (mmol/L)	$q_e$ (mmol/g)	Ad (%)
NI			
0.2	0.002	0.020	98.98
0.4	0.006	0.040	98.55
0.6	0.010	0.060	98.32
0.8	0.015	0.080	98.15
1.2	0.030	0.119	97.54
1.6	0.048	0.158	97.04
AN			
0.3	0.015	0.025	94.29
0.5	0.045	0.049	91.69
0.8	0.092	0.071	88.55
1.1	0.149	0.092	86.08
1.6	0.283	0.133	82.46
2.1	0.442	0.171	79.39
PH			
0.3	0.017	0.025	93.56
0.5	0.043	0.049	91.98
0.8	0.078	0.072	90.24
1.1	0.111	0.095	89.59
1.6	0.190	0.140	88.08
2.1	0.291	0.183	86.32

adsorption. Basically they are the extensions of single-component isotherm equations. Ideal adsorbed solution theory (IAST) model and real adsorbed solution theory (RAST) better represent the multi-component adsorption behavior. Details of these theories are given in Section 2.

In the present study, the Langmuir, Freundlich, and Redlich–Peterson models were used for the fitting of experimental equilibrium adsorption data of NI, AN, and PH. The IAST and RAST model were used for the analysis of equilibrium adsorption isotherms for three binary systems namely nitrobenzene–aniline (NI–AN), nitrobenzene–phenol (NI–PH) and phenol–aniline (PH–AN) on to GAC at 30 °C. To check the interactive effect of initial concentration of one species onto the other, a number of experiments were carried out at different initial concentration ratios. The initial concentration ratios for (NI–AN) system was 1:0.67, 1:1.3 and 1:2.6, for (NI–PH) system was 1:0.67, 1:1.3 and 1:2.6, and for (PH–AN) system was 1:0.5, 1:1 and 1:2. The RAST model is derived from IAST model under the hypothesis of adsorbed phase does not follow the ideal behavior. The non-ideal behavior of the system was taken into account by including activity coefficient in to the basic equation of IAST that represents the equality between the chemical potential of liquid and adsorbed phases for each component. The activity coefficient which is a function of spreading pressure was calculated from experimental binary adsorption data.

## 2. Theory

The models used and compared in present work are IAST and RAST, these are multicomponent adsorption model developed by Myers and Prausnitz [21] for gaseous adsorption and then modified for liquid solution by Radke and Prausnitz [22]. They provide a thermodynamically dependable and practical method for prediction of multicomponent adsorption system using single-component isotherm data [16,23]. IAST model is best suitable for a system which show non-interactive behavior. This model is based on the assumptions that all component in a mixture behave as ideal adsorbed solutes according to Raoult's law which means that there is no interaction between adsorbent–adsorbate is considered [24] as well as the chemical potential in adsorbed phase and liquid phase is equal for each component therefore, the spreading pressure is also constant for all components in a given mixture. RAST is best suitable for a system shows antagonistic

behavior (each of the adsorbates present in the mixture have interactive effect).

The basic equation that represents the equivalence between the chemical potential of liquid and adsorbed phases for each component is expressed as follows:

$$C_i = C_i^0(T, P, \psi)x_i \quad i = 1, 2, \dots, N \quad (1)$$

In case of non-ideal system Eq. (1) can be modified as follows

$$C_i = C_i^0(T, P, \psi)x_i\gamma_i \quad i = 1, 2, \dots, N \quad (2)$$

where  $N$  is the number of solutes present in a mixture,  $C_i$  is the equilibrium liquid concentration of each solute,  $C_i^0$  is the liquid phase concentration which is in equilibrium with the resultant single-component adsorption capacity ( $q_i^0$ ), at pressure ( $P$ ), temperature ( $T$ ) and spreading pressure ( $\psi$ ),  $\gamma_i$  activity coefficient of the adsorbed component and  $x_i$  is the mole fraction of each component on adsorbent, that can be expressed as:

$$x_i = \frac{q_i}{q_T} \quad i = 1, 2, \dots, N \quad (3)$$

The IAST models also assume that adsorbent is thermodynamically inert and having constant area for adsorption per mole of solute for single or mixture of components. These assumptions are expressed by following equation

$$\frac{1}{q_T} = \sum_{i=1}^N \frac{x_i}{q_i^0} \quad i = 1, 2, \dots, N \quad (4)$$

where  $q_T$  is total surface loading on adsorbent i.e. sum of adsorbate adsorption capacity of adsorbent.

For non-ideal system the total surface loading at constant temperature can be calculated from the Gibbs–Duhem [25] relation as follows

$$\frac{1}{q_T} = \sum_{i=1}^N \frac{x_i}{q_i^0} + \sum_{i=1}^N \left( x_i \left[ \frac{\partial \ln \gamma_i(\psi)}{\partial \psi} \right]_{T, x_i} \right) \quad i = 1, 2, \dots, N \quad (5)$$

The spreading pressure for single as well as multi-component system is equal and it is derived from Gibbs adsorption isotherm, as per following equation [22]:

$$\psi_i = \int_0^{C_i^0} \frac{q_i^0(C_i^0)}{C_i^0} dC_i^0 \quad i = 1, 2, \dots, N \quad (6)$$

where  $\psi_i$  is the spreading pressure for individual components which is dimensionless,  $q_i^0(C_i^0)$  is single-component adsorption isotherm.

The IAST and RAST can be combined with single component adsorption equations in order to calculate the spreading pressure. In this present work, Freundlich isotherm is incorporated into IAST and RAST to predict the multicomponent adsorption isotherm. So Eq. (6) can be modified by incorporating the Freundlich isotherm as follows:

$$\psi_i = \int_0^{C_i^0} \frac{q_i^0(C_i^0)}{C_i^0} dC_i^0 = n_i K_{Fi} C_i^{0, n_i} \quad i = 1, 2, \dots, N \quad (7)$$

where  $K_{Fi}$  and  $n_i$  are Freundlich isotherm parameters for component  $i$ .

As per the IAST theory, at equilibrium the spreading pressure for each individual as well as mixture of components is equal, as per following equation

$$\psi_1 = \psi_2 = \psi_3 = \dots = \psi_i = \dots = \psi_N = \psi \quad (8)$$

The sum of all the mole or mass fraction in each phase must be exactly equal to unity; for the solid phase

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