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Trapping of Aromatic Compounds by Adsorption on Hydrophobic Sorbents

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ABSTRACT

Trapping by adsorption on hydrophobic porous polymers was the selected method for removing aromatic compounds from aqueous diluted medium. The study was done with four aromatic compounds which are often found in foods and which play a role in organoleptic qualities at low concentrations: ethyl acetate, 2,5-dimethylpyrazine, 1-octen 3-ol, and γ-decalactone. Several sorbents were tested: activated carbon and three porous polystyren-type polymers (Porapak Q, Chromosorb 105, and Amberlite XAD-4). Kinetic and equilibrium sorptions were investigated. The adsorption isotherms were determined for the four aromatic and all the adsorbents, and equilibrium data were correlated with a Freundlich or a Langmuir-type of isotherm equation. Kinetic experimental results were simulated for 1-octen 3-ol using an internal–external mass transfer resistance model. Good agreement was observed for the diffusion coefficient in the sorbent in the range of 10^{-8} $cm^2 \cdot s^{-1}$.

INTRODUCTION

For many years, one of the aims of biotechnologists has been the production of valuable natural substances like aromatic compounds by microorganisms. One of the major problems associated with the production of aromatics from fermentation is end-product inhibition. Therefore, it is necessary to be able to extract these aromatics by suitable techniques from culture mediums at low concentrations (μg to mg per liter). The integration of the separation step with fermentation allows the reduction of this inhibition by an in-situ product recovery and an increase in the total productivity of the process (1).

The most commonly used methods to remove organic compounds from water involve solvent extraction, separation on specific membranes, and activated carbon adsorption, especially when determining organic micropolluants in water (2). More recently, however, an increasing number of reports have described an additional method which uses porous hydrophobic polymers as the sorbing agent for the removal of organics from water and, in particular, for aromatic compounds (3, 4). In this case, as in that of carbon adsorption, extraction is based on the distribution of dissolved compounds between the solid sorbent and water.

Because of their hydrophobic nature and their high specific surface area, porous hydrophobic polymers can be suitable for extracting organic compounds from water. The main avantages of these polymers can be described as follows:

- It is not necessary to heat the aromatic compounds; thus, thermal degradation products are avoided
- The adsorption of water on the polymer is minimal (5, 6)
- The polymer surface is not chemically reactive with the organic compound

Recently, both activated carbon and particular porous organic polymers have been used for the concentration of aromatic compounds. The advantage of activated carbon is its high adsorption capacity which permits the use of small amounts of sorbent for the concentration and a high thermal stability of the material up to 700°C (7). However, this also has disadvantages: the carbon does not completely adsorb all the organic compounds dissolved in water, the desorption is not always total, and the desorbed compounds are not always identical with those which were extracted from water (8, 9).

Nowadays, porous organic resins have replaced activated carbon. These resins are synthetic polymers often found in a chromatographic column. The more commonly used are: Tenax GC, based on 2,6-diphenyl-

p-pentylene oxide (7, 10); Porapak Q, an ethylvinylbenzene–divinylbenzene copolymer (7); and Chromosorbs 102, 105 (11) and Amberlite XAD-2, XAD-4, porous polystyrene-type polymers (7, 12). Despite its lower adsorption capacity (11) (specific surface area: 19 $m^2 \cdot g^{-1}$), Tenax GC has been widely used to trap high-boiling-point volatiles using the headspace method because of its thermal stability (13). Porapak Q and the Chromosorb resins have lower thermal stabilities than Tenax GC, but they provide higher specific surface areas. Chromosorb 102 is being replaced more and more by Chromosorb 105, which can develop twice the adsorption capacity (6, 11). The most widely used resin in the isolation of organic in water has been Amberlite XAD (14, 15). For example, Nielsen et al. (16) and Larsson et al. (17) used Amberlites XAD-4 and XAD-7 to improve the productivity of acetone-butanol-ethanol fermentation with *Clostridium acetobutilicum*. This resin is a low-polarity styrene–divinylbenzene copolymer which has macroreticular characteristics (18).

Although there are numerous reports in the field of adsorption of aromatic compounds on porous hydrophobic polymers, only a few studies of polymer efficiency and saturation, as well as quantitative studies in general, can be found in the literature.

To choose the best adsorbent for a given separation problem and to design the column required to perform the separation in optimal conditions, the strategy for modeling fixed-bed processes includes (19, 20): 1) determining the individual isotherm of each component on each adsorbent, and 2) investigating the mass transfer kinetics of the molecule in the film surrounding the particle and also into the adsorbent particle. For use of the homogeneous diffusion model, we need the value of the diffusion coefficient. In addition, the hydrodynamics (Peclet number) of the flow in the column must be known, but this is independant of the molecules involved and can be estimated independently; for example, using correlations of the literature.

For our experiments in the isolation and recovery of aromatic compounds from aqueous diluted medium, the aim of the work was to compare a range of hydrophobic porous polymers with regard to their efficiency as sorbents for volatile odorous components. The fundamental aspects were investigated by applying models to the adsorption isotherms and kinetic results, and comparing the results with experimental data.

The simplest and most often used models for adsorption isotherms are Langmuir and Freundlich models. In a large number of reports dealing with adsorption on activated carbon of organic compounds dissolved in water (water purification), Freundlich's equation has been used successfully. For example, to describe the adsorption of phenolicly derived substances on different activated carbon, Abid-Hacini (2) found Freundlich's model better suited to the experimental results than Langmuir's model. However, several examples show that the Langmuir model can represent experimental data very well for various systems, such as penicillin on Amberlite IRA 945 (21), bovine serum albumine (BSA) on DEAE-sepharose (20), or phenols on Duolite ES 861 (22).

EXPERIMENTAL

Material

Aromatic Compounds

Four aromatic compounds which play a role in the aromatization of foods, and which can also be produced microbiologically, were tested. There are ethyl acetate, 2,5-dimethylpyrazine, 1-octen 3-ol, and γ-decalactone. Their characteristics are shown in Table 1. Quantitative analysis of the aromatic compounds was done using a Packard 427 chromatograph. Parameters for the gas chromatographic analysis were as follow:

- Stainless-steel column (3 m length by 3 mm I.D.) Chromosorb W-AW, 100–120 mesh coated with 10% Carbowax 20M
- Flow rates of carrier gas (N_2) and hydrogen: 20 $mL \cdot min^{-1}$
- Flow rate of air: 200 $mL \cdot min^{-1}$
- Flame ionization detector and injector temperatures: 250°C
- Column temperature:
  80°C for ethyl acetate, 160°C for 2,5-dimethylpyrazine and for 1-octen 3-ol, 200°C for γ-decalactone
  Column temperature was programmed from 100 to 200°C at 4°C$\cdot min^{-1}$ for a mixture of the four compounds

An integrator (informatic system CHROMA for BIOSYSTEMES) performed the acquisitions and treatment of the data.

Sorbents

Several sorbents were tested:

- Activated carbon (Bender and Hobein)
- Three porous polystyrene-type polymers: Porapak Q (Interchim), Chromosorb 105 (Altech Associated), Amberlite XAD-4 (Prolabo)

Some of the physicochemical characteristics of the sorbents are shown in Table 2. The sorbents (activated carbon, Porapak Q, and Chromosorb 105) were initially conditioned overnight (12 hours) at 180°C in a stream of nitrogen (30 $mL \cdot min^{-1}$). Because of its instability to heat (12), the previous method conditioning the resin could not be applied to Amberlite

TABLE 1
Physicochemical Characteristics of Aromatic Compounds (23)

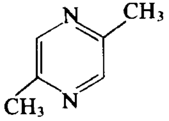
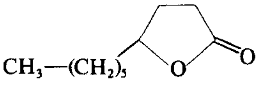
Substance	1-Octen 3-ol	Ethyl acetate	2,5-Dimethylpyrazine	γ-Decalactone
Formula	$CH_2{=}CH{-}CHOH{-}C_5H_{11}$	$CH_3{-}COO{-}C_2H_5$		
Molecular weight	128	86	108	170
Boiling point (°C)	175	76	155	281
Specific gravity at 20°C	0.84	0.90	0.99	0.98
Organoleptic properties (odor)	Mushroom (14)	Ether-like (14), pineapple (14)	Grilled nut (15)	Peach (14)

TABLE 2
Physicochemical Characteristics of Sorbents

Adsorbent	Activated charcoal	Porapak Q	Chromosorb 105	Amberlite XAD-4
Granulometry (mesh)	40–60	80–100	60–80	20–50
Surface area ($m^2 \cdot g^{-1}$)	1000	600	650	750
Temperature limit (°C)	500	180	250	—
Pore diameter (24) (μm)	0.001–0.2	0.0075–0.05	0.04–0.06	Average: 0.005

XAD-4. The purification procedure used was based on the method recommended by Junk et al. (18): Soxhlet extraction with methanol at 75°C for 24 hours, then with diethyl ether at 38°C for 24 hours, and finally drying under vacuum at 60°C.

Method

Static Adsorption Procedure

An aqueous solution of an aromatic compound at the desired concentration, always below the solubility, was prepared. Four millimeters of this solution was added to 10 mg of sorbent in a 4.5-mL hermetically sealed flask and stirred at 600 rpm at a regulated temperature of 25°C.

After reaching the equilibrium loading (from 40 to 180 minutes), the concentration of the solution was analyzed by gas chromatography. The amount adsorbed corresponded to the difference in concentration between the initial and the equilibrium concentrations.

This procedure was used to determine several items.

The Adsorption Isotherms. For the determination of adsorption isotherms, the quantity of adsorbed compounds per gram of polymer was plotted vs equilibrium concentration of the aqueous solution after equilibrium. The chosen concentrations were 100 to 2000 ppm for ethyl acetate, 2,5-dimethylpyrazine, and 1-octen 3-ol, and 100 to 600 ppm for γ-decalactone because of its limited solubility in water.

The Kinetics of 1-Octen 3-ol Trapping. The decrease of 1-octen 3-ol in the aqueous solution [initial concentration 1000 ppm ($0.84\ g \cdot L^{-1}$)] was followed by analysis every 10 minutes until the remaining quantity of 1-octen 3-ol reached equilibrium.

The Selectivity of the Polymers. The aqueous solution introduced into the 4.5-mL flask was a mixture of the four aromatic compound at 500 ppm each. When equilibrium was reached, the quantity of each compound remaining in the solution was analyzed by gas chromatography.

RESULTS AND DISCUSSION

Adsorption Isotherms

Determining the adsorption isotherm study is the first essential step in characterizing the sorbents.

Figures 1–4 present the adsorption isotherms of each aromatic compound on each adsorbent. Adsorption isotherms are classified into different types (25). For all aromatic compounds except for γ-decalactone and for all the adsorbent in the equilibrium concentration range studied, a type I isotherm is observed. This type of isotherm presents a saturation level of adsorption. It is generally characteristic for activated carbon (26) and

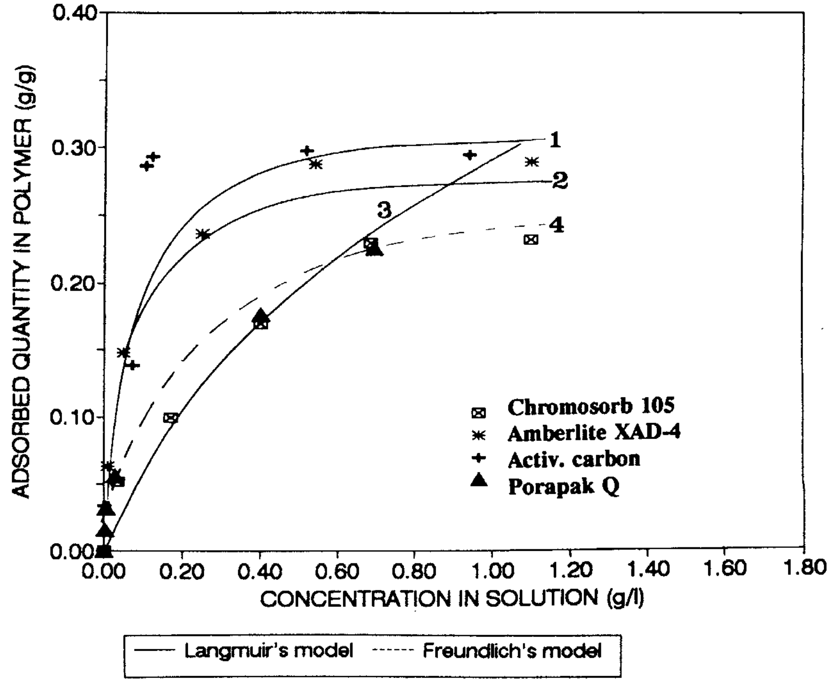


FIG. 1 Adsorption isotherm of 1-octen 3-ol on different sorbents (T = 25°C). 1: Activated carbon, 2: Amberlite XAD-4, 3: Porapak Q, 4: Chromosorb 105.

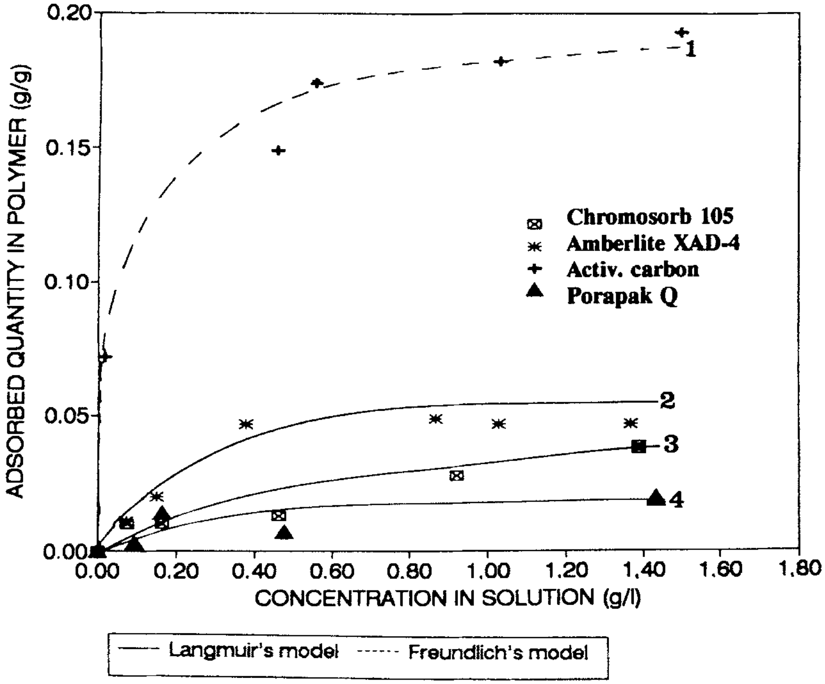


FIG. 2 Adsorption isotherm of 2,5-dimethylpyrazine on different sorbents (T = 25°C). 1: Activated carbon, 2: Amberlite XAD-4, 3: Chromosorb 105, 4: Porapak Q.

is obtained with microporous solid sorbents where the sorption is limited by the steric bulk effect to one or two molecular layers.

Isotherms of γ-decalactone for all the adsorbents were essentially linear; aspects of this observation will be discussed below.

Influence of Sorbent Nature and Physicochemical Characteristics

Activated carbon is the most efficient adsorbent for all compounds (except γ-decalactone). It gives a higher capacity at all concentrations; in addition, the curvatures of the isotherms are more pronounced. These two effects can be attributed to the high specific surface area and to the chemically complex structure of the surface of the activated carbon which allows the possibility of different types of bonds. It can adsorb four to nine times more 2,5-dimethylpyrazine than the other polymers and two

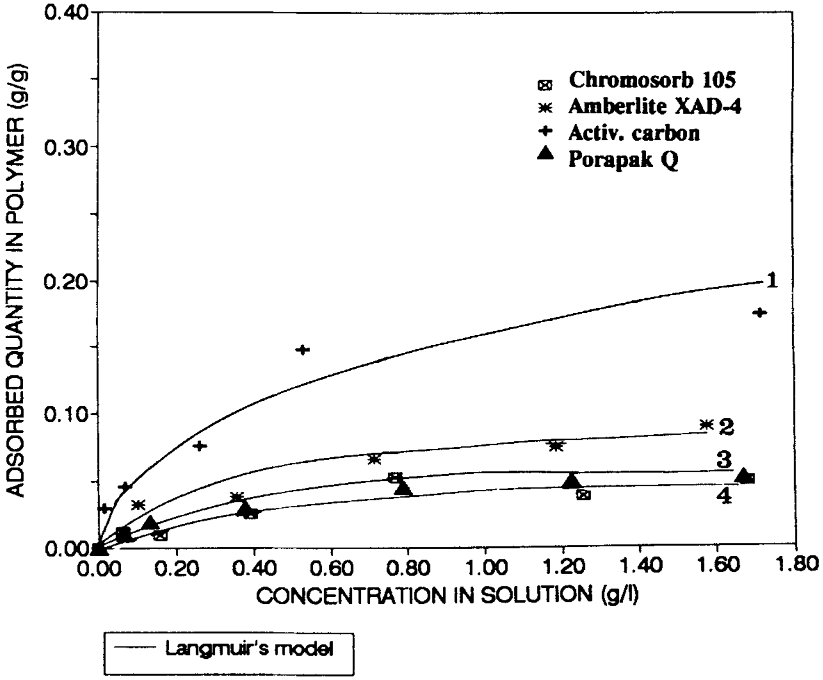


FIG. 3 Adsorption isotherm of ethyl acetate on different sorbents ($T = 25°C$). 1: Activated carbon, 2: Amberlite XAD-4, 3: Chromosorb 105, 4: Porapak Q.

times more ethyl acetate. The same behavior is observed for 1-octen 3-ol but to a lesser extent.

Amberlite XAD-4 traps aroma compounds more efficiently than Porapak Q or Chromosorb 105, which seem to have similar isotherms.

Influence of Adsorbate Nature

The four aromatic compounds are chemically very different, and it is not surprising that they exhibit different adsorption behaviors. 1-Octen 3-ol is much more easily adsorbed than the other aromatic compounds. 2,5-Dimethylpyrazine shows a marked preference for activated carbon. 2,5-Dimethylpyrazine and ethyl acetate have similar behaviors toward all the adsorbents except activated carbon. The isotherms for γ-decalactone, which has low solubility in water, have been measured over a wider range of concentrations in solution, including concentrations more than 10 times

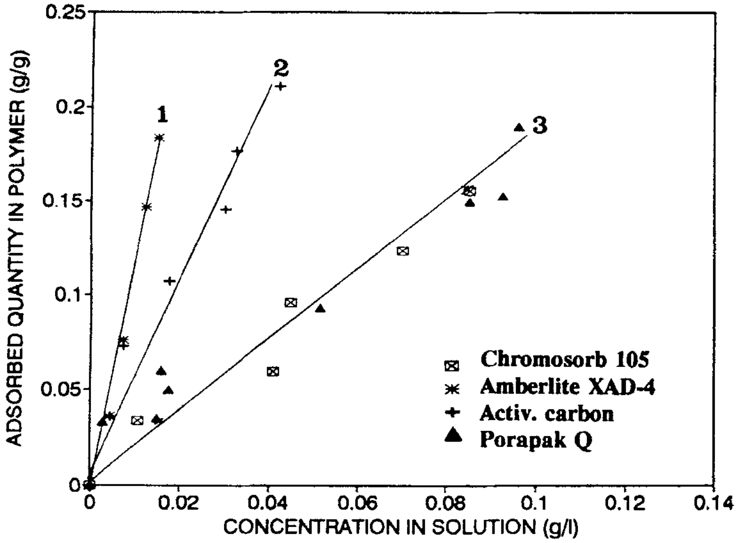


FIG. 4 Adsorption isotherm of γ-decalactone on different sorbents (T = 25°C). 1: Amberlite XAD-4, 2: activated carbon, 3: Chromosorb 105 and Porapak Q.

lower than those studied for other compounds. This probably explains the rather linear forms of these isotherms. The highest partition coefficient is for Amberlite XAD-4. The partition coefficients are much lower and equal for Chromosorb 105 and Porapak Q.

Adsorption behaviors of the aroma compound can be related to the solubilities of the compounds.

γ-Decalactone, which has a very low solubility in water (Table 1), is effectively retained by all of the studied sorbents. 1-Octen 3-ol is much better retained than ethyl acetate and 2,5-dimethylpyrazine. 1-Octen 3-ol has a lower solubility in water and therefore is the next most easily sorbed on hydrophobic porous polymers; the other two compounds are more polar and more soluble in water.

In previous studies in our laboratory we obtained similar results in trapping aromatic compounds in the vapor state (extraction by the headspace method followed by concentration on porous hydrophobic polymers): on Porapak Q, ethyl acetate was trapped at 0.8%, 1-octen 3-ol at 87.5%; on activated carbon, ethyl acetate was trapped at 15.7%, 1-octen 3-ol was adsorbed at 51% (27).

For the adsorption of organic compounds in aqueous solutions, the main factors which can play a role are

I. Interaction energy of adsorbent–organic compounds
II. Interaction energy of adsorbent–water
III. Solubility in water of the organic compound (which depends on the interaction energy of adsorbate–water)

The quantities of aromatics adsorbed are greater if the value of I is high and II and III are low. As Abid-Hacini (2) showed for benzenic compounds adsorbed on activated carbon, adsorbed quantities seem to follow the solubility in water in reverse order (Fig. 5): γ-decalactone, the less soluble substance in water, is more adsorbed than the other compounds.

Correlation of Experimental Data with the Theoretical Models

In a binary system (water–aromatic compound), the adsorption equilibrium can be characterized with the classical equations:

$$\text{Langmuir:} \qquad q = \frac{Q_0 K_L C}{1 + K_L C}$$

$$\text{Freundlich:} \qquad q = K_F C^a$$

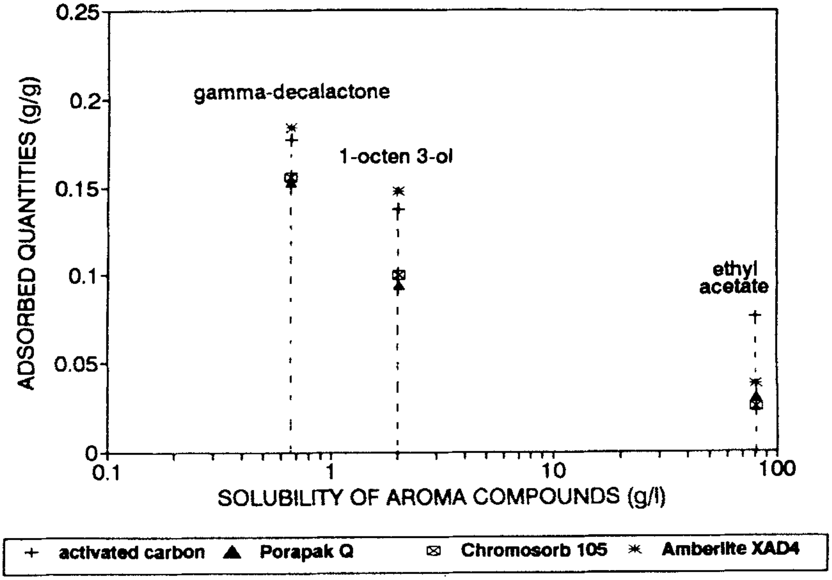


FIG. 5 Adsorbed quantities of aromatic compounds for an initial concentration of 500 ppm versus the solubility in water (T = 25°C).

where q = concentration of adsorbate in the sorbent (g/g adsorbent)
C = concentration of adsorbate in the aqueous solution (g/L)
Q_0 and K_L = Langmuir constants
K_F and a = Freundlich constants

Normally, the fitted application of the theoretical models of Langmuir and Freundlich is tested by the linearization of the equations:

$$\text{Langmuir:} \quad \frac{1}{q} = \frac{1}{Q_0 K_L C} + \frac{1}{Q_0}$$

$$\text{Freundlich:} \quad \ln q = a \ln C + \ln K_F$$

The determination of the coefficients (K_L, Q_0, K_F, and a) by linearization can be biased because the results are calculated from derivated forms of the equation and not from the basic ones. In an attempt to apply a more fitted theoretical model to our experimental data, correlation with the Langmuir and Freundlich equations was done with a numerical program, SAS. This program can test the nonlinear regression for each case and gives correlation coefficients with theoretical models. Table 3 gives the Langmuir and Freundlich coefficients. The Langmuir or Freundlich equations are suitable models for our experimental data (Figs. 1 to 3). For clarity in the figures, only examples of curves are shown. In general, both models are in good agreement with the experimental data in this study.

TABLE 3
Coefficients of the Adsorption Isotherms for the Freundlich and Langmuir Equations

Aromabic compound	Coefficients[a]	Activated carbon	Porapak Q	Chromosorb 105	Amberlite XAD-4
1-Octen 3-ol	Q_0	0.30	0.52	0.23	0.27
	K_L	335	1.29	7.67	28.0
	K_F	0.3	0.28	0.23	0.28
	a	0.26	0.46	0.28	0.24
Ethyl acetate	Q_0	0.23	0.06	0.06	0.12
	K_L	2.50	2.95	2.96	1.60
	K_F	0.16	0.04	0.04	0.06
	a	0.44	0.42	0.46	0.53
2,5-Dimethylpyrazine	Q_0	0.18	0.02	0.07	0.06
	K_L	3083	2.96	0.70	4.84
	K_F	0.18	0.02	0.03	0.05
	a	0.25	0.39	0.60	0.32

[a] Q_0, K_L: Langmuir's coefficients. K_F, a: Frendlich's coefficients.

Adsorption Kinetics

Adsorption kinetics of 1-octen 3-ol on the four studied polymers were investigated. Figures 6 and 7 show that the experimental values of concentrations in the solution decrease as a function of time, beginning with the initial concentration of 0.84 $g \cdot L^{-1}$.

The kinetics of trapping on activated carbon, Porapak Q, and Chromosorb 105 were similar, and the equilibrium was effectively reached after approximately 1 hour. On the other hand, for Amberlite XAD-4 resin the establishment of equilibrium took three times longer (180 minutes). This resin has a greater particle size than the other polymers (Table 2), but a similar specific surface area. Hence, the time required for the adsorbate to penetrate into particles is important.

The experimental kinetic results were simulated using an internal–external mass transfer resistance model in the following way. For a stirred tank, the mass balance is

$$-V\frac{dC}{dt} = v\frac{d(\rho\bar{q})}{dt}$$

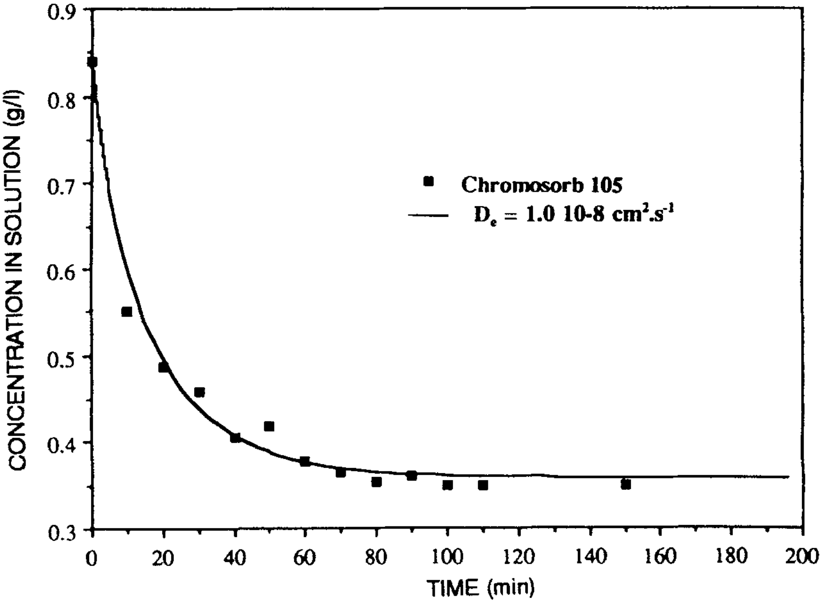


FIG. 6 Experimental results and model calculations for adsorption kinetics of 1-octen 3-ol on chromosorb 105 (C_0 = 0.84 $g \cdot L^{-1}$, m = 10 mg, v = 4 mL).

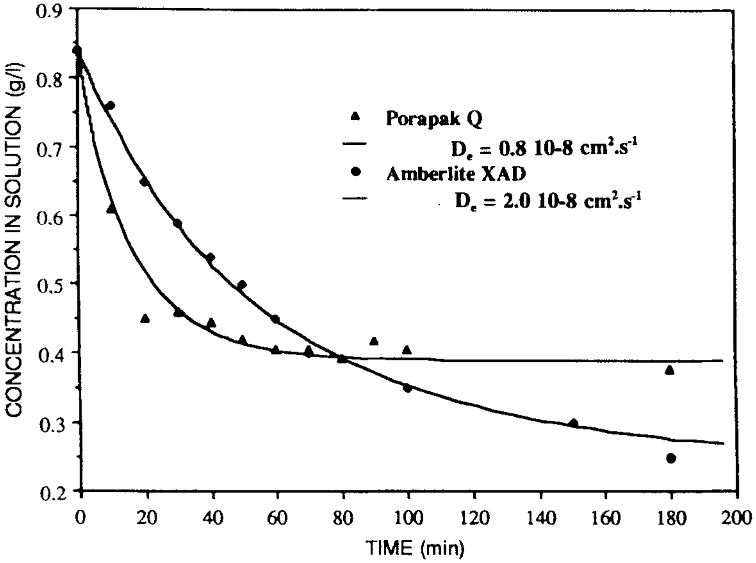


FIG. 7 Experimental results and model calculations for adsorption kinetics of 1-octen 3-ol on Porapak Q and Amberlite XAD-4 (C_0 = 0.84 g·L^{-1}, m = 10 mg, v = 4 mL).

where V is the solution volume, v and ρ are the volume and the density of sorbent, and $\bar{q}$ is the average concentration in the sorbent:

$$\bar{q} = \frac{3}{R^3}\int_0^R qr^2 dr$$

where R is the particle radius and q is the local concentration in the sorbent as a function of time and position.

The intraparticular transport mechanisms for homogeneous diffusion are described by

$$\frac{\partial q}{\partial t} = \frac{D_e}{r^2}\frac{\partial}{\partial r}\left(\frac{\partial q}{\partial r}\right)$$

where D_e is a constant effective diffusion coefficient.

For external mass transfer:

$$\frac{d(\rho\bar{q})}{dt} = \frac{3}{R}k_f(C - C^*),$$

where k_f is the liquid film mass transfer coefficient and C^* is the equilibrium concentration at the interface.

Equilibrium isotherms are obtained and modeled from experiments as shown previously. A group of parameters, including k_f, was estimated by considering that the sorbent is initially free of adsorbate, and therefore $C^* = 0$. Thus,

$$-\frac{1}{C_0}\frac{dC}{dt} = \frac{v}{V}\frac{3}{R}k_f$$

The right-hand side of this equation is estimated from the initial slope of the experimental kinetic values. Model simulations were performed with different values of the internal diffusion coefficient in order to obtain better representations of the experimental results.

Figures 6 and 7 show the simulations together with the experimental points. Good agreement is observed by using a diffusion coefficient value in the 10^{-8} $cm^2 \cdot s^{-1}$ range.

Table 4 compares the values of D_e obtained in this study with those obtained in the literature for other compounds.

Our results are of the same order of magnitude as those obtained by other authors for small molecules on activated carbons. Only a few results are available on polymeric adsorbents. On XAD-4, a value of 1.6×10^{-8} $cm^2 \cdot s^{-1}$ for *p*-chlorophenol has been reported (30).

The values of the diffusion coefficients obtained for 1-octen 3-ol are not a limiting factor for an adsorption process in a column.

Polymer Selectivity

Results of static adsorption for the four aromatic compound mixtures in water at a 500-ppm concentration are presented in Table 5. In mixtures,

TABLE 4
Diffusion Coefficients of Small Molecules in Different Adsorbents

Adsorbent	Solute	Temperature (°C)	Diffusion coefficient (D_e) $\times 10^8$ $cm^2 \cdot s^{-1}$
Activated carbon	Nitrobenzene	20	2 (28)
	n-Butanol	25	8.6 (29)
	n-Pentanol	25	6.2 (29)
Amberlite XAD-4	*p*-Chlorophenol	25	1.6 (30)
	1-Octen 3-ol	25	2[a]
Chromosorb 105	1-Octen 3-ol	25	1[a]
Porapak Q	1-Octen 3-ol	25	0.8[a]

[a] This work.

TABLE 5
Extraction Yield Obtained for Static Adsorption of the Mixture of the Four Aromatic Compounds at 500 ppm Each (multicomponent system)

	Activated carbon	Porapak Q	Chromosorb 105	Amberlite XAD-4
1-Octen 3-ol	50	38.7	43	57.5
Ethyl acetate	4.7	9.3	2.5	3.5
2,5-Dimethypyrazine	5.5	25.2	9.6	3.6
γ-decalactone	91	88.9	84	97

γ-decalactone is strongly adsorbed on all the polymers (from 84% for Chromosorb 105 to 97% for Amberlite XAD-4) to the detriment of 1-octen 3-ol, which was less adsorbed in mixtures than in a binary system with water (Fig. 8).

Once again, the adsorption can be correlated with the solubility in water of the adsorbate: γ-decalactone is preferentially sorbed over 1-octen 3-ol, which in turn is better adsorbed than ethyl acetate and 2,5-dimethylpyr-

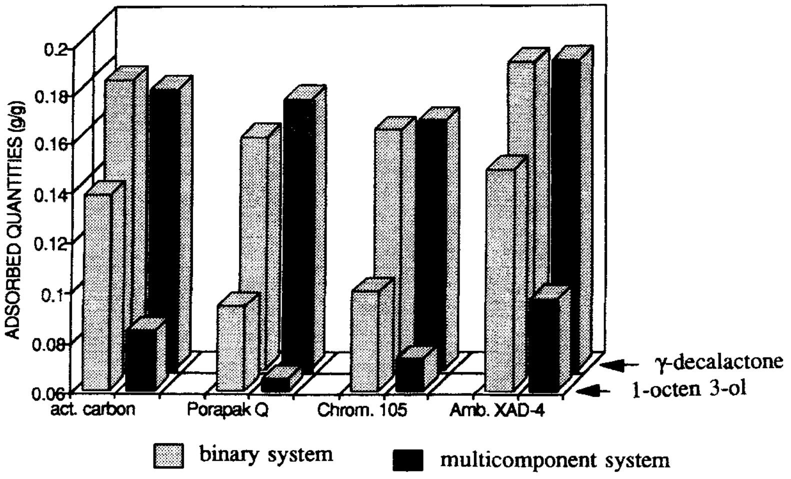


FIG. 8 Comparison of adsorbed quantities of γ-decalactone and 1-octen 3-ol in a binary system (one aromatic compound at 500 ppm + water) and in a multicomponent system (the four aromatic compounds each at 500 ppm + water).

azine. This phenomenon appears to be present in all the sorbents studied although the interaction between the solute and the solvent determines the selectivity of the resin.

CONCLUSION

Sorption on activated carbon or on porous hydrophobic polymers is a suitable method for extracting and concentrating aromatic compounds from an aqueous solution.

It appears that for the aromatic compounds studied (ethyl acetate, 2,5-dimethylpyrazine, 1-octen 3-ol, and γ-decalactone), the sorption efficiency of polymers depends on the nature and the physicochemical characteristics of both:

- The solute: the adsorbed quantities are correlated with the solubilites in water of the solute
- The adsorbent: activated carbon, which has a higher specific surface area and a chemically complex surface, is more efficient at adsorbing than polystyrene-type polymers, except for γ-decalactone which is better adsorbed on Amberlite XAD-4. This polymer, with its smaller pore size diameter, can trap aromatic compounds more efficiently than Porapak Q and Chromosorb 105, which are chemically similar

Adsorption isotherms have been described and correlated by both the Freunlich and Langmuir models except for γ-decalactone. Kinetic experimental results have been simulated for 1-octen 3-ol using an internal–external mass transfer resistance model; good agreement was observed. The diffusion coefficients obtained from the simulation show the possibility of a dynamic adsorption process in a column.

SYMBOLS

a	Freundlich isotherm coefficient
C	concentration of sorbate in aqueous solution ($g \cdot L^{-1}$)
C_0	initial value of C ($g \cdot L^{-1}$)
D_e	effective diffusion coefficient ($cm^2 \cdot s^{-1}$)
K_F	Freunlich isotherm coefficient
K_L	Langmuir isotherm coefficient
k_f	liquid film mass transfer coefficient ($L \cdot g^{-1}$)
m	mass of adsorbent (g)

Q_0	Langmuir isotherm maximum capacity (g·g^{-1} of adsorbent)
q	concentration of adsorbate in sorbent (g·g^{-1} of adsorbent)
R	mean bed radius (cm)
r	radial distance (cm)
t	time (min)
V	volume of solution (mL)
v	volume of sorbent particles (mL)
ρ	apparent density of sorbent (g/mL of particles)

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