

Modeling Activated Carbon Adsorbers for the Control of Volatile Organic Compounds in Indoor Air

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ABSTRACT

A state-of-the-art model was developed to predict adsorption performance of activated carbon adsorbers as they pertain to volatile organic compounds (VOC) control in commercial building applications. The model includes two parts: the first is for calculating indoor VOC concentrations in an occupied space with an adsorber in either mixed or recirculating air locations; the second is physical adsorption of VOC within a carbon adsorber and calculates removal efficiency versus service time. These two parts are linked together by the initial and boundary conditions of the system.

In light of the myriad of VOC mixtures in office buildings, the model along with a component grouping technique was applied to representative compounds to seek VOC efficiency and service life on the basis of total concentration.

INTRODUCTION

HVAC-compatible activated carbon adsorbers are being considered more and more frequently as a strategy for reducing indoor concentrations of volatile organic compounds (VOC) as well as other gaseous contaminants in commercial building applications. The drive for this is at least twofold: (1) outdoor air in many urban settings is of unacceptable quality for ventilation, and (2) filtration of recirculation air may be an energy-conserving alternative to augment dilution with outdoor air alone.

When such adsorbers are considered, two questions are raised: (1) what is the basis for determining required efficiency to achieve acceptable indoor air quality, and (2) which compound(s) should be used to represent VOC efficiency and adsorption capacity, given the fact that VOC mixtures in office buildings contain a large number of compounds?

The first question has been addressed with a two-step design method (Yu *et al.* 1991) using the concept of achieving indoor air quality equivalent to "100 percent" outdoor air, introduced in ASHRAE Standard 62-81. The method applies to both particulates and gases. Here, "100 percent" outdoor air is defined as the amount of fresh outdoor air deemed necessary to achieve the acceptable air quality by dilution alone, and it is not limited to the values given in Table 2 of ASHRAE Standard 62-89.

This study addresses the second question. A state-of-the-art model was developed to predict adsorption performance of activated carbon adsorbers as they pertain to VOC control in recirculation systems. The model along with a component grouping technique was applied to representative compound(s) to seek VOC efficiency and service life on the basis of total concentration. In addition, equilibrium adsorption capacity and mass transfer of VOC at ppb concentrations will be analyzed.

THEORETICAL CONSIDERATIONS

The model consists of two parts. The first part is for calculating indoor VOC concentrations in an occupied space with a carbon adsorber in either mixed or recirculating air positions (Figure 1). The second part is physical adsorption of VOC within a carbon adsorber and calculates removal efficiency versus service time. The model equations are given in the following sections.

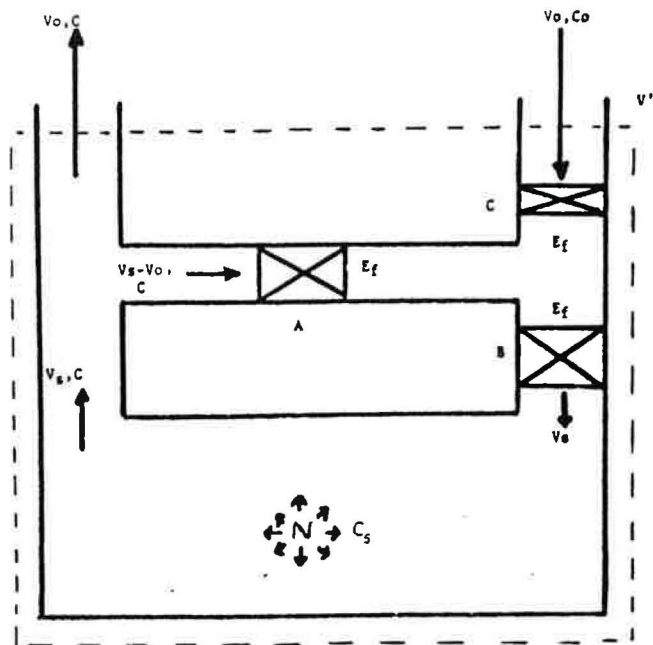


Figure 1 Filter location in single zone

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Indoor VOC Concentrations

When a carbon adsorber is located in a mixed air position (location B, Figure 1), the steady-state total concentration of a VOC mixture in an occupied space is (Yu 1990):

$$C_s = \frac{KG + C_o V_o (1 - E_f)}{V_o + E_f (V_s - V_o)} \quad (1)$$

and

$$K = \frac{(1-E_v)(1-E_f)(V_o/V_s) + [(1-E_v)E_f + E_v]}{E_v} \quad (2)$$

It should be noted that Equation (1) does not include the terms for surface adsorption or desorption. However, the term G in Equation (1) may be interpreted as net generation rate of VOC mixture.

Carbon Adsorber

The mass balance equations of component i within a carbon bed may be written:

$$\frac{\partial C_i}{\partial t} + \frac{U}{\epsilon} \frac{\partial C_i}{\partial z} + \frac{\rho_b}{\epsilon} \frac{\partial Q_i}{\partial t} = 0 \quad (3)$$

$$\frac{\partial Q_i}{\partial t} = \bar{K}_{si} (\bar{Q}_i - Q_i) = K_{si} (C_i - C_{ip}) \quad (4)$$

Adsorber efficiency on the basis of total VOC concentration is:

$$E_f(t) = 1 - C(L,t)/C(O,t) \quad (5)$$

The multicomponent adsorption theory is used to describe the competitive adsorption of a VOC mixture (Grant and Manes 1972). The equilibrium adsorption capacity of each component may be calculated from the following equations using an iteration procedure.

$$\frac{1}{\beta_1} \ln \frac{(X_1 C_{v1})}{C_1} = \frac{1}{\beta_2} \ln \frac{(X_2 C_{v2})}{C_2} = \dots = \frac{1}{\beta_n} \ln \frac{(X_n C_{vn})}{C_n} \quad (6)$$

$$\sum_{i=1}^n X_i = 1 \quad (7)$$

$$E = \frac{RT}{\beta_1} \ln \frac{(X_1 C_{v1})}{C_1} \quad (8)$$

$$V_{ads} = W_o \exp(-\alpha E^2) \quad (9)$$

$$N_T \left(\sum_{i=1}^n X_i V_i \right) = V_{ads} \quad (10)$$

$$N_i = N_T X_i \quad (11)$$

$$\bar{Q}_i = N_i M_i \quad (12)$$

The $D-R$ equation is used to relate equilibrium capacity to adsorption energy as shown in Equation (9) (Dubinin and Raduskevich 1947). In essence, the $D-R$ equation is a characteristic curve of activated carbon expressed in a function form. Alternately, the characteristic curve of a given carbon can be determined from the adsorption experiments, and the data can be fitted into a polynomial form.

To account for the effect of relative humidity, adsorption energy [Equation (8)] is empirically modified as:

$$E = \frac{RT}{\beta_1 F} \ln \left(\frac{X_1 C_{v1}}{C_1} \right) \quad (13)$$

where

$$F = a [1 + \ln(1/RH)] \quad (14)$$

The rate of adsorption in Equation (4) is expressed by a linear driving force. The mass transfer coefficient of component i (K_{si}) based on gas phase concentrations is related to film and pore diffusions in series:

$$\frac{1}{K_{si}} = \frac{R_p}{3 K_{fi}} + \frac{R_p^2}{15 D_{pi}} \quad (15)$$

and

$$\bar{K}_{si} = K_{si}/S_i \quad (16)$$

$$Sh = \frac{2K_{fi}R_p}{D_{mi}} = 2.0 + 0.6 S_c^{0.333} Re^{0.5} \quad (17)$$

$$D_{pi} = e_p D_{mi}/Z_p \quad (18)$$

EXPERIMENTAL AND MODEL RESULTS

Model Verification

At present, no data are available to test the model in a recirculation system. Nevertheless, the model will be compared with the experimental breakthrough data obtained from a few simple adsorption systems in a once-through mode. Prior to the model verification, it must be stressed that the affinity coefficient β of a specific compound, the pore structure coefficient α , and tortuosity Z_p of the coconut carbon used were deduced by fitting the model with the experimental breakthrough data (118 and 15 ppm heptane on 1-in. carbon beds at 50 fpm). Once these parameters were determined, the model was then compared with other breakthrough data. The experimental apparatus and procedures were described in a previous paper (Liu 1990).

Figure 2 tests the model at different bed depths (but the same residence time). As shown in Figure 2, the model deviations are larger for shorter bed depth/lower velocity. This may indicate the importance of axial dispersion at such conditions. Axial dispersion is not incorporated in the model.

Figure 3 tests the model at 0.71 ppm heptane. Figure 4 tests the model for competitive adsorption, a two-component system. Again, the affinity coefficient of decane was determined from its single component breakthrough curve. Figure 5 tests the model for a carbon adsorber, which consists of four 2 by 2-ft panels of 1.75-in. thickness in zigzag configuration within a standard size housing. The test was conducted in an ASHRAE test duct (once-through mode) during working hours, using 100% outdoor air (it was shut down at night and on weekends).

The flow diagram of the test apparatus is shown in Figure 6. Toluene concentration upstream of the adsorber was generated by passing the air through the bubbler (containing liquid toluene) at a low flow rate, then mixing it with 2000 cfm outdoor air. The upstream concentration of toluene was controlled by a mass flow meter (0 to 20 lpm).

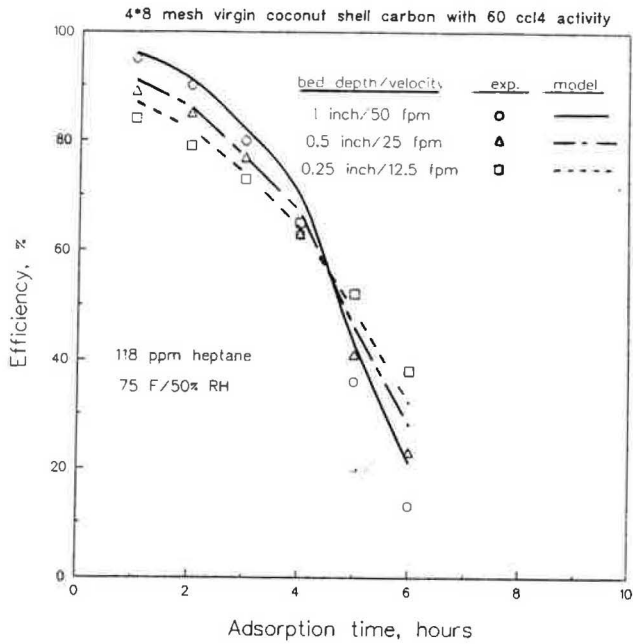


Figure 2 Efficiency curves of heptane at same residence time

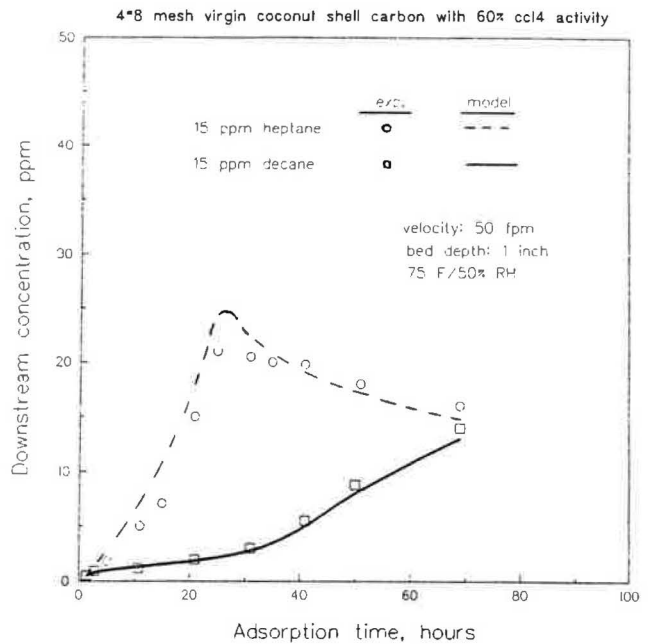


Figure 4 Breakthrough curves of a two-component system

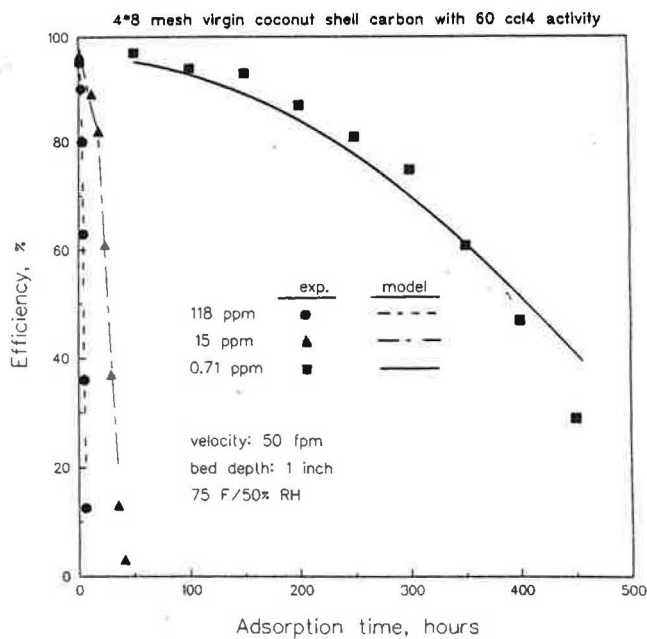


Figure 3 Efficiency curves of heptane at various concentrations

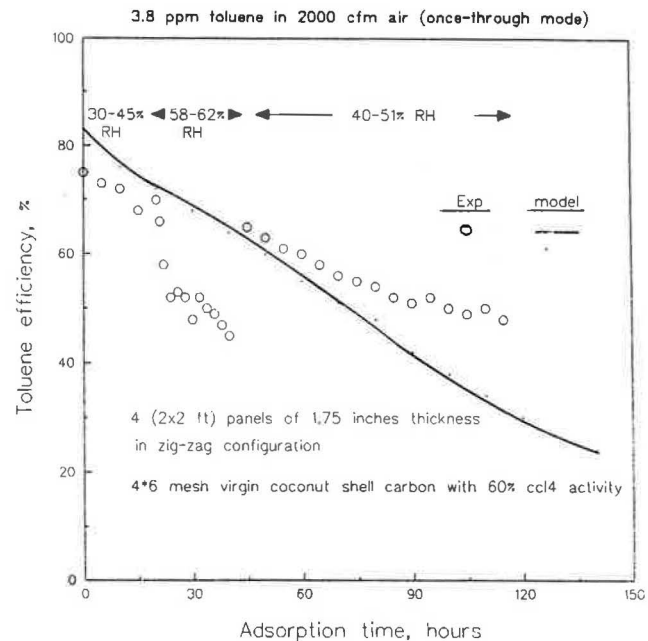
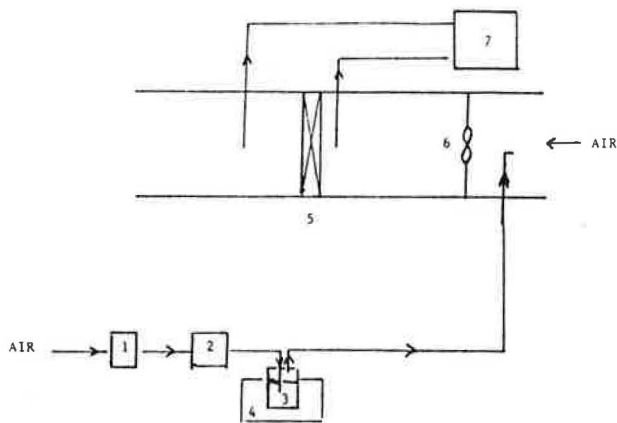


Figure 5 Toluene efficiency curve of a commercial carbon adsorber

A fan was used to ensure the complete mixing of toluene concentration inside the ASHRAE duct. A gas chromatograph (Shimadzu GC-14A with FID detector) was used to continuously monitor the removal efficiency of the adsorber. The relative humidity of outdoor air was uncontrolled but recorded. The total amount of carbon is 48 lbs. The model assumes the flow velocity is uniform across the carbon panels. For the model calculations, 50% rh was used.

Adsorption of a Single Component at ppb Concentrations

Although the model has not been tested at typical indoor concentrations (low ppb range), the insights of low concentration adsorption may be delineated by model simulations. This was done for a 1.5-in. carbon bed challenged with 100 ppb toluene at 125 fpm in a once-through mode. The carbon packing density is 0.46 g/cc. The concentration and loading profiles at different service times



1. Particulate filter
2. Mass flow meter
3. Bubbler (contains organic liquid)
4. Water bath
5. Carbon adsorber
6. Fan
7. Gas chromatograph

Figure 6 Flow diagram of test apparatus for carbon adsorber

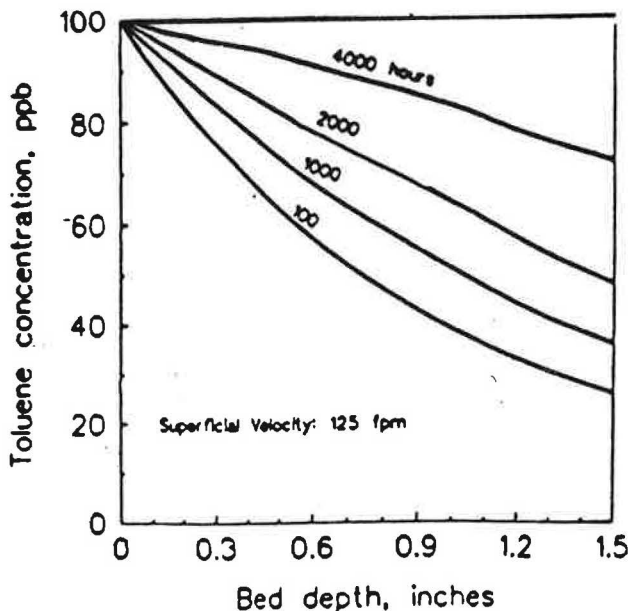


Figure 7a Toluene concentration profile within carbon bed

are shown in Figures 7a and 7b, respectively. The concentration profiles reveal typical behavior of what may be expected on adsorber efficiency. The initial efficiency is about 80%, which indicates that the length of the mass transfer zone is larger than the bed depth. As adsorption proceeds, the efficiency decreases very slowly. It takes 4000 h for the downstream concentration to increase from 20 to 72 ppb (or for efficiency to decrease from 80 to 28%), because the ratio of the equilibrium adsorption capacity to the concentration is so great that the concentration profile travels at an extremely slow rate. The uptake of toluene is also a slow process. The toluene loading at the leading edge of the bed has not even reached its equilibrium loading (14% wt) after 4000 h. This slow uptake is nothing but a starvation problem, *i.e.*, the mass flow rate of toluene

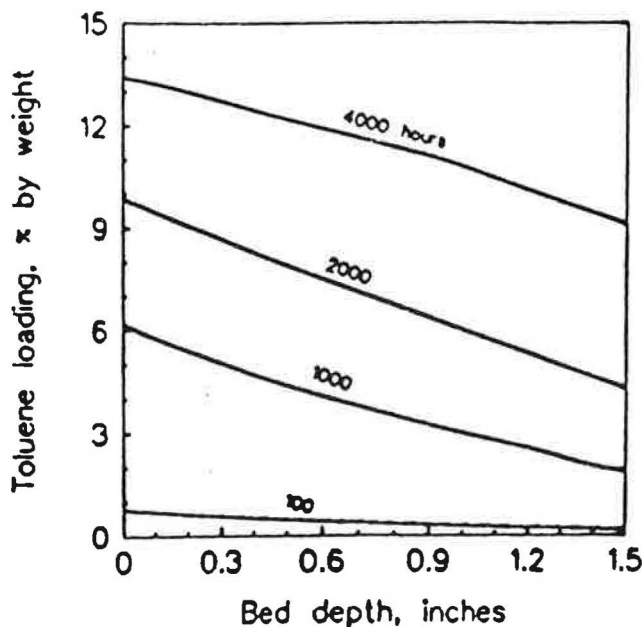


Figure 7b Toluene loading profiles within carbon bed

available for adsorption is too low compared to the amount that can be adsorbed.

Initial efficiency of a compound is primarily determined by flow velocity, carbon bed depth, carbon particle size, packing density, and relative humidity. For most compounds, the concentration and type of compound have either an insignificant or no effect on initial efficiency, except for large molecule size compounds (*e.g.*, two or three benzene rings). These compounds may have lower initial efficiencies due to the molecule sieving effect. The rate at which efficiency decreases with time (service life) is inversely proportional to the ratio of equilibrium capacity to concentration of a given compound.

Component Grouping

Adsorption of the office's VOC mixture in a carbon bed is very complicated and perhaps unmanageable if one attempts to track the efficiency and service life of individual compounds. However, if control criteria are set at total VOC concentration, methods are available to simplify it. The breakthrough curve of a complex VOC mixture in terms of total concentration may be represented by that of a single or a few compounds using component grouping techniques. This technique was first introduced by Tian *et al.* (1984, 1986) in the area of wastewater and groundwater purification with fixed-bed activated carbon adsorbers. They used a concentration-weighted average technique to reduce a large number of volatile organic compounds present in water to a few representative compounds. The resulting breakthrough curves in terms of total VOC concentration were in excellent agreement.

Now, the principle of this technique is being applied to vapor phase applications. To illustrate the technique, 20 compounds are selected and shown in Table 1. This VOC mixture covers the normal boiling point ranging from 56 to 235°C, and various types of VOC; aromatic, aliphatic, oxygenated, and chlorinated hydrocarbons. These compounds are listed in the order of increasing boiling point, and equal volumetric concentration is assigned to each

TABLE 1
List of VOC Compositions and HVAC Operating Conditions

(1) VOC Compositions		
Compound	Boiling Point, °C	Generation Rate, mg/h
Acetone	56	52
Chloroform	61	106
1,1,1-trichloroethane	74	120
MEK	80	62
Benzene	80	70
Cyclohexane	81	75
TCE	87	117
Heptane	98	89
Toluene	110	81
MIBK	117	89
Perc	121	147
Ethyl benzene	136	94
Xylene	139	94
Styrene	145	92
Nonane	151	113
Cumene	152	102
Cyclohexanone	156	87
1,3,5 trimethyl benzene	165	106
Decane	174	126
Tridecane	235	163
Total 2000 (mg/h)		

- (2) Carbon adsorber: 1.2-in. carbon bed, 125 fpm superficial velocity, packing density of 0.46 g/cc, virgin coconut shell carbon with 60 CCl₄ activity, located in a mixed air position.
- (3) Total supply air V_s: 2000 cfm (100 cfm/person)
- (4) Outdoor air V_o: 100 cfm (5 cfm/person)
- (5) Ventilation effectiveness E_v: 1
- (6) Office space: 3000 ft² with 20 occupants
- (7) Temperature/relative humidity: 75°F/50%

compound. The total internal VOC generation rate is 2000 mg/h and outdoor VOC concentration is assumed to be zero. The supply air is 2000 cfm, with 5% outdoor air. With an occupant density of 7 persons/1000 ft², this simulates an office space of 3000 ft² with 100 cfm/person supply air and 5 cfm/person outdoor air. The relative humidity and temperature of supply air are 50% and 75°F, respectively. The ventilation effectiveness equals unity.

It should be noted that the VOC composition and generation rate chosen for component grouping is only for the purpose of illustration. It does not necessarily represent actual VOC in a typical office building.

These 20 compounds are grouped into two cases. Case 2 consists of 4 grouped components—component A represents the mixture from acetone to cyclohexane; component B, the mixture from trichloroethylene to mibk; component C, the mixture from perc to nonane; and component D, the mixture from cumene to tridecane. The diffusional (diffusivity) and adsorptive properties (vapor pressure, affinity coefficient, molecular weight, and liquid molar volume) of the grouped components are calculated from their respective mixture, using a concentration-weighted average method. The concentration (or generation rate) of the grouped component is the sum of individual concentrations (or generation rates) in that mixture. Case 1 is done in the same way, except that it uses a single component to represent the entire mixture.

The model is used to calculate the indoor total VOC concentrations for the original VOC mixture (20 compounds) and Cases 1 and 2. The comparison of efficiency curves is shown in Figure 8. As shown in this figure, the efficiency curve of 4 grouped components is very close to that

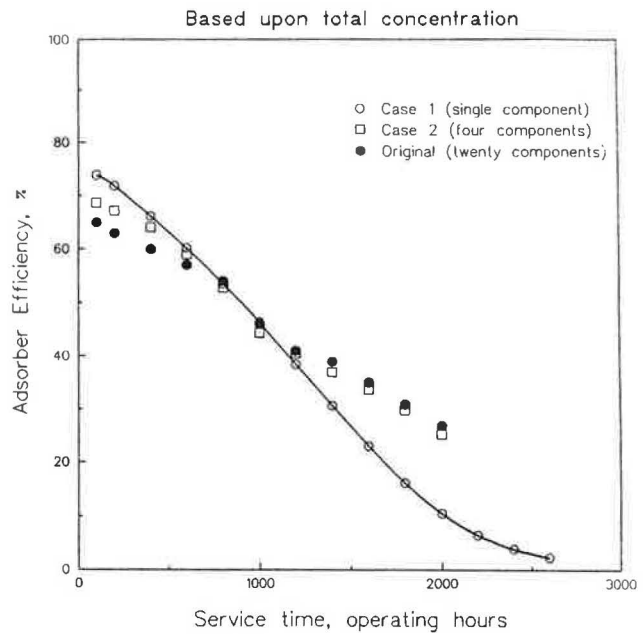


Figure 8 Comparisons of efficiency curves

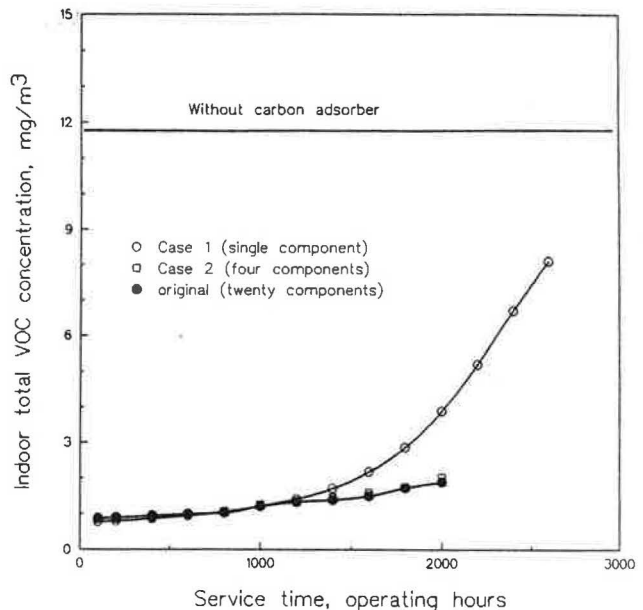


Figure 9 Comparisons of indoor VOC total concentrations

of the original 20 compounds. However, the use of a single component (Case 1) still yields a satisfactory comparison. The corresponding total VOC concentrations are shown in Figure 9. The breakthrough of indoor VOC concentration occurs when the adsorber efficiency drops below 30%. This is also the efficiency or time that the indoor concentration of Case 1 starts to deviate from that of the original mixture. For this particular case, the deviation of service time at the same breakthrough concentration is about 25% (1400 versus 1800 h). In percentage, the deviation is smaller when outdoor air is increased or when supply air is decreased.

For the purpose of estimating VOC efficiency and service life of a carbon adsorber, the use of a single component is considered adequate. In this regard, toluene is

recommended as the representative compound for VOC mixtures in commercial buildings. The basis for this is:

- The concentration-weighted average boiling point of 35 common volatile organic compounds generated from buildings is 107°C (Shah and Singh 1988).
- The concentration-averaged boiling point of organic bioeffluents from occupants is 106°C (Wang 1975).
- The boiling point of toluene is 110°C. In addition, toluene is a water-immiscible compound (subject to relative humidity effect) and has average molecular weight, liquid density, and affinity coefficient.

Once the representative compound(s) is chosen, the service life of a carbon adsorber may be determined from the available information on VOC concentrations in commercial buildings. Based on hundreds of air samples taken from a large number of office buildings in four separate studies (Weschler *et al.* 1990, Knoppel *et al.* 1989, Morey *et al.* 1989, and Grot *et al.* 1989), 80 to 90% of the buildings studied have total VOC concentrations between 0.25 and 1 mg/m³. The remaining 10 to 20%, new buildings and high human-related activity buildings, have 1 to 5 mg/m³. Assuming 10 cfm/person outdoor air, occupancy density of 7 people/1000 ft², ventilation effectiveness of 0.65 (Rask 1989) and negligible outdoor VOC concentrations, the VOC generation rates are estimated in the range of 100 to 400 mg/h-3000 ft² and 400 to 2000 mg/h-3000 ft² for low and high VOC office buildings, respectively.

With the above information and use of toluene as a representative compound, carbon usage rates are estimated for office buildings where VOC are generated primarily from internal sources. This is shown in Table 2 for the coconut shell carbon used for various VOC generation rates and adsorber efficiencies. Considering the swing of relative humidity in HVAC systems (30 to 50% in winter and 40 to 60% in summer), the carbon usage rates in Table 2 are based on 60% of its saturation (equilibrium) adsorption capacity determined at 50% rh. Since carbon service life is longer when the percentage of outdoor air is increased, the carbon usage rate at different outdoor air is divided by its normalized correction factor shown in Table 2.

TABLE 2
ESTIMATED CARBON USAGE RATES
FOR OFFICE BUILDINGS
(BASED ON TOLUENE)

VOC Generation Rate, mg/h-3000 ft ²	*Carbon Usage Rate, lbs/year-3000 ft ² , Average Adsorber Efficiency, %		
	85	50	10
100	9	8	6
400	29	27	20
800	53	50	—
1600	100	93	—

*Based on virgin coconut shell carbon of 60 CCl₄ activity, 5% outdoor air, and 1 year = 4000 HVAC operating hours.

Outdoor Air, %	Normalized Correction Factor		
	85	50	10
5	1.00	1.00	1.00
10	1.05	1.10	1.22
15	1.13	1.19	1.41
20	1.19	1.22	1.54

DISCUSSION

The experimental breakthrough data used for model verification are limited to low ppm and high ppb concentrations. Since VOC concentrations in most commercial buildings are in the low ppb range, it is pertinent to discuss the behavior of equilibrium adsorption capacity and mass transfer with regard to VOC concentrations.

The adsorption of VOC on microporous solids such as activated carbon is known as a liquid-filling process. The adsorption capacity (cc of liquid per unit weight of carbon) of a compound is equal to the cumulative micropore volume V_{ads} to a pore size r , which has the same adsorption energy E as that required to compress the molecules from the gas phase into a liquid in the micropores. As the concentration or boiling point of a compound decreases or as the temperature increases, the required work for condensation is increased too. Consequently, the adsorption capacity is lower, since only the smaller micropores have enough energy to participate in pore-filling adsorption. This may be understood by examining the following relationships:

$$E = \frac{RT}{\beta} \ln(C_v/C)$$

$$RT \ln(C_v/C) = \frac{2\sigma V \cos(\theta)}{r} \quad (\text{Kelvin Equation})$$

or

$$E = \frac{2\sigma V \cos(\theta)}{\beta r}$$

$$V_{ads} = W_o \exp(-\alpha E^2)$$

Where σ and V are surface tension and liquid molar volume of adsorbate, θ is the contact angle, and r is the pore radius.

As shown above, adsorption conditions determine the adsorption energy E or the largest pore size r that can participate in liquid-filling adsorption. The characteristic curve or micropore size distribution of activated carbon determines the volume V_{ads} of micropores available at a given adsorption energy or pore size. The $D-R$ equation assumes that the characteristic curve of activated carbon takes the form of Gaussian distribution.

In essence, the adsorption of VOC mixtures at a low ppb range can only use a portion of the total micropore volume. The micropore size distribution of a typical virgin coconut shell carbon of 60% CCl₄ activity is shown in Figure 10. If the average boiling point of VOC mixtures in office buildings is assumed to be 110°C (e.g., toluene), the adsorption capacity at 50% rh is 17 cc/100g carbon or 14% wt at 100 ppb total concentration. This amounts to 40% of the total micropore volume. Figure 10 also shows that the toluene isotherm is still highly nonlinear at low ppb concentrations (e.g., 10% wt at 10 ppb). In one study (Graham 1990), the reported adsorption capacity of carbon samples serving HVAC applications (office building, hospital, and library) were 4 to 15% wt at estimated VOC concentrations between 10 and 150 ppb. Their lower loading data are usually accompanied by higher water loadings, an indication of high relative humidity applications.

It is advantageous to use coconut shell activated carbons because of their superior micropore structure. Virgin coconut shell carbon, activated to 60 CCl₄ activity in

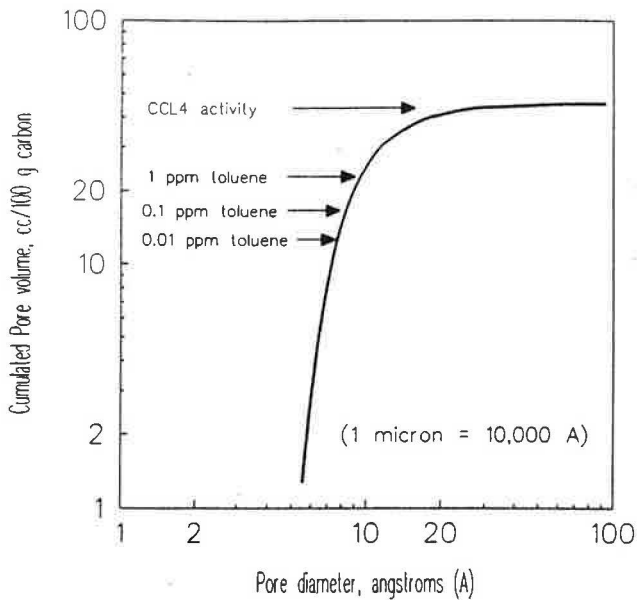


Figure 10 Micropore structure of 60 CCl_4 activity—Coconut shell carbon

manufacture, is the recommended choice of activated carbon for VOC control in commercial building applications. Overactivated or improperly regenerated carbons may actually have a lower usable micropore volume even though they have the same or higher CCl_4 activity.

Mass Transfer at Low ppb Concentrations

The length of the mass transfer zone of a compound is independent of its challenging concentration. Since the length of the mass transfer zone is determined by the rate of adsorption (into the carbon) against its mass flow rate (along the carbon bed), as the concentration decreases, the rate of adsorption expressed by a linear driving force is proportionally decreased (but mass transfer coefficient K as well as the mass flow rate of the compound remain the same) (Figure 2). In Figure 3, the initial efficiencies (an indicator for length of mass transfer zone) are about the same as the heptane concentration decreases from 118 ppm to 0.71 ppm.

Multicomponent adsorption of VOC mixtures is competitive in nature, since the mixtures are all adsorbed in the same adsorption space, *i.e.*, in the micropores. If the control of VOC is based on total concentration, the effect of competitive adsorption is neutralized, and the adsorption capacity may be estimated from the concentration-weighted average method, as shown in this study. This effect becomes unfavorable and adsorption capacity is lower if the control is based on weaker components; the reverse is true if based on stronger components.

It seems that the recent trend of health studies on VOC favors the use of total concentration. Molhave (1990) uses total concentration in his tentative health guideline for VOC.

CONCLUSIONS

The framework of the carbon bed modeling shows that the adsorption of a complex VOC mixture can be represented by a few compounds or even by a single compound with the aid of a component grouping technique. Based on data of existing VOC compositions in office build-

ings, toluene is selected as the representative compound for rating VOC efficiency and adsorption capacity of activated carbon adsorbers. This greatly simplifies the use of activated carbon for commercial building applications.

For the lack of low concentration VOC sensors at the present time, the calculated data in Table 2 is recommended for carbon service life in office buildings where VOC are generated primarily from internal sources. However, it is only applicable to virgin coconut shell carbon with 60 CCl_4 activity.

NOMENCLATURE

- a = empirical coefficient in the modified $D-R$ equation (reflecting the affinity of activated carbon toward water vapor)
- $C_i(z,t)$ = concentration of component i within the carbon bed
- $C(o,t)$ = total VOC concentration upstream of carbon adsorber
- $C(L,t)$ = total VOC concentration downstream of carbon adsorber
- C_{ip} = concentration of component i in the interior of a carbon particle
- C_o = total VOC concentration from outdoor air
- C_s = total VOC concentration in occupied space
- C_{vi} = vapor pressure of component i
- D_{mi} = gas phase diffusivity of component i
- D_{pi} = pore diffusivity of component i
- E = adsorption energy in potential theory
- E_f = adsorber efficiency based on total upstream and downstream VOC concentrations
- E_v = ventilation effectiveness, defined as fraction of supply air delivered to occupied space
- G = net generation rate of total VOC within an occupied space
- G_i = net generation rate of component i within an occupied space
- \bar{K}_{si} = overall mass transfer coefficient of component i based on adsorbed phase concentration (loading)
- K_{si} = overall mass transfer coefficient of component i based on gas phase concentration
- K_{fi} = mass transfer coefficient of component i for boundary layer (film) diffusion
- L = length of carbon bed
- M_i = molecule weight of component i
- n = number of components in VOC mixture
- N_i = moles of component i adsorbed on carbon
- N_T = total moles of VOC mixture adsorbed on carbon
- $Q_i(z,t)$ = loading of component i within the carbon bed
- Q_i = equilibrium adsorption capacity of component i based on local concentration
- R = gas constant
- R_p = particle size of activated carbon
- rh = relative humidity of airflow, fractional value
- S_i = ratio of equilibrium loading to concentration for component i
- T = adsorption temperature
- t = time
- U = superficial velocity of air through carbon bed
- V_o = flow rate of outdoor air
- V_s = flow rate of supply air, defined as the sum of recirculation and outdoor airflow rates
- V_{ads} = equilibrium adsorption capacity of VOC mixture based on local concentrations
- V_i = liquid volume of component i
- W_o = total micropore volume of activated carbon
- X_i = mole fraction of component i adsorbed on carbon
- z = axial direction of carbon bed
- Z_p = tortuosity of activated carbon
- ϵ = void fraction of carbon bed

β_i = affinity coefficient of component i
 α = pore structure coefficient in the $D-R$ equation
 ϵ_p = porosity of activated carbon
 ρ_b = packing density of carbon bed
 Sh = Sherwood number
 Sc = Schmidt number
 Re = Reynolds number

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