

Modelling of a Passive Adsorption Sheet to Purify Indoor Air

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Abstract

In this paper the use of a thin adsorbent sheet composed of activated carbon particles to purify indoor air is modelled. A loose sheet with high porosity appears more effective than a dense one. The carbon sheet can be replaced by a fresh sheet after a certain period of use, thus keeping the volatile organic compound (VOC) level low in the remaining years. The model has been used to predict the optimal replacement time. Binary VOCs are modelled. The results turn out to be close to those from single component calculations, which suggests that the efficiency of the carbon sheet to one VOC is negligibly affected by the presence of other VOCs at ppb levels.

KEY WORDS:

Indoor air purification, Adsorption, Compartment model, Binary VOCs, Replacement of adsorbent sheet

Introduction

Volatile organic compounds (VOCs) emitted from modern building materials or household cleaning agents into indoor air can cause health problems. Some sorbing materials such as furniture, books and curtains in a building will sorb and reemit VOCs, thus extending the presence of VOCs in indoor air (Neretnieks et al., 1993; Christiansson et al., 1992). Ventilation in ordinary dwelling houses is often insufficient to reduce VOC levels.

In a previous study we investigated the effect of a thin adsorbent sheet composed of activated carbon particles on reducing the concentration of a VOC in a hypothetical ventilated room containing a VOC-emitting source as well as sorbing materials (Yu and Neretnieks, 1993). A mathematical model was used to simulate the emission and sorption processes. We concluded that an activated carbon sheet can reduce the concentration of the VOC. On the other hand, it was shown that when a dense sheet with its porosity equal to 0.4 is used, the resistance to mass transfer in the laminar gas film surrounding the activated carbon sheet and in the stagnant void gas in the sheet will decrease the adsorption rate significantly, thus limiting the efficiency of the activated carbon sheet.

In this paper we model an activated carbon sheet that has a loose structure with its porosity equal to 0.9. The high porosity of the sheet increases the airflow through the voids between the activated carbon particles. Consequently the mass transfer into the sheet is not only by diffusion through the gas film and the voids, but also by convective flow. We intend to learn whether it will raise the effect of the activated carbon sheet.

With the mathematical model we are to analyse the placement scheme of the activated carbon sheet. Instead of placing a large sheet once and for all, we put a smaller sheet into the hypothetical room, and replace it with a fresh one after a period of time.

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The aim is to see which scheme is most appropriate and what replacement time is optimal if the latter scheme is employed.

Usually more than one VOC is present in indoor air. The VOC less strongly adsorbed by the adsorbent would probably be displaced by a stronger one, thus making the adsorbent sheet inefficient to the weaker VOC. In this work we model also the binary situation with the adsorption equilibria to be expressed by the multicomponent Langmuir isotherm.

Methods

The Hypothetical Room

The hypothetical room contains a PVC flooring which is the initial emission source of the VOC 2-ethylhexanol, an activated carbon sheet, walls, a door, a ceiling, tables, drawers, book-shelves, books, binders, filing cabinets, curtains, and some stuffed furniture that functions as sorbing and re-emitting material. The ventilation rate is assumed to be 0.5 exchanges per hour. The adsorbent sheet is assumed to be composed of activated carbon particles of 1 millimeter in diameter. One placement scheme of the activated carbon sheet is that one $2 \times 5 \times 0.002 \text{ m}^3$ sheet is placed in the room all the time. Alternative schemes are that the sheet is divided into two sheets, $2 \times 2.5 \times 0.002 \text{ m}^3$ each, with one of them being placed from the beginning and then replaced by the other after some time. The porosity of the activated carbon sheet is 0.9. The sizes and properties of the other objects in the room are the same as in the previous work (Yu and Neretnieks, 1993).

The Mathematical Model

The mathematical model is an adaptation of the compartment model proposed by Romero et al. (1991). Based on the compartment model, the system is represented by a number of compartments in contact with each other. The compartments are porous media that have absorption/adsorption capacities to the VOCs, depending on the VOC concentrations in the pore volumes of the compartments. The mass transfer in the compartments is assumed by diffusion in general and by fluid flow in some cases. The mass flux between two adjacent compartments is described by a linear-driving-force approximation. The air in the room is represented by a compartment. Each piece or each type of building material and each piece of furniture is represented by one or more compartments. The activated

carbon sheet is represented by two compartments, one for the interparticle voids and the other for the carbon particles. The whole room is represented by 23 compartments in the model. A more detailed description of the model is referred to elsewhere (Yu and Neretnieks, 1993).

The equation of mass balance for each compartment can be generally expressed as

$$\frac{dc_i}{dt} = \frac{1}{V_i[\varepsilon_i + (1 - \varepsilon_i)K_i]} \sum_{j \neq i} k_{ij}(c_j - c_i) \quad (1)$$

where c_i = gas phase concentration in the compartment i , c_j = gas phase concentration in the compartment j that is in contact with the compartment i , t = time, k_{ij} = mass transfer coefficient, V_i = volume of the compartment i , ε_i = porosity, and K_i = sorption equilibrium constant.

For the compartment representing the room air, the porosity is unity and there is a ventilation term for the mass balance equation:

$$\frac{dc_i}{dt} = \frac{1}{V_i} \sum_{j \neq i} k_{ij}(c_j - c_i) - \frac{Fc_i}{V_i} \quad (2)$$

where F = the flow rate of ventilation.

The equilibrium relation for adsorption of the VOC on activated carbon is usually nonlinear. Therefore the equilibrium constant K_i is substituted with the tangent of the adsorption isotherm curve, which is a function of the concentration.

The mass transfer coefficient k_{ij} is expressed as

$$k_{ij} = A_{ij} / \left[\left(\frac{\Delta x}{D} \right)_i + \left(\frac{\Delta x}{D} \right)_j \right] \quad (3)$$

where A_{ij} = contact area between compartments i and j , Δx = mass transfer distance, and D = diffusion coefficient of the VOC.

When a considerable amount of air flows through the activated carbon sheet, the mass transfer coefficient for the mass transfer between the room air and the interparticle voids should include a flow term:

$$k_{ij} = A_{ij} u + A_{ij} / \left[\left(\frac{\Delta x}{D} \right)_i + \left(\frac{\Delta x}{D} \right)_j \right] \quad (4)$$

where u = airflow velocity in the voids.

The mass transfer distance from the interparticle voids to the outer surface of the carbon particles is

estimated by the following equation based on the Carberry equation (Carberry, 1960):

$$\Delta x = d_p / (1.15 \text{Re}^{1/2} \text{Sc}^{1/3}) \quad (5)$$

where d_p = diameter of the particles, Re = the Reynolds number, and Sc = the Schmidt number.

The contact area between the room air and the interparticle voids is equal to the total outer surface area (both sides) of the carbon sheet times the porosity. The contact area between the interparticle voids and the carbon particles is equal to the total outer surface area of all carbon particles.

Simultaneous Adsorption of Two VOCs

When there are two VOCs present in indoor air, both VOCs will compete for the adsorption surface of the activated carbon sheet. Consequently the adsorption equilibrium relation will be affected by both components. To simulate the simultaneous adsorption process, we use the multicomponent Langmuir isotherm to describe the binary adsorption equilibrium:

$$c_{si} = \frac{c_{mi} b_i c_{ai}}{1 + b_1 c_{a1} + b_2 c_{a2}} \quad i = 1, 2 \quad (6)$$

where c_{s1} , c_{s2} = adsorbed phase concentrations of components 1 and 2, c_{m1} , c_{m2} = limiting adsorbed phase concentrations, b_1 , b_2 = single component adsorption constants, and c_{a1} , c_{a2} = gas phase concentrations of components 1 and 2 in the particle pores.

The mass balance equation for the compartment representing the carbon particles becomes

$$V_a \varepsilon_a \frac{dc_{ai}}{dt} + V_a (1 - \varepsilon_a) \left(\frac{\partial c_{si}}{\partial c_{a1}} \frac{dc_{a1}}{dt} + \frac{\partial c_{si}}{\partial c_{a2}} \frac{dc_{a2}}{dt} \right) = k_{avi} (c_{vi} - c_{ai}) \quad i = 1, 2 \quad (7)$$

where V_a = volume of the compartment, ε_a = porosity of the compartment, t = time, k_{av1} , k_{av2} = mass transfer coefficients between the compartment for the interparticle voids and the compartment for the particles, and c_{v1} , c_{v2} = gas phase concentrations of components 1 and 2 in the compartment for the interparticle voids.

For simplicity, in the simulation of two VOCs we assume that the hypothetical ventilated room contains only a PVC flooring as the emission source and an activated carbon sheet. Other sorbing materials are not included in this simulation.

Results

In all the calculations the laminar air film over all objects in the room is assumed to be 3.5 cm thick. The airflow velocity in the interparticle voids of the loose carbon sheet is assumed to be 0.01 m/s.

The concentration of 2-ethylhexanol in the room air using a loose activated carbon sheet ($2 \times 5 \times 0.002 \text{ m}^3$, $\varepsilon = 0.9$) is compared with one using a dense sheet ($\varepsilon = 0.4$) with the same dimension (Yu and Neretnieks, 1993) (Figure 1). The concentration is also shown in Figure 1 when a $2 \times 2.5 \times 0.002 \text{ m}^3$ loose carbon sheet is used and replaced by a fresh sheet of similar size after 1 year.

Figure 2 shows the concentrations from sequential placement of two $2 \times 2.5 \times 0.002 \text{ m}^3$, $\varepsilon = 0.9$ sheets with different replacement times. The different placement schemes result in different accumulated exposures to the VOC, which are listed in Table 1.

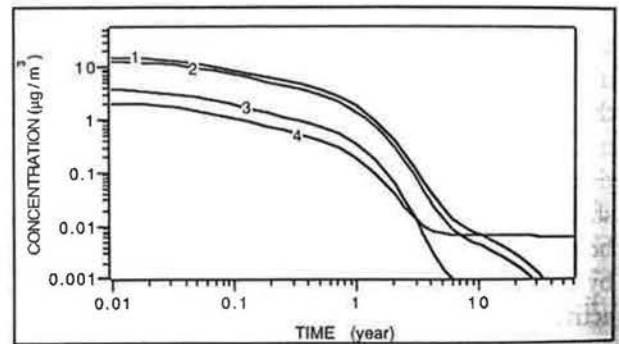


Fig. 1 The concentrations of 2-ethylhexanol in the room air. Without carbon sheet (-1-). With a dense sheet (-2-). With a loose sheet (-4-). With a half-sized, loose sheet, replaced by a fresh sheet after 1 year (-3-).

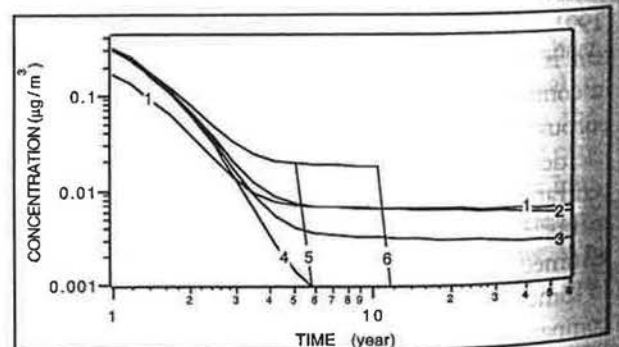


Fig. 2 The concentrations of 2-ethylhexanol in the room air, calculated by assuming placement of a small sheet ($2 \times 2.5 \times 0.002 \text{ m}^3$), replaced by a fresh sheet after 3 months (-2-), 6 months (-3-), 1 year (-4-), 5 years (-5-), and 10 years (-6-). Single large sheet ($2 \times 5 \times 0.002 \text{ m}^3$) without replacement (-1-).

Table 1 Accumulated exposures to the VOC with different placement schemes of carbon sheets ($\text{hour} \cdot \text{mg}/\text{m}^3$)

Period	Placement scheme							
	No carbon	dense ^a	loose ^b	3 months ^c	6 months	1 year	5 years	10 years
0-1 year	38.9	31.3	4.49	8.04	8.05	8.08	8.08	8.08
1-60 year	12.2	9.04	4.29	4.86	3.28	2.05	2.48	3.38
0-60 year	51.1	40.3	8.78	12.9	11.3	10.1	10.6	11.5

^aMono-placement of a dense carbon sheet ($2 \times 5 \times 0.002 \text{ m}^3$, $\epsilon = 0.4$). ^bMono-placement of a loose carbon sheet ($2 \times 5 \times 0.002 \text{ m}^3$, $\epsilon = 0.9$). ^cSequential placement of two loose carbon sheets ($2 \times 2.5 \times 0.002 \text{ m}^3$, $\epsilon = 0.9$). The second sheet replaces the first one after 3 months, 6 months, etc.

For the calculation of simultaneous emission of two VOCs, we assume the VOCs to be methylcyclohexane and toluene. The initial concentrations in the PVC flooring are assumed to be $40 \text{ g}/\text{m}^3$ for methylcyclohexane and $120 \text{ g}/\text{m}^3$ for toluene. Their diffusion coefficients in air are $8.9 \times 10^{-6} \text{ m}^2/\text{s}$ and $8.7 \times 10^{-6} \text{ m}^2/\text{s}$ respectively (Perry et al., 1984). Their diffusion coefficients in the PVC flooring are assumed to be $8.5 \times 10^{-14} \text{ m}^2/\text{s}$ and $1.4 \times 10^{-13} \text{ m}^2/\text{s}$ respectively. The diffusion coefficients in the activated carbon particles are estimated from previous work (Yu, 1987) as $2.84 \times 10^{-6} \text{ m}^2/\text{s}$ for methylcyclohexane and $1.93 \times 10^{-6} \text{ m}^2/\text{s}$ for toluene. The binary Langmuir isotherm constants are obtained from Yu and Neretnieks (1990). The concentrations of methylcyclohexane and toluene present simultaneously in the room air and their concentrations present as a single component are shown in Figure 3.

Discussion

The mathematical model uses linear-driving-force approximation for the true concentration gradient. Owing to lack of experimental data a number of data values are assumed in the calculations. These facts will introduce errors, but a certain understanding may be drawn from the results. Experimental work is needed to validate the modelling.

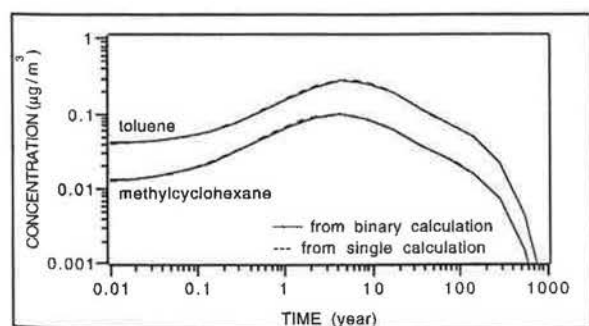


Fig. 3 Concentrations in the room air, from binary calculation and single component calculation.

Figure 1 indicates that a loose activated carbon sheet has increased effects compared to a dense sheet of the same size, while the loose sheet has only one sixth of the amount of activated carbon of the dense sheet. As we can see in Figure 1, however, the VOC concentration in the room air will stay higher after seven years when we use a loose sheet than when we use a dense one. Curve 4 has a plateau-shaped tail. This is because the activated carbon is saturated by the VOC at that time and starts to function as a re-emission source. This drawback can be solved by replacing the saturated sheet with a fresh sheet. Although the total carbon amounts are the same, the sequential placement of two half-sized sheets results in a rather different concentration history from the mono-placement, as shown by curves 3 and 4 in Figure 1. With sequential placement the concentration of the VOC in the room air is higher during the first two years, but it is considerably lower in the remaining years. Table 1 indicates that if we use a single loose sheet, the people who stay in the room will have an accumulated exposure to the VOC of $4.49 \text{ hour} \cdot \text{mg}/\text{m}^3$ during the first year and $4.29 \text{ hour} \cdot \text{mg}/\text{m}^3$ during the period 1-60 years, whereas if we use two sequential sheets with the replacement after one year, the accumulated exposure will be 8.08 and $2.05 \text{ hour} \cdot \text{mg}/\text{m}^3$ respectively. Thus we can choose the placement scheme according to the period of interest. When we require lower concentration and accumulated exposure in the first year, we should place a single large sheet. When we place more attention on the remaining longer period, then it is preferable to use sequential placement schemes.

According to the results shown in Figure 2 and Table 1, the optimal replacement time of the carbon sheet is about 1 year for the current conditions.

Figure 3 shows that the concentrations calculated for simultaneous binary VOCs are close to the concentrations from single VOC calculations, implying that in the region of very low concentrations, which

we are investigating, the adsorption of VOCs appears minimally competitive. Since ppb levels are commonly encountered in indoor air problems, we may treat simultaneous VOCs separately as if they were not interactive. The efficiency of the activated carbon sheet to one VOC will be nearly unaffected by the presence of other VOCs.

Acknowledgement

We wish to thank the Swedish Council for Building Research for financial aid.

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