Indoor Air 1993, 3: 2-11 Printed in Denmark = all rights reserved 并 6つ 8 4 Copyright © Munksgaard 1993 Indoor Air

LSSN 0907-2055

Modelling of Emission and Re-emission of Volatile Organic Compounds from Building Materials with Indoor Air Applications

Ivars Neretnieks¹, Jan Christiansson¹, Leonardo Romero¹, Lars Dagerholt¹, Ji-Wei Yu¹

Abstract

Polymer materials and their additives are today ever present in our daily surroundings. These materials have been found to emit a number of different volatile organic compounds (VOCs) into the ambient air, thus affecting the quality of the indoor air. VOCs with detectable concentrations are exchanged between the different materials and indoor air. Materials present in the system act as sorbents as well as sources of emission, depending on the concentration of the VOCs in the air at a specific time. This work demonstrates a method of studying the phenomena of absorption/re-emission. A hypothetical room that resembles a furnished office has been studied. A PVC flooring material was used as a primary emission source in a system where materials such as wood, paint, cloth, chipboard, and cellulose were present. Mass transfer in the solid materials was assumed to be by diffusion. The results show that the mechanism of absorption/ re-emission of volatiles may extend the time of residence in an indoor system considerably. A person working in this environment could risk longer exposure to toxic volatiles than if there were no absorption/re-emission effects.

KEY WORDS:

Indoor air quality, Compartment model, Absorption, Emission, PVC flooring, Volatile organic compounds (VOCs).

Manuscript received: 16 March 1992 Accepted for publication: 21 January 1993

Introduction

The "sick building syndrome" is an effect of many synergic conditions of the indoor environment. One of these conditions is the presence of irritants in indoor air. These may have a number of origins, for example fumes from traffic, tobacco smoke, etc. Another origin of substances that may have an adverse effect on health is various organic volatile compounds (VOCs) emitted from construction and furnishing materials.

The concentrations of VOCs due to emission are usually quite low. However, a number of factors suggest that this would not necessarily mean that the risk to human health is low. It is believed that the sensory reaction of the human body to odorous substances in our surroundings in many cases is proportional to the logarithm of the exposure to the specific irritant (Berglund et al., 1985). Another factor stressing the risk of VOCs is long exposure even at low concentrations. With regard to exposure to carcinogens, multiple exposure to lower concentrations may be even more harmful than exposure to isolated peak concentrations (Holmberg, 1977).

The construction and furnishing materials that do not contain any VOCs will also play a role in the "sick building" although they are not the primary emission sources of VOCs. A material in contact with indoor air will act as a sorbing material as long as the concentration of the specific compound in the air is higher than the gas phase concentration within the material. When the concentration in the air later decreases due to ventilation, the material will evolve to become an emitting source of the compound as the difference in concentration has reversed. In this way a number of capacitors have been acquired, delaying the expulsion of the volatiles from the building. Slow emission (if the volatile has been absorbed deeply into the material) can result in the indoor air containing VOCs for long periods of time.

Department of Chemical Engineering, Royal Institute of Technology, S-100 44 Stockholm, Sweden, Telefax: +46 8 105228

This work sets out to identify some relevant secondary sources of emission, and to show the extent of their effect on indoor air. This has been done by using a computer model and applying measured data found in literature as well as estimated values where no data have been found.

A hypothetical room has been constructed containing a number of commonly used materials in the furniture and building-industry. To this room, a primary emission source has been added in the form of a 1.9 mm thick PVC flooring. The variables in the system have been the materials present in the room as well as the ventilation of the room. 2-ethylhexanol was chosen as the VOC studied.

It should be noted that this is not a comprehensive study of all common building materials or VOCs. The primary aim of this work is to demonstrate a method of studying the phenomena of absorption/re-emission of VOCs in an indoor environment. This work may also indicate in which areas further work may be needed for a better understanding of the mechanisms that govern the presence of hazardous VOCs in an indoor environment.

A Basic Sample-Case

This work is carried out by a basic sample-case in which a ventilated room is constructed containing a number of objects based on an actual office space. The room has a PVC flooring as the only primary emitting source of VOC. Other objects present in the room include: walls, a ceiling, a door, tables, bookshelves, cabinets, books, binders, filing cabinets, curtains, and upholstered furniture. These objects function as both sorbing sinks and secondary emitting sources. Only one VOC is considered in this work.

In the beginning, the PVC flooring, the primary emitting source, is assumed to contain 2-ethylhexanol as the VOC. The other objects in the room do not contain any VOC. The room air is also assumed to be free of VOC.

The conditions in the room are then simulated by a model, which yields the concentrations in various objects in the room as well as in the room air at different times.

Description of the Conceptual Model

The dynamics of emission, sorption, and re-emission processes of the VOC in the room is complicated. It depends on the initial content of the VOC, the ventilation rate, the dimensions of each object in the room, the physical, chemical and transport properties of each material, and the sorption equilibria. The complexity is also due to the irregular geometric structure of some objects. Some materials are porous and some have heterogeneous properties, which also contribute to the complexity in description of the conditions in the room.

To make a quick but meaningful investigation, a compartment model developed by Romero et al. (1991) is applied to the basic sample-case. The compartment model assumes that the system to be modelled is built up by a number of compartments in contact with each other. Each object in the system consists of one or more compartments. The basic sample-case in this work is assumed to consist of 21 compartments, as illustrated in Figure 1. In the 21compartment model, compartment No. 2 represents the room air. The ceiling, the door, the wall, and the upholstered furniture are each divided into two compartments, because these objects are made of composite materials with layers of different properties.

The compartment model assumes that the concentration in each compartment is represented by an average concentration. For some materials having high concentration gradient this assumption may introduce considerable error. Therefore the compartments for the PVC flooring and all chipboard compartments (the ceiling, the wall, the drawers, and the upholstered furniture) are further divided into two compartments each where the compart-



Fig. 1 Illustration of a 21-compartment model.

ment closest to the room air has the thickness of 1/3 of the original compartment.

The VOCs can in principle be held by a material in three different ways, in three different parts of the material:

- in the gas in porous cavities in the material, which may be open or closed;
- by absorption into an absorbing component within the material; examples of absorbing components may be for textiles fat/wax (natural fats within the fibres, additives from processing, or dirt), colouring, hydrophobic compounds, preservatives, softeners, as well as glues;
- by adsorption onto the surfaces of an adsorbing component in the material; adsorption may be present both in the macroscopic and microscopic scale.

Thus a compartment for sorbing material can be subdivided into four parts, as shown in Figure 2.

In addition to the above assumptions, a number of assumptions have been made to simplify the problem of calculating the exchange of the VOC between the materials.

- All transport within a material is by diffusion.
- No irreversible chemical reactions occur.
- An ideal solution is assumed when the VOC is absorbed in the absorbing component. The equilibrium between the concentration of an absorbed component and the concentration in the gas phase is expressed by Raoult's law.

Adsorption is not included in this work, though its role is significant in the re-emission problem. We have taken adsorption into account in another work, where the effect of adsorption was shown (Christiansson et al., 1992).

Total compartment V

Inert	Adsorbing component	Absorbing component	Porous volume
V _{inert}	V _{ads}	Va	V _{por}

Fig. 2 Each material can be divided into the four parts, absorbing component, adsorbing component, porous volumes, and inert component.

Definition of the Mathematical Model

Conservation of Matter

For practical reasons we have chosen to formulate the model based on the concentrations in the room air, and the air in the pores of all materials, c_j . The total concentration in a compartment, c'_{ij} , is the product of the concentration in the porous volume, c_j , and an equilibrium constant, K_i , related to the concentration in the air (gas) in a compartment. That is

$$\mathbf{c'_{j}} = \mathbf{K_{j}} \mathbf{c_{j}} \tag{1}$$

The equilibrium constant K_i describes the equilibrium within each compartment, between the concentration in the porous volumes of air and the total compartment including voids, inert, and sorbing fractions. The compartment model formulates the equation for the conservation of matter in a compartment representing a sorbing material as follows:

$$K_{j}V_{j} \frac{dc_{j}}{dt} = \sum_{i\neq j} k_{ji}(c_{i}-c_{j})$$
⁽²⁾

The term on the right side of the equation accounts for the transport by diffusion in and out of the compartment from all adjacent compartments. The lefthand term describes the accumulation of the volatile organic compound within each compartment j including sorption effects.

In the case of compartment j being the air in the room, the effect of the ventilation is added:

$$K_{i}V_{i} \frac{dc_{i}}{dt} = \sum_{i\neq j} k_{ji}(c_{i}-c_{j}) - Qc_{j}$$
(3)

where Q defines the volumetric ventilation rate.

Equations (2) and (3) can also be expressed as:

$$\frac{dc_i}{dt} = \sum_i g_{ii}c_i \tag{4}$$

where

$$g_{ji} = \frac{k_{ji}}{K_j V_j} \qquad i \neq j$$
(5)

$$\mathbf{g}_{jj} = -\sum_{i\neq j} \mathbf{g}_{ji} \tag{6}$$

11

for all compartments except the compartment for the room air, and

$$g_{jj} = -\sum_{i\neq j} g_{ji} \frac{Q}{K_i V_j}$$
(7)

for the compartment representing the room air.

The Equilibrium Constant

Each compartment can be looked upon as consisting of four parts which react differently with respect to the VOCs: a porous volume, an inert part that does not take part in withholding the VOCs, an absorbing part, and an adsorbing part. The equilibrium constant, K_i , depends on all and is the sum of all effects. It is different for each volatile. A mass balance over the whole compartment gives

$$V_j c'_j = v_a c_{abs} + v_{ads} c_{ads} + v_{por} c_j$$
(8)

or

$$c'_{i} = \frac{v_{a}}{V_{j}} c_{abs} + \frac{v_{ads}}{V_{j}} c_{ads} + \frac{v_{por}}{V_{j}} c_{j}$$

$$\tag{9}$$

The effects of adsorption have not been considered in this work. Hence Equation (9) becomes

$$\mathbf{c'_{i}} = \frac{\mathbf{v_{a}}}{\mathbf{V_{j}}} \mathbf{c_{abs}} + \frac{\mathbf{v_{por}}}{\mathbf{V_{j}}} \mathbf{c_{i}} = \left(\frac{\mathbf{v_{a}}}{\mathbf{V_{j}}} \frac{\mathbf{c_{abs}}}{\mathbf{C_{j}}} + \frac{\mathbf{v_{por}}}{\mathbf{V_{j}}}\right) \mathbf{c_{j}}$$
(10)

The equilibrium relation for absorption can be derived based on vapour-liquid equilibrium and by assuming the ideal gas law.

$$c_{abs} = \frac{\rho_a RT}{M_a \gamma P^o} c_j \tag{11}$$

where the absorbed mole fraction is approximated by the number of moles of the volatile divided by the number of moles of the absorbing component. A combination of Equations (1), (10) and (11) leads to

$$K_{j} = \frac{v_{a}}{V_{j}} \cdot \frac{\rho_{a} RT}{M_{a} \gamma P^{o}} + \frac{v_{por}}{V_{j}}$$

$$(12)$$

At present we assume that the absorbed VOC and the absorbing component form an ideal solution, which leads to a unity activity coefficient.

The Rate Constant

The rate constant when diffusion dominates is:

$$k_{ji} = \frac{A_{ji}}{\left(\frac{\Delta x}{D}\right)_{ji}}$$
(13)

where the term $(\Delta \times /D)_{ji}$ accounts for the resistance to mass transfer between the compartments j and i depending on the two diffusion resistances $(\Delta \times /D)$ on either side of the interface, coupled in series.

$$\left(\frac{\Delta x}{D}\right)_{ji} = \left(\frac{\Delta x}{D}\right)_{i} + \left(\frac{\Delta x}{D}\right)_{j}$$
(14)

Estimation of **D**ata

Diffusivities and Initial Concentration

Mass transfer in porous solids involves gaseous diffusion, surface diffusion, convective flow due to diffusion, and viscous flow. Both gaseous and surface diffusion fluxes follow Fick's first law (Yang, 1987). For diffusion of dilute VOCs in air as in this work, the convective flow will be negligible. The viscous flow is usually small and will therefore be neglected. The effective diffusivity for the migration of a VOC, 2-ethylhexanol, in the primary emission source, the PVC flooring, has been collected from the experimental work of Christiansson (1991). The same source has also supplied the data on initial concentration that can be expected in PVC-flooring materials. The diffusivities of the VOC in other materials have been estimated based on data from chamber experiments of Ulrich et.al. (1982) and Meyer (1984). The data used in the calculations, except the data for the PVC flooring, are based on estimates. Further material studies are needed for more accurate assessments.

Porosities

The porosities of the wood material have been derived from data on the density and molar weight of the cellulose fibres and the porosities of other materials have been guessed. The model is very insensitive to uncertainties in the porosities.

Ventilation Flow

Ventilation has a large impact on the concentrations of volatiles in indoor air. Swedish building standards define a ventilation flow in occupational and public buildings to be at least 0.5 exchanges per hour. However, the efficiencies of ventilation systems are seldom 100%. Short-circuiting of ventila-

	Compartment		Material	Width	Length	Thickness [m]
1	flooring		plasticized PVC	5.0	4.0	6.333×10 ⁻⁴
2	room air			5.0	4.0	2.4
3	wall	surface	acrylic latexpaint	18.0	2.4	0.0003
4	wall	inner layer	chipboard	18.0	2.4	0.005
5	door	surface	teakwood	1.0	1.9	0.002
6	door	inner layer	fiberboard	1.0	1.9	0.004
7	ceiling	surface	acrylic latexpaint	5.0	4.0	0.0003
8	ceiling	inner layer	chipboard	5.0	4.0	0.005
9	tables		oak	1.0	4.0	0.02
10	bookshelves		oak	1.0	4.0	0.02
11	drawers		chipboard	1.0	2.2	0.005
12	books		cellulose	0.5	19.0	0.10
13	binders		plastic	1.0	0.6	0.002
14	filing cabinet		varnish	1.0	2.2	0.0002
15	curtains		cotton cellulose	1.0	6.0	0.0005
16	uph. furn.	surface layer	cotton cellulose	1.0	2.8	0.0005
17	uph. furn.	upholstery	poly-urethane	1.0	2.8	0.1
18	wall	inner layer	chipboard	18.0	2.4	0.010
19	ceiling	inner layer	chipboard	5.0	4.0	0.010
20	drawers		chipboard	1.0	2.2	0.010
21	flooring		plasticized PVC	5.0	4.0	1.266×10 ⁻³

Table 1 The compartment dimensions

tion flow within a room is common as well as hindrance by the furniture arrangement etc. It is not uncommon that the ventilation efficiency within a room is considerably less than 20%, resulting in an actual ventilation of rooms or sections thereof that is considerably lower than the 0.5 exchanges defined by the building standards.

Three different ventilation flows have been used in the model. The normal ventilation was defined as 0.5 exchanges per hour; this is the flow specified by the Swedish building standards. Higher ventilation can be found in old buildings with inferior insulation. The value used for high ventilation is 5 exchanges per hour. Considering the very low actual local ventilation, the value used for low ventilation flow in the model is 0.05 exchanges per hour. The ventilation in the present model runs is continuous.

Resistance to Mass Transfer in the Laminar Air Layer Adjacent to the Solid Surfaces

The resistance to mass transfer in the room air film adjacent to the materials is taken into account in the model. For all compartments in direct contact with the room air this film thickness is fixed at 3.5 cm, based on air velocity equal to 10 cm/s and a relation for the mass transfer resistance at different velocities (Zimmerli, 1982). This is a representative value 5 cm above the floor in ventilated dwellings (Kovanen et al., 1987). Table 2 Data used for equilibrium constant

rtm./ ing	ρ_a	Ma	$\nu_a\!/V_j$	v_{por}/V_{j}	K _i
-	(kg/m ³)	(g/mo	ol)		
DOP	98 0	391	0.28	0.006	2.61 × 10 ⁵
(=		-	0	1	1
PEG	1120	600	0.15	0.003	1.04×10^{5}
REO	1030	600	0.1	0.57	6.38×10^{4}
ABA	1030	302	0.1	0.68	1.27×10^{5}
ABA	1030	302	0.05	0.55	6.34×10^{4}
PEG	1120	600	0.15	0.003	1.04×10^{5}
REO	1030	600	0.1	0.57	6.38×10^{4}
ABA	1030	302	0.02	0.49	2.54×10^{4}
ABA	1030	302	0.02	0.49	2.54×10^{4}
REO	1030	600	0.1	0.57	6.38×10^{4}
ABA	1030	302	0.02	0.56	2.54×10^{4}
PEG	1120	600	0.05	0.06	3.47×10^{4}
PEG	1120	600	0.02	0.02	1.39×10^{4}
ABA	1030	302	0.003	0.81	3.80×10^{3}
ABA	1030	302	0.003	0.68	3.80×10^{3}
DDB	900	264	0.03	0.96	3.80×10^{4}
	Ttm./ ing DOP PEG REO ABA ABA PEG REO ABA ABA REO ABA ABA PEG PEG ABA ABA DDB	$\begin{array}{c} rtm./ \\ ng \\ (kg/m^3) \\ \hline \\ DOP \\ 980 \\ \hline \\ PEG \\ 1120 \\ REO \\ 1030 \\ ABA \\ 1030 \\ PEG \\ 1120 \\ PEG \\ 1120 \\ PEG \\ 1120 \\ ABA \\ 1030 \\ ABA \\ 100 \\ 100 \\ ABA \\ 100 \\ 100 \\ 100 \\ 100 \\ 100 \\ 100 \\ 100 \\ 100 \\$	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$

Abbreviations: ABA = abietic acid, DDB = dodecylic benzene, DOP = di-2-ethylhexyl phthalate, PEG = polyethylene glycol (M = 600 g/mol), REO = resin oil (M = 600 g/mol).

Calculations and Results

The system of Equation (4) is solved by a program initially prepared by Romero et al. (1991). It was used to model solute transport in a repository for radioactive waste. This program has been modified to suit the needs of this work. The program uses standard numerical techniques through the Stiff solver based on Gear's method. The solver makes use

Compartment	D_i/K_i (m²/s)	Δx (m)	k _{ii} (m³/s)	
1	1.0×10^{-13}	3.17 × 10-4	$k_{1,2} = 1.21 \times 10^{-3}$	$k_{1,21} = 5.49 \times 10^{-4}$
2	7.9×10^{-6}	3.50×10^{-2}	$k_{2,i} = k_{i,2}$ see other compartments	
2	8.0×10^{-15}	1.50×10^{-4}	$k_{3,2} = 2.34 \times 10^{-4}$	$k_{3,4} = 2.33 \times 10^{-4}$
4	8.0×10^{-12}	2.50×10^{-3}	$k_{4,3} = 2.33 \times 10^{-4}$	$k_{4,18} = 2.94 \times 10^{-3}$
5	8.0×10^{-13}	1.00×10^{-3}	$k_{5,2} = 1.33 \times 10^{-4}$	$k_{5,6} = 1.38 \times 10^{-4}$
6	8.0×10^{-12}	2.00×10^{-3}	$k_{6.5} = 1.38 \times 10^{-4}$	
7	8.0×10^{-15}	1.50×10^{-4}	$k_{7,2} = 1.08 \times 10^{-4}$	$k_{7,8} = 1.08 \times 10^{-4}$
8	8.0×10^{-12}	2.50×10^{-3}	$k_{8,7} = 1.08 \times 10^{-4}$	$k_{8,19} = 1.36 \times 10^{-3}$
9	8.0×10^{-13}	1.00×10^{-2}	$k_{9,2} = 8.04 \times 10^{-6}$	
10	8.0×10^{-13}	1.00×10^{-2}	$k_{10,2} = 8.04 \times 10^{-6}$	
11	8.0×10^{-12}	2.50×10^{-3}	$k_{11,2} = 2.40 \times 10^{-4}$	$k_{11,20} = 1.52 \times 10^{-4}$
12	3.1×10^{-12}	5.00×10^{-2}	$k_{12,2} = 1.50 \times 10^{-5}$	
13	$1.0 imes 10^{-14}$	1.00×10^{-3}	$k_{13,2} = 2.08 \times 10^{-7}$	
14	6.0×10^{-15}	1.00×10^{-4}	$k_{14,2} = 1.86 \times 10^{-6}$	
15	2.1×10^{-9}	2.50×10^{-4}	$k_{15,2} = 1.35 \times 10^{-3}$	
16	2.1×10^{-9}	2.50×10^{-4}	$k_{16,2} = 6.28 \times 10^{-4}$	$k_{16,17} = 4.45 \times 10^{-4}$
17	2.1×10^{-9}	5.00×10^{-2}	$k_{17,16} = 4.45 \times 10^{-4}$	
18	8.0×10^{-12}	5.00×10^{-3}	$k_{18,4} = 2.94 \times 10^{-3}$	
19	8.0×10^{-12}	5.00×10^{-3}	$k_{19,8} = 1.36 \times 10^{-3}$	
20	8.0×10^{-12}	5.00×10^{-3}	$k_{20,11} = 1.52 \times 10^{-4}$	
21	$1.0 imes 10^{-13}$	6.33×10-4	$k_{21,1} = 5.49 \times 10^{-4}$	

Table 3 Data used for mass transfer rate constant

of the function SDRIV2 to solve n ordinary differential equations of the form $d\mathbf{Y}(\mathbf{I})/d\mathbf{t} = \mathbf{F}(\mathbf{Y}(\mathbf{I}), \mathbf{t})$, given the initial conditions $\mathbf{Y}(\mathbf{I}) = \mathbf{Y}\mathbf{I}$ (Kahaner et.al., 1988). The compartment model has been verified by Romero et al. (1992). Its accuracy has been compared with an analytical solution and another numerical solution to the diffusion equation in a simple mass transfer problem. The results obtained using the very simple compartment model deviate from the exact solution, especially for early times, due to the coarse discretization of compartments. The errors are deemed to be acceptable, considering the uncertainties in other data used for the calculations. The accuracy of the numeric results can be considerably increased by using finer discretizations of the compartment, if needed.

The input provided to the model was data on the dimension of each compartment (listed in Table 1) as well as such properties as other physical and chemical properties of both the VOC and the compartment (listed in Tables 2 and 3).

The vapour pressure of 2-ethylhexanol is 6.7 Pa at 298 K. Its initial concentration in the PVC flooring is 0.032 kg/m^3 . The other compartments contain no VOC initially.



Fig. 3 Results of 3-compartment model. Total concentration in each compartment at normal ventilation flow, 0.5 exchanges/h.





The Reference Calculation

The first calculations were made with only three compartments, two representing the PVC flooring and one representing the room air. The results of these calculations are taken as reference to the influence of the other compartments in the system.

All calculations have been made using the three different values of ventilation flow. The calculation with normal ventilation flow renders the following concentrations in each compartment with respect to time (note: 1 year $\approx 10^4$ hours).

Figure 3 shows that it takes one year for any significant changes in the concentration of the VOC in the room air to occur. This is the result when no other materials are present. It can also be observed that the decrease in concentration in the PVC flooring is very low for times less than a year. In the case with higher and lower ventilation flow, the maximum concentration is considerably changed, as well as the time for the VOC to be exhausted from the system (Figure 4).

The Calculation for the Basic Sample-Case

The 21-compartment model renders a much different result compared to the 3-compartment model. The changes in concentration at the end of the cycle are slower. The concentration stays high for a longer period of time.

The concentrations in the different compartments displayed in Figure 5 can be divided into two groups: the compartments that have concentrations that generally follow the dynamics of the room air (3, 5, 6, 7, 11, 14, 15, 16, 17, and 20), and those where there is a delayed effect (4, 8, 9, 10, 12, 13, 18, 19). The latter are to a large extent responsible for the delay
 Table 4 The compartments with delayed reactions to the concentration changes in the room air

Compartment:		Material:		
4	wall	chipboard (coated)		
18	wall	chipboard, inner compartment		
8	ceiling	chipboard (coated)		
19	ceiling	chipboard, inner compartment		
9	table	solid wood		
10	bookshelves	solid wood		
12	books	cellulose		
13	plastic binders	polystyrene		

of the decrease of the concentration in the room air. Table 4 summarizes the materials that have delayed reactions.

Figure 6 showing the comparison between different ventilation flows also shows inflexion points in the room air concentration transient after about 5 years.

The total exposure to a volatile compound in the room air can be obtained by integrating the concentration/time graph, as shown in Figure 7.

Discussion

A simple compartment model has been used to study the transport of VOCs between the room air and the different materials in a room. The model, although very simple in concept, is a useful tool which can be used to study the absorption and reemisson of VOCs between different materials in a room. It is very flexible and can easily be extended to include an arbitrary number of materials. It can be used for scoping calculations with a few compartments when high accuracy computations are not warranted because data are not accurate. While the compartment model uses a linear-driving-force approximation instead of the real concentration gradient to calculate the diffusion flux, its computational accuracy can easily be improved by subdivision of compartments when material data are well known. It can also be used to assess which materials in a room are important and which are not important.



Fig. 6 Results of the 21-compartment model. Concentrations in the room air at different ventilation flows, 0.05, 0.5, and 5 exchanges/h.



The results of the 3-compartment model show how the concentration of the VOC in the room air is relatively constant for a long period of time until the PVC flooring is exhausted of its content of the volatile. Depending on the ventilation, the concentration can be said to have significantly decreased (less than 0.1 µg/m3 after 3 years at normal ventilation. With low ventilation this time is extended to 11 years.

The effect of the addition of furniture, walls, and ceiling is demonstrated by the 21-compartment model. The time until the concentration of the VOC in the room air has reached a level below 0.1 $\mu g/m^3$ is still 3 years at normal ventilation. This is in accord with the 3-compartment model. At concentrations below 0.1 µg/m3 the case is different, and here we can see the re-emission effects of the additional compartments. The decrease in concentration is considerably slower than in the case with only three compartments.

When the ventilation is lower, the influence of the additional compartments is greater. The time until the air concentration reaches a level below 0.1 μ g/m³ 34 years at low ventilation. This is an increase by a factor 6 compared to the case with no other compartments than the PVC flooring and the ventilated room.

The concentration of the VOC in the air at early times is slightly lower in the 21 compartment model $(1.6\times 10^{-8} kg/m^3)$ than in the 3-compartment model $(1.7 \times 10^{-8} \text{kg/m}^3)$ at normal ventilation. This is due to the absorption of the VOC by the other compartments, walls, furniture, and books, in the room.

Figure 7 shows that the exposure increases considerably when the ventilation decreases. For a period of more than one year, the total exposure is approximately proportional to the ventilation exchange rate.

Conclusions

The addition of sorbing materials to a ventilated system with VOCs will alter the dynamic behaviour of the concentration in indoor air significantly.

The concentration of 2-ethylhexanol in the room air is in the range of $\mu g/m^3$. This is a substantial concentration when it may be expected that people will be exposed to this air for a long period of time. The time until the total amount of the VOC in the system diminishes is long.

Those compartments that show a delayed reaction to the changes in the concentration of the room air are the compartments responsible for the delay of the ventilation of the system. These are the compartments made of solid wood, chipboard, cellulose, and plastic (Figure 5).

It should be emphasized that the case study results presented here are hypothetical. Experimental measurements are expected to validate the applicability of the modeling. To acquire more reliable results from the calculations, work is needed to establish data for the materials involved such as diffusivities and equilibrium data. This is an area where not much data is available.

Acknowledgements

This work was funded by the Swedish Council for Building Research which we gratefully acknowledge.

Notation T

\mathbf{A}_{ji}	The area of the interface	
	between compartments i and i	m²
Cabs	Concentration of the volatile	111
	in the absorbed phase	ka/m ³
C _{ads}	Concentration of the volatile	к <u>ө</u> /ш
	in the adsorbed phase	ka/m ³
$\mathbf{c}_{\mathbf{j}}$	Concentration of the volatile	K6/111
-	in the air phase within compartment	i ka/m ³
c'i	Total contration of the volatile	.) Kg/III
	within compartment i	ka/m3
\mathbf{D}_{i}	Diffusivity of volatile in compartment	$m^{2/c}$
\mathbf{g}_{ji}	Model parameter	n) m/s
\mathbf{K}_{j}	The equilibrium constant describing	3
	the equilibrium between the concen-	
	trations of the volatile in compart-	
	ment j and the concentration in the	
	porous volume of compartment i	
k _{ji}	The rate constant describing the rate	
	of mass transfer from compartment i	to i $m^{3/s}$
$M_{ m a}$	Molar mass of absorbing compound	kg/mol
\mathbf{P}^{o}	Vapour pressure of volatile	Pa
Q	Ventilation flow rate	m ³ /s
R	Gas-law constant	I/mol·K
Т	Temperature	K K
t	Time	
\mathbf{V}_{j}	Volume of the compartment i	m ³
Va	Volume of the absorbing portion	111
	of compartment j	m ³
Vads	Volume of the adsorbing portion	411
	of compartment j	m ³
	1	111

Vinert	Volume of the inert portion	
	of compartment j	m ³
Vpor	Volume of the porous volume	
	within compartment j	m ³
Δx	Diffusion length	m

- γ Activity coefficient
- $\begin{array}{c} \rho_a & \mbox{ Density of the absorbing component} \\ & \mbox{ of a compartment} & \mbox{ kg/m}^3 \end{array}$

References

- Berglund, B., Berglund, U., Högman, L., Johansson, I. and Lindvall, T. (1985) "Measurement of formaldehyde odor indoors". In: Fanger, P.O. (ed.) Proceedings of the Clima 2000 World Congress on Heating, Ventilating, and Air-Conditioning, Copenhagen, VVS Kongres – VVS Messe, Vol. 4: Indoor Climate, pp. 251-256.
- Christiansson J. (1991) Emission of Organic Compounds from Floorings of Plasticized PVC, Stockholm, Department of Chemical Engineering, Royal Institute of Technology, Stockholm (in Swedish).
- Christiansson, J., Neretnieks, I. and Yu, J.-W. (1992) Compartment Modeling of Emission, Uptake, and Reemission of Volatile Air Pollutants in a Ventilated, Furnished room. Paper presented at the conference Indoor Air Quality'92: Environments for People, San Francisco, California, October, 1992.

- Holmberg, B. (1977) Some Ideas on Chemically Induced Cancer, from a Toxicologic View, Swedish Board of Occupational Health (Arbetarskyddsstyrelsen) Report 1977:37 (in Swedish).
- Kahaner, D., Moler, C. and Nash, S. (1988) Numerical Methods and Software, Englewood Cliffs, New Jersey, Prentice Hall.
- Kovanen, K., Seppänen, O., Sirèn, K. and Majanen, A. (1987) "Turbulent air flow measurements in ventilated spaces". In: Indoor Air '87, Berlin, conference report 3, 329-333.
- Meyer, B. (1984) "Formaldehyde release from building products". In: Berglund, B., Lindvall, T. and Sundell, J. (eds) *Proceedings* of Indoor Air '84, Stockholm, Swedish Council for Building Research, Vol. 3, pp. 29-34.
- Romero, L., Moreno, L. and Neretnieks, I. (1991) "A compartment model for solute transport in the near field of a repository for radioactive waste". Paper presented at the MRS meeting, Strasbourg, Nov 4-7, 1991.
- Romero, L., Moreno, L. and Neretnieks, I. (1992) Verification of the Compartment Model, Code for Calculating Radionuclides Release in the Near Field of a Repository, Swedish Nuclear Fuel and Waste Management Co.(SKB), SKB Report AR-xx, (in print).
- Ulrich, D., Nagel, R. and Seifert, B. (1982) "The influence of lacquer coatings on the indoor air quality; Radiator lacquer as an example". In: Aurand, B., Seifert, B. and Wagner, J. (eds) Luftqualität in Innenraumen, pp. 283-298.
- Yang, R. T. (1987) Gas Separation by Adsorption Processes, Boston, Butterworths.
- Zimmerli, B. (1982) "Modelling the transfer of pollutants from painted surfaces to the surrounding air". In: Aurand, B., Seifert, B. and Wagner, J. (eds) *Luftqualität in Innenräumen*, pp. 235-267.