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# A method for measuring internal diffusion and equilibrium partition coefficients of volatile organic compounds for building materials

A. Bodalal<sup>a</sup>, J.S. Zhang<sup>b,\*</sup>, E.G. Plett<sup>a</sup>

<sup>a</sup>Department of Mechanical and Aerospace Engineering, Carleton University, Ottawa, Canada, K1S 5B6

<sup>b</sup>Institute for Research in Construction (IRC), National Research Council (NRC) of Canada, Ottawa, Canada, K1A 0R6

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## Abstract

An experimental method for the determination of the internal diffusion coefficient ( $D$ ) and partition coefficient ( $k_c$ ) of volatile organic compounds (VOCs) is developed for dry building materials (such as carpet, vinyl flooring, plywood, etc.). The method is used to determine  $D$  and  $k_c$  for four VOCs (toluene, nonane, decane, and undecane) through the backing material of a carpet specimen, for four VOCs (ethylbenzene, nonane, decane, and undecane) through a floor tile specimen, and three VOCs (cyclohexene, ethylbenzene, and decane) through a plywood specimen. It was found that the values of diffusion coefficients for a given material are inversely proportional to the molecular weights of the VOCs, whereas the value of the partition coefficients are proportional to the vapour pressures of the VOCs. The measured diffusion and partition coefficients are useful for predicting the emission rates of VOCs from building materials. Crown Copyright © 1999 Published by Elsevier Science Ltd. All rights reserved.

## 1. Introduction

A wide variety of dry materials (e.g. carpet, vinyl, plywood, wall papers, etc.) are used to construct and furnish residential and commercial buildings. It is important to understand and determine the VOC emission characteristics of these materials in order to evaluate their impact on the indoor air quality. With the growing awareness of the problems associated with indoor air quality, there is now a strong impetus for manufacturing, and selecting building materials with low VOC emissions. Success in both manufacturing and choosing environmentally conscious building materials will be greatly facilitated by the availability of mathematical models for predicting the emission rates of VOCs from these materials.

Emission rates of VOCs from dry materials are primarily controlled by the diffusion within the material (i.e. internal diffusion) [1–3]. The diffusion process in its simplest form, may be described by:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \quad (1)$$

Where,  $D$  is the diffusion coefficient of a VOC in the material;  $C$  is the concentration in the material;  $x$  is the spatial coordinate (assuming 1-D diffusion).

In order to apply the diffusion model for predicting the VOC emission rates, it is necessary to know the diffusion coefficient ( $D$ ). However, data on the diffusion coefficients for building materials are very limited. A previous method for determining the diffusion coefficients used the concentration data obtained from a dynamic chamber test for VOC emissions [4]. The method requires the knowledge of the initial concentration within the region of interest. Mathematically, the initial concentration may be treated as an ad-

\* Corresponding author. Tel.: +1-613-993-9538; fax: +1-613-954-3733.

E-mail address: jianshun.zhang@nrc.ca (J.S. Zhang)

### Nomenclature

|          |   |        |   |
|----------|---|--------|---|
| $A$      | area of the specimen ( $\text{m}^2$ )   | $L$    | thickness of the specimen under investigation (m)                 |
| $B_{pt}$ | boiling point of the compound ( $^{\circ}\text{C}$ )                                | $M_w$  | molecular weight of the compound                                  |
| $C$      | concentration of the compound within the specimen ( $\text{mg}/\text{m}^3$ )        | $P$    | Laplace–Carson transformation operator                            |
| $C_0$    | initial concentration of the compound in the specimen ( $\text{mg}/\text{m}^3$ );   | $q_1$  | first positive root of the characteristic equation [Eq. (18)]     |
| $c$      | concentration of the compound in the chamber air ( $\text{mg}/\text{m}^3$ )         | $r$    | slope of the straight line ( $r = -q_1 D_i L^2$ )                 |
| $c_0$    | initial concentration of the compound in the chamber air ( $\text{mg}/\text{m}^3$ ) | RH     | relative humidity   |
| $D$      | diffusion coefficient of the compound within the specimen ( $\text{m}^2/\text{s}$ ) | $t$    | time (s)  |
| IAQ      | indoor air quality  | $S, s$ | transformation of $C$ and $c$ respectively                        |
| $k_e$    | equilibrium partition coefficient between the specimen and the air (dimensionless)  | $u$    | intercept of the straight line ( $u = \text{Ln}(c_2 - c_1)/c_0$ ) |
|          |   | $V$    | volume of the chamber air ( $\text{m}^3$ )                        |
|          |   | VOC    | Volatile Organic Compound   |
|          |   | $x$    | linear distance (m)   |

ditional parameter to be estimated from the concentration data. This will increase the number of parameters to be estimated in a single least-square regression analysis, which may result in a large estimation error due to inter-dependency of the parameters in the regression analysis process. This work is aimed at developing a novel method to determine the diffusion coefficients more accurately. The partition coefficients for VOCs at the solid/gas interface can also be determined by the method (it is a coefficient used to describe the relationship between the concentration in the gas phase and the concentration in the solid phase).

## 2. Theory

An experiment will be described later in this paper in which the diffusion rate through a test specimen is observed by measuring concentrations on the two sides of the sample. Initially, the diffusing species is only in one compartment, and an impermeable membrane prevents this material from contacting the test sample. The thickness of a test specimen (e.g. a carpet backing material), separating the two compartments (Fig. 1) will be designated as  $l$ . The concentration in one compartment (of volume  $V_2$ ) at the beginning of the experiment is  $c_0$ ; after time  $t$  from the time the membrane is broken, its value decreases to  $c_2(t)$  due to diffusion through the test specimen. Meanwhile, the concentration in the second compartment (of volume  $V_1$ ) rises from the zero initial value to  $c_1(t)$ . The gas mixture in both compartments is stirred so that the concentration is uniform in each compartment.

The concentration of the diffusing substance at time  $t$  in the test specimen at a point whose distance is  $x$

from the top surface is designated as  $C(x, t)$ .  $A$  is the total frontal area of the specimen exposed to the diffusing species and  $D$  is the diffusion coefficient of the specific compound under study.

On the assumption that the VOC concentration on the specimen (carpet backing) surface is proportional to the concentration of the compound in contact with this surface ( $k_e$  is the equilibrium partition coefficient), the process can be described by Eq. (1) subject to the following boundary and initial conditions:

Boundary conditions

$$\text{At } x = 0 \quad C = k_e c_1 \quad (2a)$$

$$\text{At } x = l \quad C = k_e c_2 \quad (2b)$$

Initial condition

$$\text{At } t = 0, \quad 0 \leq x \leq l \quad C = 0 \quad (2c)$$

The concentration in the low and high concentration compartments can be expressed by Eqs. (3) and (4), respectively,

$$C_1 = (DA/V_1) \int_0^t \left( \frac{\partial C}{\partial x} \right)_{x=0} dt \quad (3)$$

$$c_2 = c_0 - (DA/V_2) \int_0^t \left( \frac{\partial C}{\partial x} \right)_{x=l} dt \quad (4)$$

Since the surface chemistry phenomena is extremely important in the case of gas/solid interfaces, it is crucial to select a suitable model so that the adsorption at the solid surface will be accounted for [namely the boundary condition Eqs. (2a) and (2b)]. Atoms at the surface of a solid exert an attractive force normal to

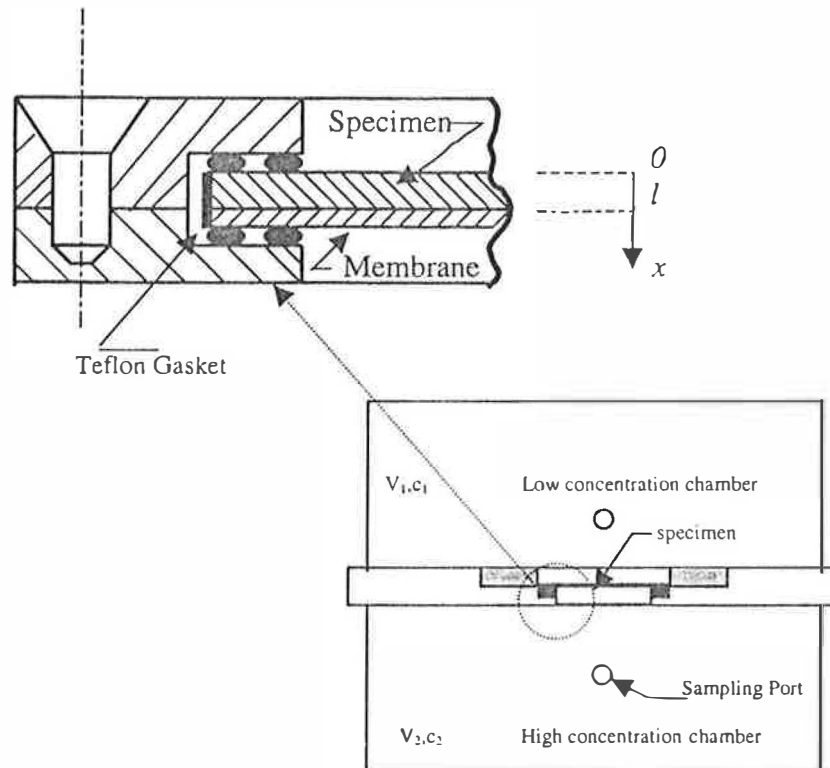


Fig. 1. Diffusionmetric apparatus.

the surface plane. Consequently, the concentration of adsorbed gas at a *gas/solid interface* exceeds that in the gas phase [5,6]. The excess concentration at the surface is caused by *adsorption*; the solid is the adsorbent and the gas the *adsorbate*. For isothermal conditions at atmospheric pressure, equilibrium relations between the concentration of the adsorbate molecules in the air-phase ' $c$ ', and the sorbed-phase ' $C$ ' identified as *adsorption isotherms* may be represented functionally as  $C=f_s(c)$ , where  $f$  is a function that is unique for each species/solid system. Linear, Langmuir, BET, Freundlich, and Polanyi DR are the most common isotherm models which may be used to describe the adsorption process [5]. For the sorption of trace concentration air-pollutants on building materials, the Langmuir model or its low-concentration asymptote, the Linear model is a reasonable first candidate [5]. Therefore, in this study the *linear isotherm model* ( $C=k_e c$ ) was used to describe the near surface concentration [i.e. the boundary conditions Eqs. (2a) and (2b)] where,  $k_e$  is the equilibrium partition coefficient. An important assumption is that the concentration at the surface (i.e.  $x=l$ ) increased from 0 to  $k_e c_2$  within an infinitely small period of time. In other words, the equilibrium between the surface concentration and the gas phase concentration occurred instantaneously (at least relative to the time scale of any measurement taken). The instantaneous equilibrium assumption ( $C=k_e c$ ) has been used previously by many other in-

vestigators. For example, Little et al. [4,7] used this assumption when they studied the emission from carpets in the full scale chamber. Similar assumptions were also adopted by Chang et al. [8] and Tichenor et al. [9].

Eqs. (1) to (4) can be solved by means of the Laplace-Carson Transformation. If we let  $S$ ,  $s_1$ ,  $s_2$  be the Laplace-Carson Transforms of concentrations  $C$ ,  $c_1$ ,  $c_2$ , respectively we may write;

$$S(x,p) = \mathcal{L}\{C(x,t)\} = p \int_0^{\infty} C(x,t) \exp\{-pt\} dt \quad (5)$$

$$s_1(p) = \mathcal{L}\{c_1(t)\} = p \int_0^{\infty} c_1(t) \exp\{-pt\} dt \quad (6)$$

$$s_2(p) = \mathcal{L}\{c_2(t)\} = p \int_0^{\infty} c_2(t) \exp\{-pt\} dt \quad (7)$$

When this transform is used with Eq. (1), an ordinary differential equation results, as given by Eq. (8).

$$D \frac{d^2 S}{dx^2} = p(S - C(x,0)) \quad (8)$$

Similarly, Eqs. (3) and (4) are transformed to take the following forms.

$$s_1(p) = (DA/V_1P) \left( \frac{dS}{dx} \right)_{x=0} \quad (9)$$

and

$$s_2(p) = c_0 - (DA/V_2P) \left( \frac{dS}{dx} \right)_{x=l} \quad (10)$$

Upon imposing the initial condition [Eq. (2c)], the solution of the ordinary differential equation [Eq. (8)] has the form:

$$S = \lambda_1 \sinh[x(p/D)^{0.5}] + \lambda_2 \cosh[x(p/D)^{0.5}] \quad (11)$$

Evaluating the integration constants  $\lambda_1$  and  $\lambda_2$  with boundary conditions [Eqs. (2a) and (2b)], yields:

$$s_1(q) = \frac{x_1 c_0}{(x_1 x_2 / q^2 - 1)q \sin(q) + (x_1 + x_2) \cos(q)} \quad (12)$$

and

$$s_2(q) = \frac{(x_1 \cos(q) - q \sin(q))c_0}{(x_1 x_2 / q^2 - 1)q \sin(q) + (x_1 + x_2) \cos(q)} \quad (13)$$

where:

$$q = k(p/D)^{0.5}, \quad x_1 = \frac{k_e A l}{V_1}, \quad \text{and} \quad x_2 = \frac{k_e A l}{V_2} \quad (13a)$$

If  $V_1$  and  $V_2$  are equal, the sum  $(x_1 + x_2)$  in the numerator of the characteristic equation  $\tan(q) = (x_1 + x_2)/ (q^2 - x_1 x_2)$ , can be replaced by  $2x$  and the product  $x_1 x_2$  can be replaced by  $x^2$ .

The inverse transformation of Eqs. (12) and (13) according to the generalized Heaviside Theorem [10] yields the relationships for measurable quantities  $c_1$  and  $c_2$ .

$$\frac{(c_2 - c_1)}{c_0} = \sum_{i=1}^{\infty} 4x [q_i^2 + x(2+x)]^{-1} \exp\{-q_i^2 D t / l^2\} \quad (14)$$

Where  $q_i$  are the positive roots of the characteristic equation;

$$\tan(q) = \frac{2x q_i}{(q_i^2 - x^2)} \quad (15)$$

The infinite series (14) converges rapidly, so that for sufficiently large  $t$  only the first term  $q_1$  is significant. That is:

$$\frac{(c_2 - c_1)}{c_0} = \frac{4x}{q_1^2 + x(2+x)} \exp\left\{ \frac{-q_1^2 D t}{l^2} \right\} \quad (16a)$$

Taking the natural log of both sides of the above equation [Eq. (16a)] yields:

$$\ln \frac{(c_2 - c_1)}{c_0} = \ln \left\{ \frac{4x}{q_1^2 + x(2+x)} \right\} - \frac{q_1^2 D}{l^2} t \quad (16b)$$

Hence, from Eq. (16b), the dependence of  $\text{Ln}\{(c_2 - c_1)/c_0\}$  on  $t$  approaches a straight line, as  $t$  increases with the slope:

$$r = \frac{-q_1^2 D}{l^2} \quad (17)$$

That intersects the  $\text{Ln}\{(c_2 - c_1)/c_0\}$  axis at:

$$u = \ln \left\{ \frac{4x}{q_1^2 + x(2+x)} \right\} \quad (18)$$

On solving Eqs. (15), (17) and (18), the auxiliary parameters,  $q_1$  and the quantities  $D$  and  $x$  can be computed from experimentally determined values  $r$  and  $u$ . The partition coefficient  $k_e$  can then be determined by Eq. (13a) where  $x_1 = x_2 = x$ .

### 3. Experimental set-up and procedure

The experimental set-up consists of two identical chambers of 50 l in volume, each having its own sampling port. As shown in Fig. 1, a test specimen separates the two chambers, and the VOC compound (or VOCs mixture) under investigation is introduced into the high concentration chamber. Gas samples are collected from the sampling port of each chamber by drawing the gas through a commercially available sorption tube for collecting VOCs. The sorption tube is 4 mm inside diameter and 229 mm long with three layers of sorbents: glass beads, 150 mg of Tenex TM of 25 to 35 mesh, and 150 mg of 25 to 35 mesh. The choice of a proper sampling volume is important because a large sampling volume would create a pressure difference between the two chambers, and the assumption of pure diffusion would no longer be valid, while on the other hand a high sampling volume is desired for measuring low concentrations. For this study a sampling volume of 3 to 4 ml was found to be suitable. Gas samples collected by the adsorbent tubes were analyzed by a thermal desorption GC/FID system to determine the VOC concentrations in both chambers.

All the components of the experimental set up were fabricated from electro-polished stainless steel. To insure good gas mixing, each chamber was equipped with a small DC fan. The whole test facility was located in a room with a constant temperature ( $23 \pm 1^\circ\text{C}$ ).

#### 4. Test material and specimen preparation

Samples of plywood, vinyl floor tile, and a residential carpet were tested. As indicated by its label, the carpet contained nylon fibers and a secondary backing consisting of a coarse polypropylene mesh bonded to the primary backing with styrene-butadiene rubber (SBR) latex adhesive. The plywood belonged to the G1 S (Good One Side) group (i.e. 'Sanded, best appearance one side only, and may contain neat wood patches, inlays or synthetic patching material'). This kind of plywood is used where the appearance on one side is important such as in the case of furniture, cabinet doors, partitions, shelving, and concrete formwork. The floor tile tested was vinyl based.

The materials were cut in to circular specimens (60 mm in diameter), and placed on a glass substrate in an environmentally controlled room with a clean air supply for a minimum of 8 weeks before testing. Air conditions were maintained at  $23 \pm 1^\circ\text{C}$  and  $50\% \pm 5\%$  RH. This allowed VOCs remaining in the specimens to be minimal and the materials to be in equilibrium with the test condition. Special attention was paid to the sealing of the specimen edges. As shown in Fig. 1, Teflon gaskets are used for sealing the edges.

#### 5. Evaluation of the test facility

##### 5.1. Air mixing and velocity level within the two chambers

A number of preliminary tests were conducted for the purpose of refining the experimental procedures and determining the most suitable initial concentration and sampling volume. The main points of concern were the homogeneity of the concentration inside the two chambers and the repeatability of the test data. To simplify the analysis of the test results, it is convenient to assume that the extracted air sample is representative of the air throughout the test chambers. In other words, it is assumed that the VOCs are homogeneously distributed throughout the air volume of the two chambers. The first objective of the preliminary experiments was therefore to provide for the interior air movement to achieve a close approach to homogeneity. As stated earlier, an interior air circulation fan was introduced in both chambers to ensure complete air mixing. The air velocity inside the two chambers were measured at different locations (bottom, middle and 1 cm above the specimen surface) to insure proper air circulation (mixing level). The velocity inside the two chambers was measured by using thermal anemometer. The measured velocities at bot-

tom, middle and 1 cm above the specimen were 0.55, 0.25 and 0.6 m/s, respectively.

If we define the convective resistance to mass transfer as  $R_{\text{gas}}$ , where  $R_{\text{gas}}$  is the ratio of the boundary layer thickness ( $\delta$ ) divided by the diffusivity of the compound in the air ( $D_{\text{air}}$ ), and the  $R_{\text{solid}}$  as the resistance to mass transfer within the solid (diffusive resistance), where  $R_{\text{solid}}$  is the ratio of the specimen thickness ( $L$ ) divided by the diffusivity of the compound within the specimen ( $D_{\text{solid}}$ ), the order of magnitude of both mass transfer resistances can be estimated. For example, for ethylbenzene within the plywood, the values of  $R_{\text{gas}}$ , and  $R_{\text{solid}}$  were 0.985 hr/m and  $4.09 \times 10^4$  hr,m (assuming turbulent flow with 0.6 m/s velocity above the specimen surface) respectively. Therefore, for the compounds tested in this study, the order of magnitude of the convective resistance ( $R_{\text{gas}}$ ) is negligible comparing to the diffusive mass transfer resistance ( $R_{\text{solid}}$ ).

##### 5.2. Air-tightness of the test facility

Air leakage is one of the most serious sources of error in the diffusion measurement. Many precautions were made to eliminate air leakage in the test facility. This included: balancing the pressure of both chambers with the ambient pressure (i.e. the pressure in the high concentration chamber, the pressure in the low concentration chamber, and the ambient pressure are equal), taping the specimen/stainless steel interface with more than one layer of Teflon tape (namely, four Teflon gaskets were used, two above and two underneath the specimen), and fastening the test specimen to the specimen holder by 12 bolts. The air tightness of the two chambers at 5 Pa pressure difference across the chamber walls was about 0.08 l/min, and was considered negligible under the zero pressure difference during the diffusion measurements conducted.

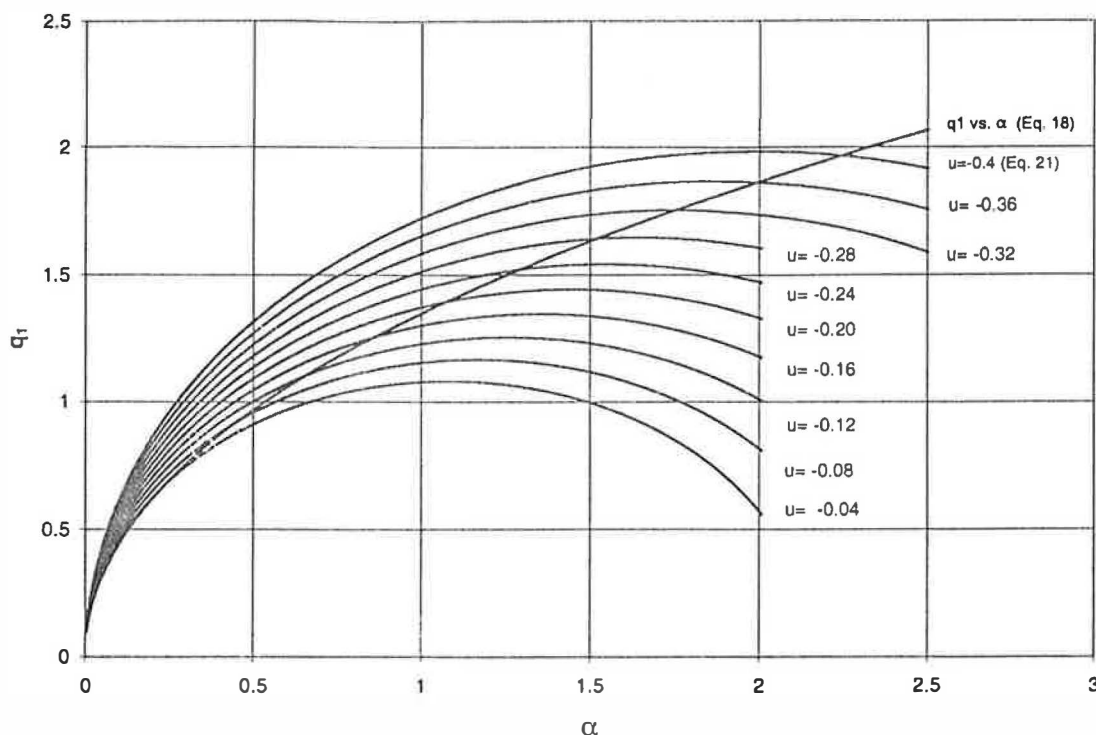
##### 5.3. The impact of possible sink effect

Some consideration was also given to the problem of adsorption of volatiles VOCs on the walls of the test chambers (the sink effect), and its impact on the measured parameters. Previous sink studies showed that the sink strength of an empty stainless steel chamber [9,15] is very small, and thus, can be neglected for compounds investigated in this study.

#### 6. Solution procedure

The following procedure was used:

1. From the straight line part of the plot  $\text{Ln}\{(c_2 - c_1)/c_0\}$  vs  $t$  determined from experiments, the quantities

Fig. 2.  $q_1$  vs  $\alpha$ .

$r$  and  $u$  (the slope and the negative intercept) were calculated by the least-square regression method.

- The root  $q$  of the characteristic equation [Eq. (15)] was first computed by using the Bisection method [11] for selected values of  $\alpha$  as shown in Fig. 2 (Note: until now the correct values of  $\alpha$  and  $q$  were unknown).
- From Eq. (18),  $q_1$  values were calculated and plotted against  $\alpha$  for a given  $u$  (Fig. 2 illustrates curves for a range of  $u$  values).
- The values  $q_1$  and  $\alpha$  corresponding to the intercept between Eq. (15) and Eq. (18) for the experimentally determined  $u$  are the correct  $q_1$  and  $\alpha$  values.
- Finally, the diffusion ( $D$ ) and partition ( $k_c$ ) coefficients were calculated using Eqs. (17) and (13a), respectively.

## 7. Results and discussion

The experimental results for selected compounds are shown in Figs. 3, 4 and 5 for carpet, plywood and the floor tile, respectively. The linearity shown by the measured  $\ln(c_2 - c_1)/c_0$  vs time confirmed the validity of the approximation in Eq. (16a). The parameter values ( $D$  and  $k_c$ ) for each compound are given in Tables 1, 2 and 3, respectively. Diffusion and partition coefficients for VOCs depend on the chemical and physical properties of the compound such as the mol-

ecular weight, vapour pressure, polarity, etc. Schwöpe et al. [12] correlated diffusion coefficients for a wide range of VOCs in six polymers as a function of molecular weight, showing that diffusivity increases with the inverse of the molecular weight. As shown in Tables 1, 2 and 3 and Fig. 6 the range of measured values of ' $D$ ' for carpet is  $4.3 \times 10^{-11}$  to  $2.8 \times 10^{-12}$   $m^2/s$  for the compounds with molecular weights varying between 92 to 157. For the plywood, the range of measured values of ' $D$ ' was  $1.55 \times 10^{-10}$  to  $1.28 \times 10^{-11}$   $m^2/s$  for the compounds with molecular weight varying between 84 to 143. For the floor tile, the range of measured values of ' $D$ ' was from  $1.6 \times 10^{-11}$  to  $8.55 \times 10^{-13}$   $m^2/s$ , for the compounds with molecular weight varying between 116 to 156. The largest molecule has the smallest diffusion coefficient, which is true for all three materials tested. The partition coefficient ( $k_c$ ) is expected to increase as the vapour pressure of the compound decreases. As shown in Tables 1, 2 and 3 and Fig. 7, Undecane has the lowest vapour pressure, and the measured value of ' $k_c$ ' is indeed the largest. Based on the measured data, relationships between  $D$  vs  $1/MW$  and between  $k_c$  vs  $1/P$  were shown in Figs. 6 and 7 respectively. It should be noted that the trends are shown only to illustrate the relationship between  $D$  vs  $1/MW$  and between  $k_c$  vs  $1/P$ . More data are necessary to obtain more accurate correlations. Park et al. [13] measured the diffusion and partition coefficients for a range of VOCs in the Styrene-Butadiene Rubber (SBR) (which is the main

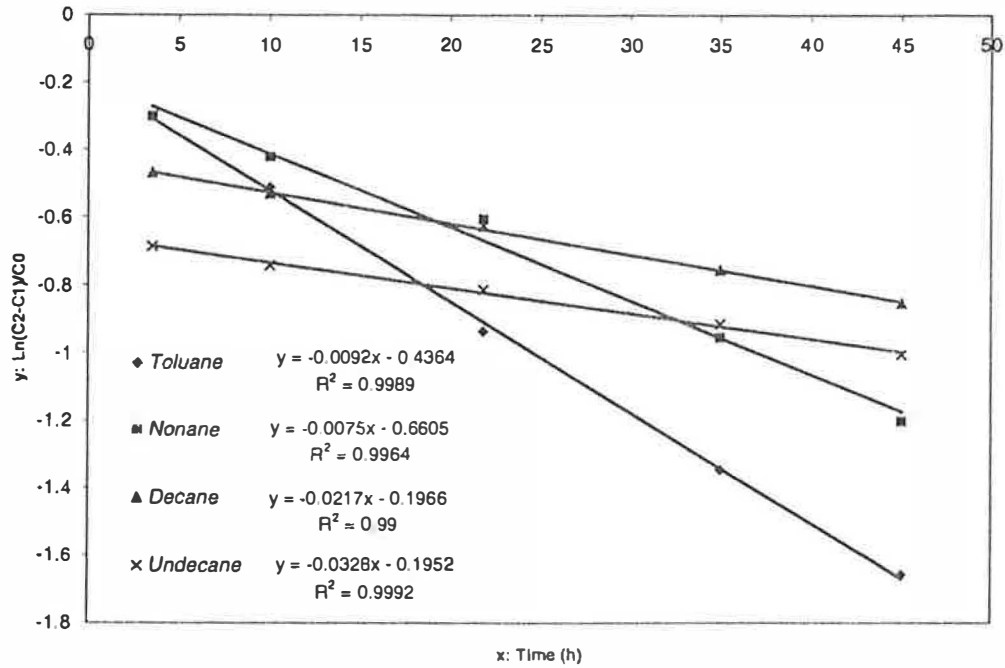


Fig. 3.  $\ln(c_2-c_1)/c_0$  vs time.

component of the carpet backing material), and found values of 'D' varying between  $2.3 \times 10^{-12}$  to  $1.0 \times 10^{-12}$  m<sup>2</sup>/s, and  $k_e$  varying between 200 to 28000 for molecular weights varying from 72 to 166. Also Little et al. [4] studied the emission from carpet in the full scale chamber, and fit the data to a mass transfer

based model. They calculated the diffusion, and partition coefficient for the VOCs with molecular weight varying from 30 to 158, obtaining 'D' ranging from  $0.5 \times 10^{-12}$  to  $1.0 \times 10^{-11}$  m<sup>2</sup>/s, and the value of 'k<sub>e</sub>' varying from 1400 to 170,000. These values are close to those obtained from this experimental study.

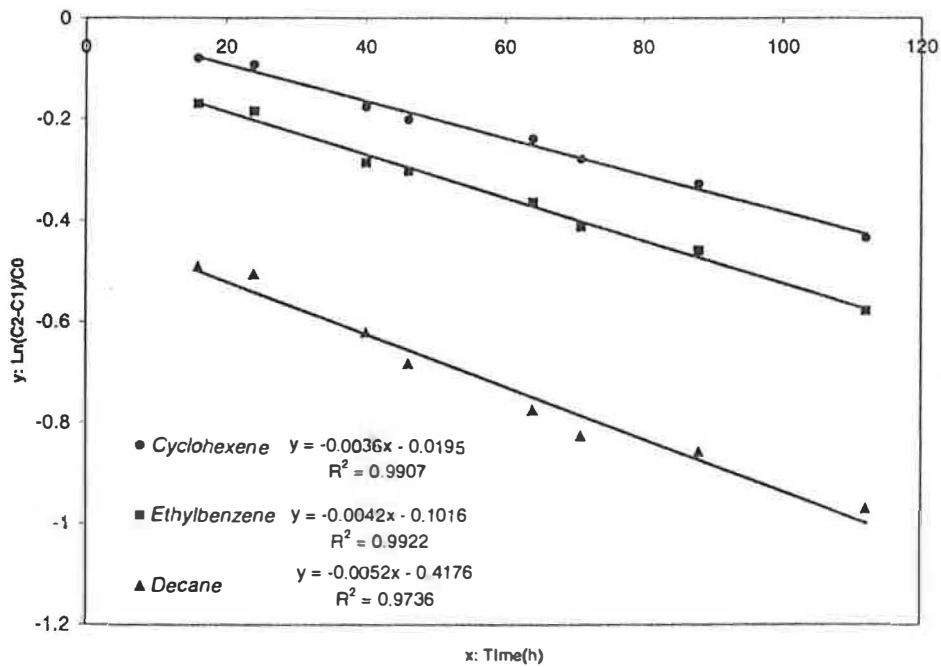
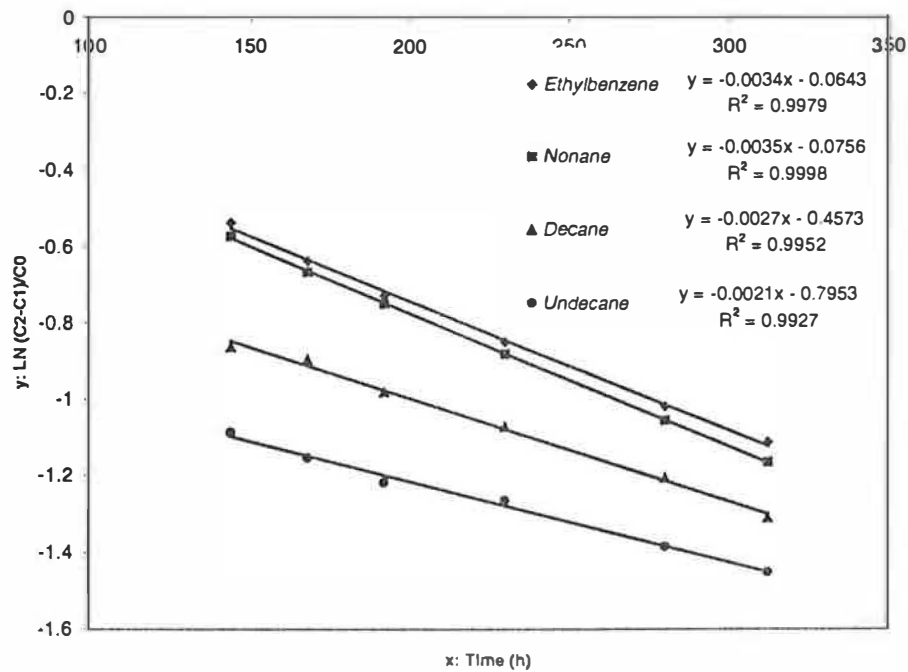


Fig. 4.  $\ln(c_2-c_1)/c_0$  vs time.

Fig. 5.  $\ln(c_2 - c_1) / c_0$  vs time.Table 1  
Parameters for the carpet backing material

| Compound name | Molecular weight | Vapour pressure (mm-Hg) at 23 C | Diffusion coefficient 'D' ( $m^2 s$ ) | Partition coefficient 'k <sub>v</sub> ' |
|---------------|------------------|---------------------------------|---------------------------------------|---|
| Toluene       | 92.14            | 25.64                           | $4.31 \times 10^{-11}$                | 6171                                    |
| Nonane        | 128.26           | 3.93                            | $2.83 \times 10^{-11}$                | 6216                                    |
| Decane        | 142.29           | 1.25                            | $5.42 \times 10^{-12}$                | 14,617                                  |
| Undecane      | 156.31           | 0.35                            | $2.79 \times 10^{-12}$                | 24,255                                  |

Table 2  
Parameters for the plywood

| Compound name | Molecular weight | Vapour pressure (mm-Hg) at 23 C | Diffusion coefficient 'D' ( $m^2 s$ ) | Partition coefficient 'k <sub>v</sub> ' |
|---------------|------------------|---------------------------------|---------------------------------------|---|
| Cyclohexane   | 84               | 35.6                            | $1.55 \times 10^{-10}$                | 348                                     |
| Ethybenzene   | 116.25           | 8.58                            | $4.04 \times 10^{-11}$                | 1636                                    |
| Decane        | 142.29           | 1.25                            | $1.28 \times 10^{-11}$                | 6948                                    |

Table 3  
Parameters for the floor tile

| Compound name | Molecular weight | Vapour pressure (mm-Hg) at 23 C | Diffusion coefficient 'D' ( $m^2 s$ ) | Partition coefficient 'k <sub>v</sub> ' |
|---------------|------------------|---------------------------------|---------------------------------------|---|
| Ethybenzene   | 116.25           | 8.58                            | $1.6 \times 10^{-11}$                 | 1920                                    |
| Nonane        | 128.26           | 3.93                            | $1.48 \times 10^{-11}$                | 2142                                    |
| Decane        | 142.29           | 1.25                            | $2.09 \times 10^{-12}$                | 13,045                                  |
| Undecane      | 156.31           | 0.35                            | $8.55 \times 10^{-13}$                | 26,647                                  |



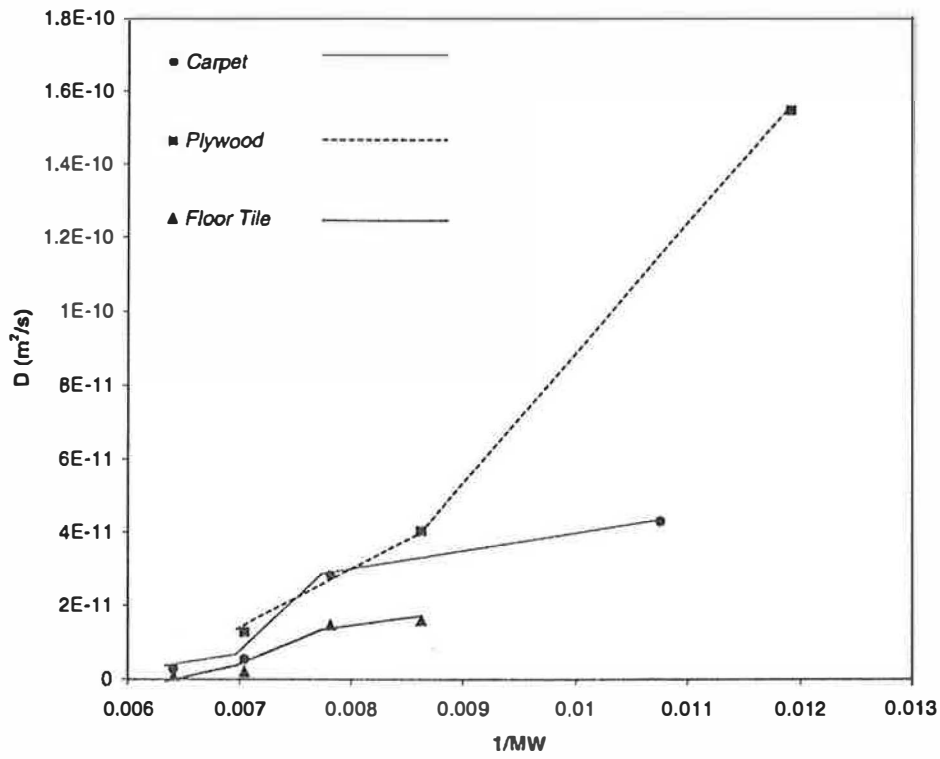


Fig. 6. Diffusion coefficient vs  $1/MW$ .

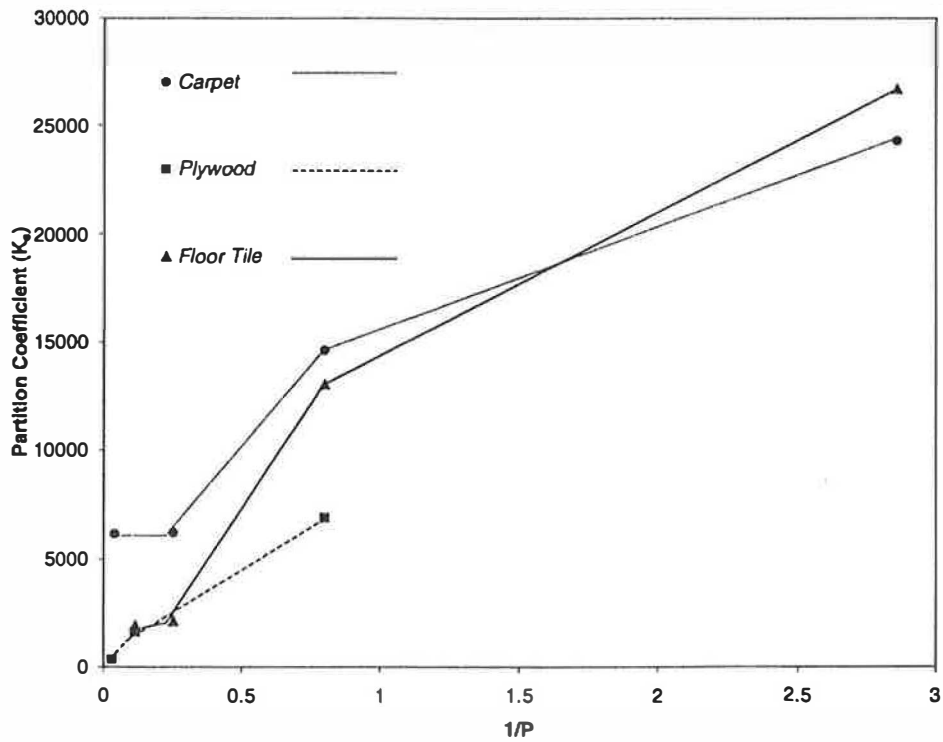


Fig. 7. Partition coefficient vs  $1/P$ .

As mentioned above, emission from dry materials is mainly controlled by diffusion within the source. The resulting mass transfer model usually contains three mass transfer parameters [3,4,7]:

1. diffusion coefficient within the source ' $D$ ';
2. initial concentrations of VOCs in the source ' $C_0$ ';
3. partition coefficient ' $k_e$ '.

The experimental method developed in this study will give  $D$  and  $k_e$ .  $C_0$  can be determined by conducting a static chamber test (headspace test). In the headspace test, a specimen is placed in an air-tight chamber under a pre-specified condition (e.g. 23°C, 50% RH) for a period of time that is sufficient for reaching the equilibrium between the specimen and the air in the chamber. The air concentration ( $C_{\text{space}}$ ) in the chamber is measured (i.e. the headspace concentration) [14].  $C_0$  is determined by  $C_0 = k_e C_{\text{space}}$ . This will facilitate the prediction of the emission rates without the need of a dynamic chamber test.

## 8. Summary and conclusions

A new experimental method for the determination of diffusion and partition coefficients of VOCs is developed for dry building materials based on the solution of Fick's law equation of diffusion with appropriate boundary conditions. Using the new experimental method developed, the diffusion and partition coefficients were determined for three building materials including carpet, plywood and vinyl tile. It was found that, for all three materials tested, the VOCs with the largest molecular weight had the smallest diffusion coefficient, and the VOCs with lowest vapour pressure had the largest partition coefficient.

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