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Correlations Between the Internal Diffusion and Equilibrium Partition Coefficients of Volatile Organic Compounds (VOCs) in Building Materials and the VOC Properties

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ABSTRACT

In this study, a novel experimental method that was previously developed was used to directly measure the internal diffusion (D) and the equilibrium partition coefficients (k_e) for three classes of volatile organic compound (VOC), (1) aliphatic hydrocarbons, (2) aromatic hydrocarbons, and (3) aliphatic aldehydes, through typical dry building materials (plywood, particleboard, vinyl floor tile, gypsum board, subfloor tile, and OSB). For each chemical class, correlations between D and the VOC molecular weight and between k_e and the vapor pressure of VOCs were developed for every product. These correlations can be used to estimate D and k_e when direct measurement data are not available and, thus, facilitate the prediction of VOC emissions from the building materials using mass transfer theory. It was found that the values of diffusion coefficients for a given material are inversely proportional to the molecular weights of the VOCs, and the values of the partition coefficients are also inversely proportional to the vapor pressures of the VOCs. The measured diffusion and partition coefficients are useful for predicting the emission rates of VOCs from building materials.

INTRODUCTION

A wide variety of dry materials (e.g., vinyl tiles and plywood) are used in residential and commercial buildings. It is important to understand and determine the volatile organic compound (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) (Roache et al. 1994; Little et al. 1994; Christianson et al. 1993). 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, and x is the spatial coordinate (assuming 1-D diffusion).

In order to apply a diffusion-based model for predicting the VOC emission rates, it is necessary to know the diffusion coefficient (D) and the equilibrium partition coefficient k_e (k_e is a coefficient used to describe the relationship between the concentration in the gas phase and the concentration in the solid phase). However, data on these coefficients for building materials are very limited.

Little et al. (1994) proposed a method for determining these coefficients using the concentration data obtained from a dynamic chamber test for VOC emissions. It requires knowledge of the initial concentration within the region of interest. Mathematically, the initial concentration may be treated as an additional parameter to be estimated from the concentration data. This will increase the number of parameters to be estimated in a single least-squares regression analysis, which may result in a large estimation error due to inter-dependency of the parameters in the regression analysis process.

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This work reports the results of measurements conducted to determine the diffusion and equilibrium partition coefficients for selected VOCs from three classes (aliphatic hydrocarbons, aromatic hydrocarbons, and aliphatic aldehydes) and limonene through typical dry building materials (plywood, particleboard, vinyl floor tile, gypsum board, subfloor tile, and OSB). It also reports the correlations that existed between these coefficients and the physical and chemical properties of the VOCs.

METHOD

The measurement of the diffusion and partition coefficients was based on a method developed by Bodalal et al. 1999 that is briefly described below (Bodalal et al. 1999).

Consider a control volume consisting of two stainless steel chambers separated by test specimen with a thickness of l (Figure 1). Initially, the diffusing VOC is in one compartment only (chamber 2, high concentration chamber) where the concentration at the beginning of the experiment is c_0 . After time t , its value decreases to $c_2(t)$ due to diffusion through the test specimen. Meanwhile, the concentration in the other chamber (chamber 1, low concentration chamber) rises from the zero initial value to $c_1(t)$. Both chambers are well mixed so that the concentrations are uniform. 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 $C(x, t)$.

On the assumption that the VOC concentration on the specimen surface is proportional to the concentration of the compound in contact with this surface (the proportional constant k_e is known as the equilibrium partition coefficient), the process can be described by Equation 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 concentrations in the low and high concentration chambers can be expressed by Equations 3 and 4, respectively.

$$c_1 = (DA/V_1) \int_0^l \left(\frac{\partial C}{\partial x} \right)_{x=0} dx \quad (3)$$

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

where 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.

Solution of the above equations by mean of the Laplace-Carson transformation yields the relationships for measurable

quantities c_1 and c_2 (complete details of the solution procedures are given by Bodalal et al. 1999).

$$\ln \frac{(c_2 - c_1)}{c_0} = \ln \left(\frac{4\alpha}{q_1^2 + \alpha(2 + \alpha)} \right) - \left(\frac{-q_1^2 D}{l^2} \right) t \quad (5)$$

Equation 5, indicates that $\ln \frac{(c_2 - c_1)}{c_0}$ decreases linearly as t increases with the slope:

$$r = \frac{-q_1^2 D}{l^2} \quad (6)$$

That straight line intersects the $\ln \frac{(c_2 - c_1)}{c_0}$ axis at

$$u = \ln \left(\frac{4\alpha}{q_1^2 + \alpha(2 + \alpha)} \right), \quad (7)$$

where q_1 are the positive roots of the characteristic equation

$$\tan(q) = \frac{2\alpha q_i}{(q_i^2 - \alpha^2)} \quad (8)$$

On solving Equations 6, 7, and 8, the auxiliary parameters, q_1 , and the quantities D and α can be computed from experimentally determined values r and u . The partition coefficient k_e can then be determined by

$$k_e = \frac{\alpha V}{Al} \quad (9)$$

EXPERIMENTAL SETUP AND PROCEDURE

The experimental setup consists of two identical chambers of 50 L in volume, each having its own sampling port (Bodalal et al. 1999). As shown in Figure 1, a test specimen separates the two chambers, and the VOC compound (or

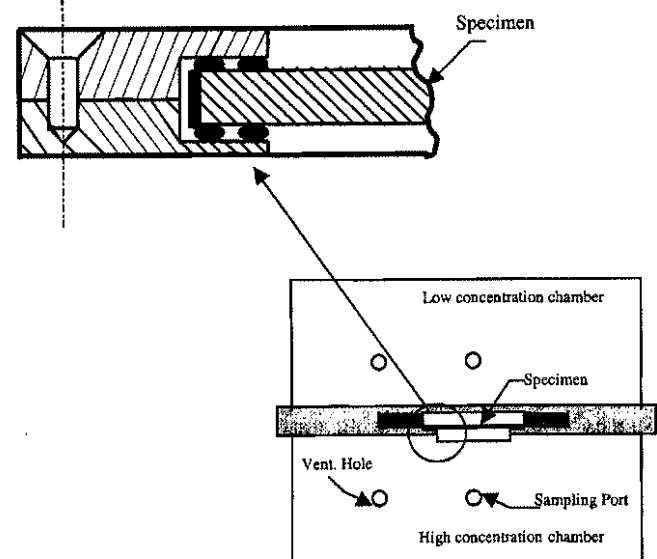


Figure 1 Diffusiometric apparatus.

VOCs mixture) under investigation is introduced into the high concentration chamber only. Gas samples are collected from the sampling port of each chamber using commercially available three-layer sorption tubes. 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 large sampling volume is necessary for measuring low concentrations. For this study, a sampling volume of 50 to 60 mL was found to be suitable. Gas samples collected were analyzed by a thermal desorption GC/FID system to determine the VOC concentrations in both chambers. All the components of the experimental setup were fabricated from electro-polished stainless steel. To ensure 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 ($23^{\circ}\text{C} \pm 1^{\circ}\text{C}$).

TEST MATERIAL AND SPECIMEN PREPARATION

Test samples included plywood, particleboard, fire resistant gypsum board, subfloor tile, vinyl floor tile, and oriented strand board (OSB). Except for the subfloor tile, all test materials are commonly used in building construction. The subfloor tile tested in this study is a new product that has recently been introduced to the market as a building material, and the main component of it is recycled automobile tires.

The automobile tires are treated chemically (recycled), melted, and cast again in the form of sheets with different dimensions ($1.5\text{ m} \times 1.8\text{ m}$). These sheets are used indoors as a part of the floors to absorb sound and vibrations.

The materials were cut into circular specimens (80 mm in diameter) and placed on a glass substrate in an environmentally controlled room with a clean air supply for a minimum of eight weeks before testing. Air conditions were maintained at $23^{\circ}\text{C} \pm 1^{\circ}\text{C}$ and $50\% \pm 5\% \text{ RH}$. This allowed VOCs remaining in the specimens to be minimized and the materials to be in equilibrium with the test condition. Special attention was given to the sealing of the specimen edges.

TEST PLAN

Table 1 summarizes the test plan and shows the physico-chemical properties of the targeted compounds. As can be seen, the targeted compounds included selected VOCs from three main chemical classes (aliphatic hydrocarbons, aromatic hydrocarbons, and aliphatic aldehydes) and limonene (for particle board and plywood only). Both the VOCs and the test materials were carefully chosen to meet the following criteria.

1. The selected materials are the most common products used indoors.
2. The selection of the targeted VOCs was based on the results of the GC/MS screening of each product.

TABLE 1
Diffusion Test Plan and Physical Properties of Target Compounds

Material	Chemical Class	Compound Name	Polarity	Molecular Weight	Vapor Pressure* (mm-Hg)	Boiling Point $^{\circ}\text{C}$
(1) Vinyl floor tile	Aliphatic-hydrocarbon	Heptane	Nonpolar	100.21	41.18	98
		Octane		114.23	12.56	125
		Nonane		128.26	3.93	151
(2) OSB		Decane		142.29	1.25	174
		Undecane		156.3	0.35	196
(1) Subfloor (recycled automobile tires)	Aromatic-hydrocarbon	Benzene	Semi-polar	84.07	81.4	80
		Toluene		92.14	25.64	110
		P-xylene		106.2	7.92	138.4
(2) Plywood		Ethylbenzene		116.25	8.58	136
(3) Vinyl floor tiles		Propyl-benzene		120.2	3.02	159.2
(4) Gypsum board		Butyl-benzene		134.22	0.89	183
(5) Particle board						
(1) Particle-board	Aliphatic-aldehydes	Pentanal	Polar	86.1	30.88	103
		Hexanal		100.16	10.00	131
(2) Plywood		Heptanal		114.19	3.10	153
		Octanal		128.22	1.02	171
	Terpenes	Limonene	Semi-polar	136.24	1.74	176

* Vapor pressure of all compounds at 23°C .

- The targeted compounds have a wide range of molecular size and vapor pressure so that the correlations between diffusion coefficient and molecular weight and between partition coefficient and vapor pressure of each product can be developed.
- The selected compounds have different degrees of polarity and cover a wide range of boiling points and vapor pressure.

RESULTS

To determine the diffusion coefficients, it is necessary to know the values of r (Equation 6) and u (Equation 7). These values were obtained from the measured concentrations. As an example, the measured concentrations for five aliphatic hydrocarbon species (heptane, octane, nonane, decane, and undecane) are shown in Figures 2 and 3 for vinyl floor tile and OSB, respectively. From the fitted curves, the value of r (slope) and u (intercept at $t=0$) can be determined. The values of r and u obtained for all tested building materials and VOCs are given in Table 2. Based on these values, D and k_e were calculated from Equations 7, 8, and 9 for each tested building material and are given in Tables 3 through 8.

TABLE 2a
Values of r and u for Equations 6 and 7 for Vinyl Flooring

VOCs	r	u	R^2
Heptane	-0.0039	-0.0616	0.9963
Octane	-0.0039	-0.0528	0.9968
Nonane	-0.0038	-0.1752	0.9982
Decane	-0.0037	-0.5104	0.986
Undecane	-0.0043	-1.182	0.9746
Benzene	-0.0043	-0.0104	0.9993
Toluene	-0.0037	-0.0267	0.9933
Ethyl-benzene	-0.004	-0.0428	0.9902
Propyl-benzene	-0.0044	-0.1436	0.9821
Butyl-benzene	-0.0068	-0.4276	0.9988

TABLE 2b
Values of r and u for Equations 6 and 7 for Oriented Strand Board (OSB)

VOCs	r	u	R^2
Heptane	-0.0087	0.0046	0.9783
Octane	-0.008	-0.0802	0.9948
Nonane	-0.0081	-0.0862	0.9781
Decane	-0.0081	-0.6074	0.9975
Undecane	-0.0107	-1.0671	0.9968

TABLE 2c
Values of r and u for Equations 6 and 7 for Fire Resistant Gypsum Board

VOCs	r	u	R^2
Benzene	-0.0048	-0.0135	0.9919
Toluene	-0.0044	-0.077	0.9955
Ethyl-benzene	-0.0045	-0.0713	0.9976
Propyl-benzene	-0.005	-0.2153	0.9852
Butyl-benzene	-0.006	-0.6949	0.9908

TABLE 2d
Values of r and u for Equations 6 and 7 for Particle Board

VOCs	r	u	R^2
Pentanal	-0.0135	0.0228	0.9979
Hexanal	-0.0152	-0.0695	0.9926
Heptanal	-0.0123	-0.377	0.991
Octanal	-0.0086	-0.9652	0.9737
Limonene	-0.0079	-0.2871	0.9886
Benzene	-0.0151	-0.0788	0.989
Toluene	-0.0141	-0.0544	0.9958
Ethyl-benzene	-0.0124	-0.0936	0.9933
Propyl-benzene	-0.0106	-0.2601	0.9928
Butyl-benzene	-0.0106	-0.76	0.991

TABLE 2e
Values of r and u for Equations 6 and 7 for Plywood

VOCs	r	u	R^2
Benzene	-0.0061	-0.0055	0.9599
Toluene	-0.0056	-0.02	0.9925
Ethyl-benzene	-0.0053	-0.156	0.9812
Propyl-benzene	-0.005	-0.2043	0.9589
Butyl-benzene	-0.0046	-0.6947	0.9664
Pentanal	-0.0041	-0.0318	0.9929
Hexanal	-0.0043	-0.0965	0.9931
Heptanal	-0.0064	-0.2183	0.9856
Octanal	-0.0065	-0.582	0.9711
Limonene	-0.0038	-0.2085	0.9885

TABLE 2f
Values of r and u for Equations 6 and 7 for Subfloor Tile

VOCs	r	u	R^2
Benzene	-0.005	-0.0097	0.9917
Toluene	-0.005	-0.0569	0.9901
P-xylene	-0.0055	-0.1992	0.9841

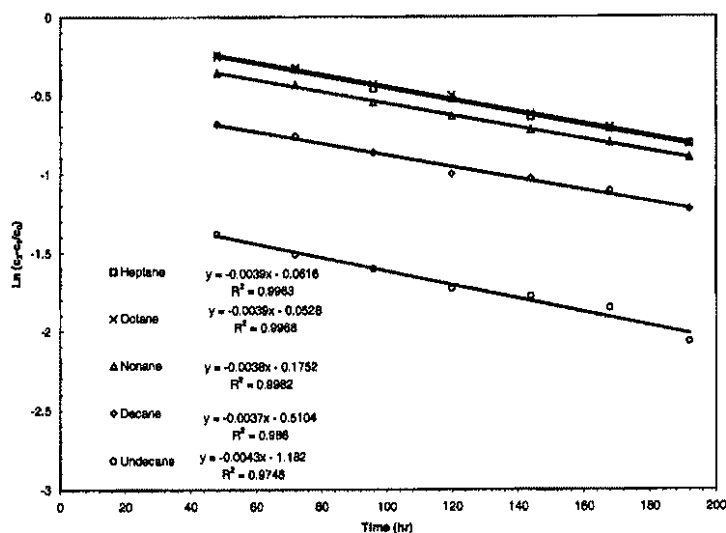


Figure 2 $\ln\{(c_2 - c_1)/c_0\}$ vs. time (vinyl flooring).

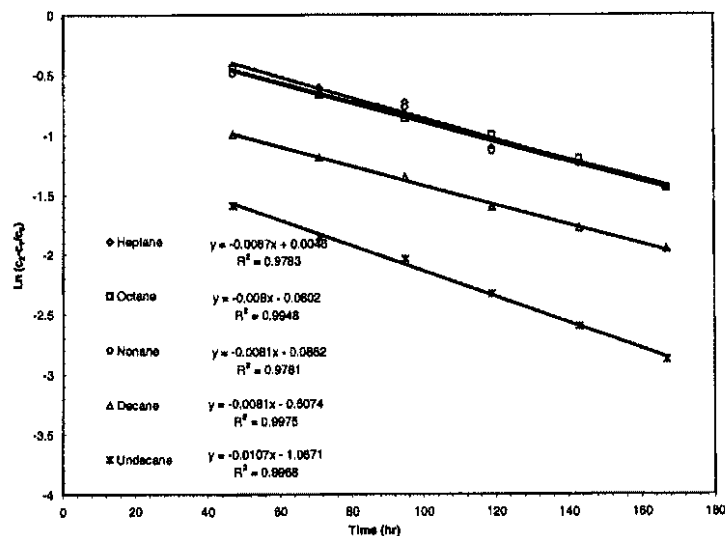


Figure 3 $\ln\{(c_2 - c_1)/c_0\}$ vs. time (OSB).

As shown in Table 3, the values of D for the vinyl floor tile vary from $2.35 \times 10^{-11} \text{ m}^2/\text{s}$ to $2.01 \times 10^{-12} \text{ m}^2/\text{s}$ for aliphatic hydrocarbon compounds with molecular weight varying between 100 and 157. For the OSB, the values of D vary from $2.34 \times 10^{-10} \text{ m}^2/\text{s}$ to $7.24 \times 10^{-12} \text{ m}^2/\text{s}$, for the compounds with the same range of molecular weight.

Figures 4 and 5 show the correlations between D and molecular weight for OSB and vinyl tile, respectively (note that the units of D used in these figures are m^2/h while the units in Table 3 are m^2/s). Figures 6 and 7 show the correlations between k_e and vapor pressure for these two building materials. The results indicate that the diffusion coefficient is inversely proportional to the molecular weight. Also, the partition coefficient is inversely proportional to vapor pressure at a given temperature.

The correlation between D and molecular weight (M_w) can be expressed by

$$D = a / M_w^{n1} \quad (10)$$

Also, the correlation between k_e and vapor pressure (P) is

$$k_e = b / P^{n2} \quad (11)$$

The values of a , $n1$, b , and $n2$ are given in Tables 3 through 8.

The diffusion and partition coefficients of five aromatic hydrocarbons (benzene, toluene, ethyl-benzene, propyl-benzene, and butyl-benzene) through gypsum board, vinyl flooring tile, subfloor tile (recycled tires), plywood, and particle board are given in Tables 5 and 6. As shown in Table 5, the values of D for the gypsum board vary from $7.05 \times 10^{-12} \text{ m}^2/\text{s}$ to

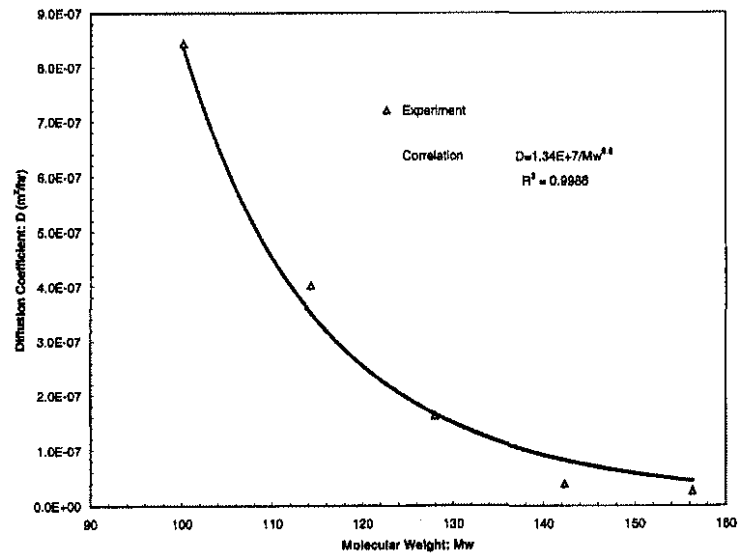


Figure 4 Diffusion coefficient vs. M_w through OSB.

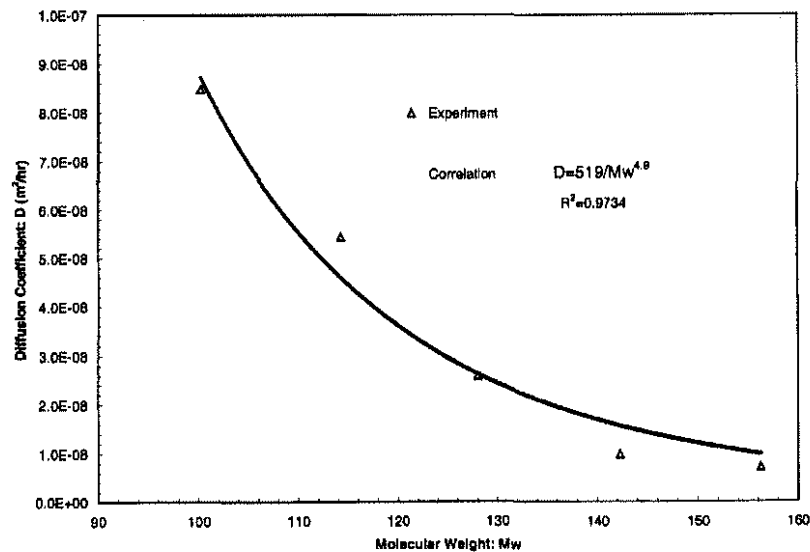


Figure 5 Diffusion coefficient vs. M_w through vinyl flooring.

TABLE 3
Diffusion Coefficients for Vinyl Tile and OSB

Compound Name	Diffusion Coefficient D (m ² /s) {Vinyl Tile}	Diffusion Coefficient D (m ² /s) {OSB}
Heptane	2.35×10^{-11}	2.34×10^{-10}
Octane	1.50×10^{-11}	1.12×10^{-10}
Nonane	7.22×10^{-12}	4.51×10^{-11}
Decane	2.74×10^{-12}	1.07×10^{-11}
Undecane	2.01×10^{-12}	7.24×10^{-12}
Coefficient and exponent, Equation 10		
a	21.044	14,500,426
$n1$	5.942	8.355
R^2	0.98643	0.98664

TABLE 4
Partition Coefficients for Vinyl Tile and OSB

Compound Name	Partition Coefficient k_p {Vinyl Tile}	Partition Coefficient k_p {OSB}
Heptane	408	472
Octane	1421	998
Nonane	4821	2369
Decane	16,072	12,027
Undecane	61,250	25,931
Coefficient and exponent, Equation 11		
b	20,318	10,733
$n2$	1.051	0.886
R^2	0.99999	0.98949

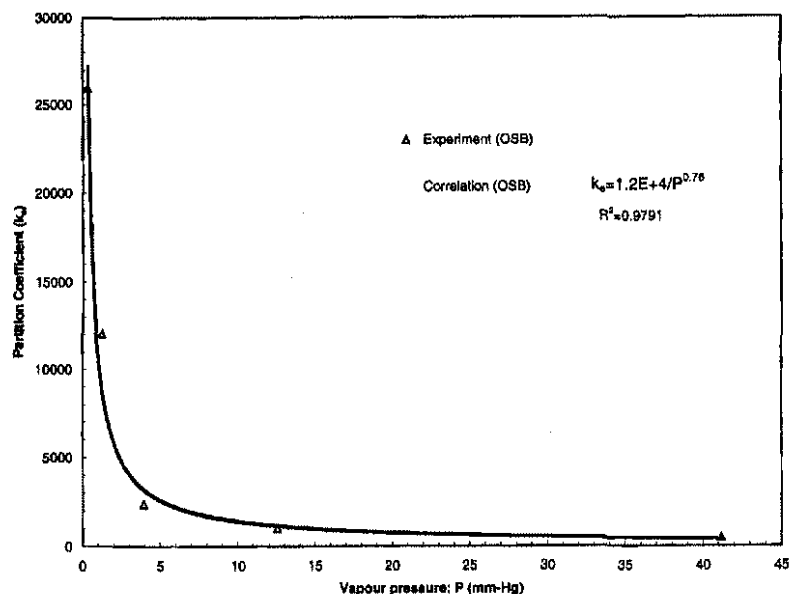


Figure 6 Partition coefficient vs. vapor pressure for OSB.

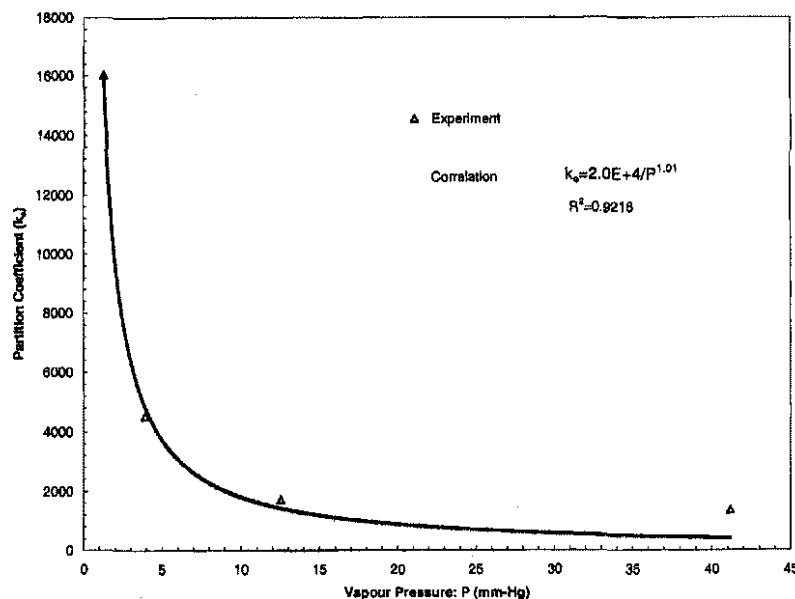


Figure 7 Partition coefficient vs. vapor pressure for vinyl flooring.

$1.42 \times 10^{-10} \text{ m}^2/\text{s}$ for the aromatic hydrocarbon compounds with molecular weights varying from 84 to 134. For the vinyl floor tile, the values of D vary from $1.06 \times 10^{-10} \text{ m}^2/\text{s}$ to $4.64 \times 10^{-12} \text{ m}^2/\text{s}$ for the aromatic hydrocarbon compounds with molecular weights varying from 84 to 134. For the subfloor tile, the range of D is from $2.78 \times 10^{-11} \text{ m}^2/\text{s}$ to $3.9 \times 10^{-12} \text{ m}^2/\text{s}$ for the compounds with molecular weights varying from 116 to 156. Also, for the plywood and the particle board, the range of D is from $4.92 \times 10^{-10} \text{ m}^2/\text{s}$ to $7.55 \times 10^{-12} \text{ m}^2/\text{s}$ and from $7.33 \times 10^{-10} \text{ m}^2/\text{s}$ to $8.97 \times 10^{-12} \text{ m}^2/\text{s}$, respectively.

As an example, Figure 8 shows the relationship between D and molecular weight for plywood (note that the units of D

used in these figures are m^2/h while the units in Table 5 are m^2/s). Figure 9 shows the correlations between k_e and vapor pressure for plywood. The results also suggest that similar to aliphatic hydrocarbons, for the selected aromatic hydrocarbons, the diffusion coefficient is inversely proportional to the molecular weight and that the partition coefficient is inversely proportional to vapor pressure at a given temperature. The values of a , n_1 , b , and n_2 are given in Tables 5 and 6.

The values of D and k_e of four aldehydes (pentanal, hexanal, heptanal, and octanal) and limonene through particle-board and plywood are given in Tables 7 and 8.

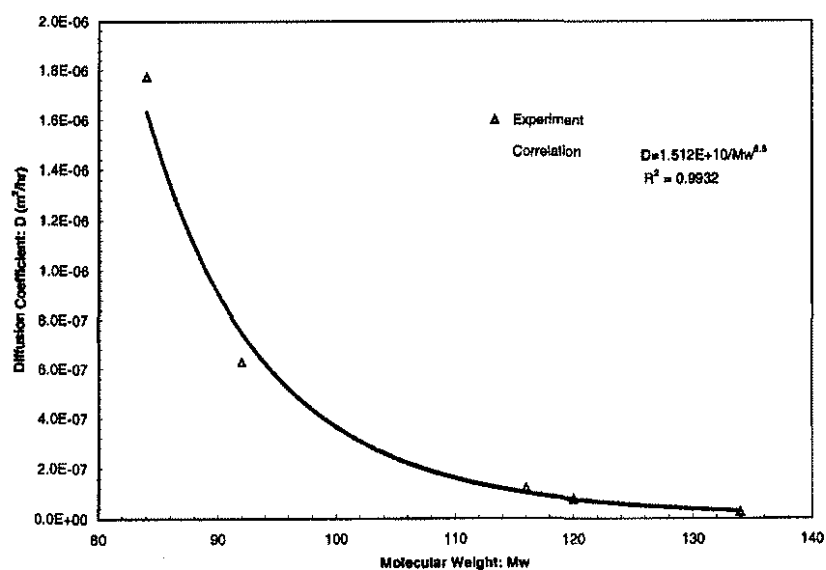


Figure 8 Diffusion coefficient vs. M_w through plywood.

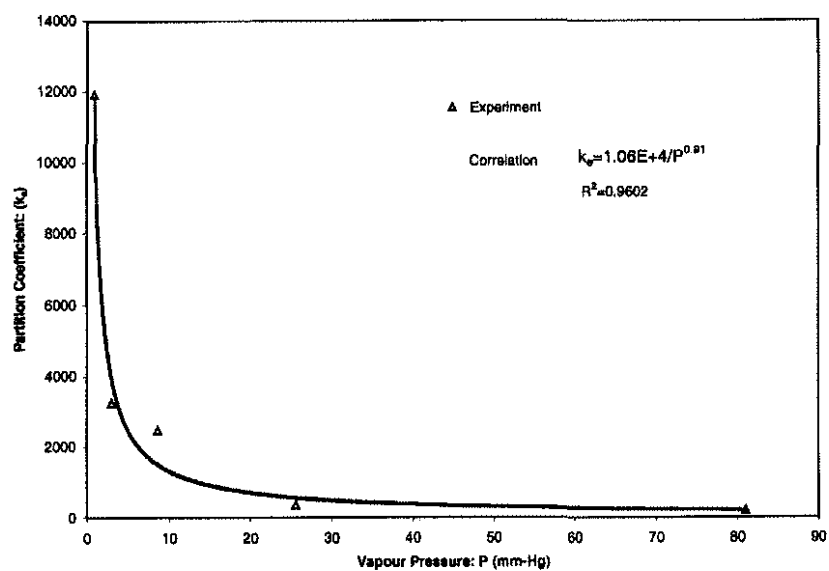


Figure 9 Partition coefficient vs. vapor pressure for plywood.

TABLE 5
Diffusion Coefficients for Gypsum Board, Vinyl Tile, Subfloor Tile, Plywood, and Particle Board

Compound Name	Diffusion Coefficient D (m ² /s) {Gypsum board}	Diffusion Coefficient D (m ² /s) {Vinyl Tile}	Diffusion Coefficient D (m ² /s) {Subfloor Tile}	Diffusion Coefficient D (m ² /s) {Plywood}	Diffusion Coefficient D (m ² /s) {Particle board}
Benzene	1.42×10^{-10}	1.06×10^{-10}	2.78×10^{-11}	4.92×10^{-10}	7.33×10^{-10}
Toluene	6.38×10^{-11}	5.42×10^{-11}	1.09×10^{-11}	1.75×10^{-10}	2.68×10^{-10}
Ethyl-benzene	2.77×10^{-11}	2.02×10^{-11}	3.89×10^{-12}	3.33×10^{-11}	1.05×10^{-10}
Propyl-benzene	1.41×10^{-11}	8.03×10^{-12}	NA	2.16×10^{-11}	3.42×10^{-11}
Butyl-benzene	7.05×10^{-12}	4.64×10^{-12}	NA	7.55×10^{-12}	8.97×10^{-12}
Coefficient and exponent, Equation 10					
a	44.81	361.73		13,372,310	16,921,219
$n1$	5.99	6.51		8.56	8.5
R^2	0.98162	0.97893		0.99687	0.96179

TABLE 6
Partition Coefficients for Gypsum Board, Vinyl Tile, Subfloor Tile, Plywood, and Particle Board

Compound Name	Partition Coefficient k_e {Gypsum board}	Partition Coefficient k_e {Vinyl Tile}	Partition Coefficient k_e {Subfloor Tile}	Partition Coefficient k_e Plywood	Partition Coefficient k_e Particle Board
Benzene	416	310	425	184	266
Toluene	941	539	2376	358	968
Ethyl-benzene	1360	1522	4675	2476	1237
Propyl-benzene	4562	4520	NA	3249	4388
Butyl-benzene	14031	13,356	NA	11,918	18,042
Coefficient and exponent, Equation 11					
b	10,693.	11,110.		11,080.	13,051
$n2$	0.772	0.863		0.944	0.892
R^2	0.98532	0.99329		0.98012	0.98339

TABLE 7
Diffusion Coefficients for Particle Board and Plywood

Compound Name	Diffusion Coefficient D (m ² /s) {Particle Board}	Diffusion Coefficient D (m ² /s) {Plywood}
Pentanal	3.66×10^{-10}	9.05×10^{-11}
Hexanal	7.42×10^{-11}	3.58×10^{-11}
Heptanal	2.22×10^{-11}	2.13×10^{-11}
Octanal	1.26×10^{-12}	1.138×10^{-11}
Limonene	1.83×10^{-11}	2.27×10^{-11}
*Coefficient and exponent, Equation 10		
a	339,627,424	0.00079
$n1$	9.33	3.637
R^2	0.83278	0.88018

* Excluding limonene

TABLE 8
Partition Coefficients for Particle Board and Plywood

Compound Name	Partition Coefficient k_e {Particle Board}	Partition Coefficient k_e {Plywood}
Pentanal	1980	680
Hexanal	2602	1845
Heptanal	7714	3117
Octanal	11,591	9226
Limonene *	5864	2839
*Coefficient and exponent, Equation 11		
b	10,366.	6,581
$n2$	0.51	0.644
R^2	0.94663	0.94122

* Excluding limonene

Figures 10 and 11 show examples of the relationships between D and molecular weight (note that the unit of D in these figures is in m^2/h while the unit in Table 5 is in m^2/s) and between k_e and vapor pressure for particle board. The results also suggest that for the four selected aldehyde compounds, the diffusion coefficient is inversely proportional to the molecular weight and that the partition coefficient is inversely proportional to vapor pressure at a given temperature. The values of a , n_1 , b , and n_2 are given in Tables 7 and 8.

DISCUSSION

The linearity shown by the measured $\ln(c_2 - c_1) / c_0$ versus time confirmed the validity of the approximation in Equation 5.

Park et al. (1989) measured the diffusion and partition coefficients for a range of VOCs in styrene-butadiene rubber (SBR) and found values of D varying between $2.3 \times 10^{-12} \text{ m}^2/\text{s}$ and $1.0 \times 10^{-12} \text{ m}^2/\text{s}$ and k_e varying between 200 and 28,000 for molecular weights varying from 72 to 166. They also reported that for the VOCs with molecular weight varying from 30 to 158, the diffusion coefficients

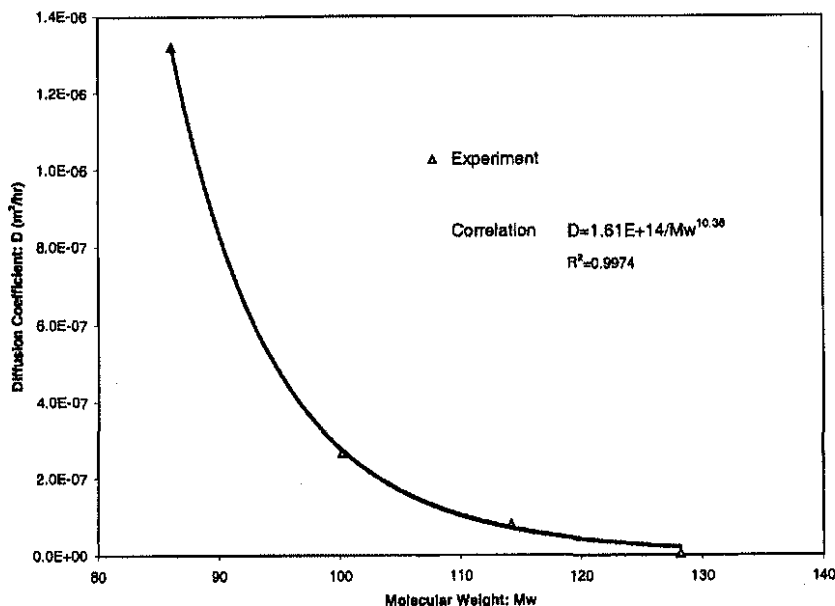


Figure 10 Diffusion coefficient vs. M_w through particle board.

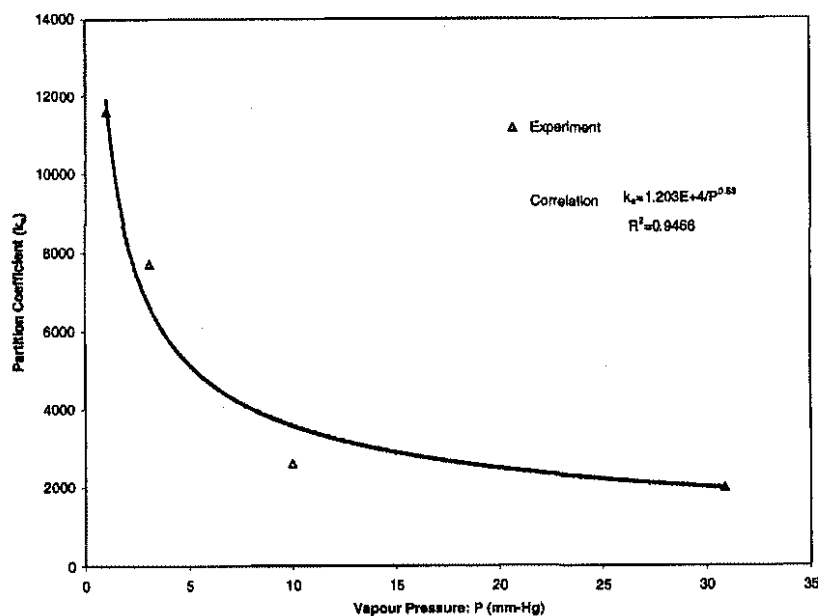


Figure 11 Partition coefficient vs. vapor pressure for particle board.

ranged from $0.5 \times 10^{-12} \text{ m}^2/\text{s}$ to $1.0 \times 10^{-11} \text{ m}^2/\text{s}$, and the values of k_e varied from 1400 to 170,000. These values are similar to those obtained from this study.

Diffusion and partition coefficients for VOCs depend on chemical and physical properties of the compound, such as the molecular weight, vapor pressure, and polarity. Schwöpe et al. (1989) correlated diffusion coefficients for a wide range of VOCs in six polymers as a function of molecular weight. They indicated that diffusivity increases as the molecular weight decreases. The present study also shows a similar conclusion.

As shown in Tables 1, 3, and 4 and Figures 6 and 7, undecane has the lowest vapor pressure and the largest k_e . Based on the measured data, relationships between D and molecular weight and between k_e and vapor pressure were obtained. More data are needed in order to obtain more accurate correlations.

IMPLICATION OF THIS STUDY

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 (Christiansson et al. 1993; Little et al. 1994, 1995): (1) diffusion coefficient within the source D , (2) initial concentrations of VOCs in the source C_0 , and (3) partition coefficient k_e . The experimental correlations (or data) 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 airtight 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 measured concentration in the chamber is C_{space} (i.e., the headspace concentration) (ASTM D 5116-97). C_0 can then be determined by $C_0 = k_e C_{space}$. This will facilitate the prediction of the emission rates without the need of a costly dynamic chamber test.

SUMMARY AND CONCLUSIONS

The diffusion and partition coefficients of six dry building materials were determined for selected VOCs. These building materials are plywood, particleboard, gypsum board, subfloor tile, vinyl floor tile, and oriented strand board (OSB).

The correlations obtained for predicting D and k_e based solely on commonly available properties, such as molecular weight and vapor pressure, were proposed for every product and three VOC classes. These correlations can be used to estimate the D and k_e when direct measurement data are not available. It was found that for all six materials tested, the VOC with the largest molecular weight had the smallest diffusion coefficient, and that the VOC with the lowest vapor pressure had the largest partition coefficient.

NOMENCLATURE

A = area of the specimen (m^2)
 $b.p.$ = boiling point of the compound ($^{\circ}\text{C}$)

C = concentration of the compound within the specimen (mg/m^3)
 C_0 = initial concentration of the compound in the specimen (mg/m^3)
 c = concentration of the compound in the chamber air (mg/m^3)
 c_0 = initial concentration of the compound in the chamber air (mg/m^3)
 D = diffusion coefficient of the compound within the specimen (m^2/s)
 IAQ = indoor air quality
 k_e = equilibrium partition coefficient between the specimen and the air
 l = thickness of the specimen under investigation (m)
 M_w = molecular weight of the compound
 OSB = oriented strand board
 p = Laplace-Carson transformation operator
 P = vapor pressure (mm-Hg)
 q_1 = first positive root of the characteristic equation
 r = slope of the straight line ($r = -q_1 D / l^2$)
 RH = relative humidity
 t = time (s)
 S, s = transformation of C and c , respectively
 u = intercept of the straight line ($u = \ln(c_2 - c_1) / c_0$)
 V = volume of the chamber air (m^3)
 VOC = volatile organic compound
 x = linear distance (m)

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