

## **Effects of Environmental Conditions on the Sorption of VOCs on Building Materials-Part II: Model Evaluation (RP-1097)**

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**ABSTRACT:** Sorption data obtained by using small environmental chambers under different environmental conditions (air temperature, relative humidity, and air velocity) have been used to evaluate the linear Langmuir model and the diffusion model for VOC sorption by different building materials. The two models were evaluated (1) by the goodness of model curve-fitting to the experimental data according to the ASTM recommended statistical indices; and (2) by the ability in predicting the desorption period based on the data from the adsorption period. The linear Langmuir model appeared to be suitable for the painted drywall and ceiling tile while the diffusion model seems more suitable for carpet. The variations of the sorption model parameters are not always in consistence with the changes of the environmental conditions.

**KEYWORDS:** Sorption, adsorption, chamber, indoor air quality, modeling

### **INTRODUCTION**

Most numerical and empirical models are the simplifications of the reality, and should be evaluated for their applicability, accuracy, and limitations. Sorption models are no exceptions to this rule. For model users, model evaluation will provide them with a clear view of the conditions under which the model can be applied and the associated prediction uncertainties. Such information may prevent the user from misusing the models. For model developers, proper evaluation will identify areas for model improvement and for developing more advanced models. Two typical sorption models: the linear Langmuir model and the diffusion model, have been widely used by researchers in this area as reviewed by Zhang et al. (2002a). Tichenor et al. (1991) evaluated the linear Langmuir model by the goodness of fitting the model to the sorption of ethylbenzene and perchloroethylene on a wallboard, ceiling tile and window glass. According to the standard deviation of the model parameters and correlation coefficient from curve-fitting, An et al. (1999) found that the linear Langmuir model was acceptable in fitting the experimental data for the equilibrium constant ( $k_e$ ) from 0.004 to 22.2 m. For the diffusion model, Little et al. (1996) found that it can fit the experimental data reasonably well. They also proposed some independent methods to measure the partition coefficient and the diffusion coefficient.

However, there seemed to be no direct comparison between the prediction using the measured partition and diffusion coefficients and the chamber test data. Due to the lack

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of experimental data, the two typical sorption models are generally validated only by curve-fitting without quantitative indices. They still need to be validated using more data, especially independent experimental data. Moreover, the effects of environmental conditions (air temperature, relative humidity and air velocity over the material surface) on the sorption and thus on the parameters of sorption model have not been studied previously. Therefore, the objective of this paper is to evaluate the two models using experimental VOC sorption data obtained from a test chamber under different environmental conditions for three typical building materials: a painted gypsum wallboard, a ceiling tile, and a carpet. The VOCs used for the test are ethylbenzene (EB), benzaldehyde (BZA), decane (DEC), 1,4-dichlorobenzene (DCB), undecane (UND), and dodecane (DOD). The test conditions for each material are listed in Table 1 that represent a wide variation of air temperature, relative humidity and air velocity. Detailed information on the experimental set-up may be found in a paper published earlier by the authors (Zhang et al. 2002b).

In order to accomplish the objective, this paper first describes briefly the two sorption models, outlines the evaluation methods using the statistical tools recommended by ASTM D5157 (1997), and selects the sorption data for model evaluation. Then the paper will present the model evaluation results together with a discussion on the effects of environmental conditions on the model parameters.

## SORPTION MODELS

The two sorption models can be clearly described by using the schematic presented in Figure 1 that shows a test specimen at the bottom of a small test chamber. The volume of the chamber is  $V$  and the surface area of the test specimen is  $A$ . The air inflow rate to the chamber is  $Q$  with a VOC concentration of  $C_{in}(t)$ .  $C_{in}(t) = C_{in}$  when  $t < t_a$  and  $C_{in}(t) = 0$  when  $t > t_a$ . The VOC concentration in the chamber and at the exhaust outlet are  $C_a(t)$ .

### The Linear Langmuir Model

The linear Langmuir model assumes that (Tichenor et al. 1991): (a) the sorption happens only on the “surface” of the material (including external and interior surfaces); (b) all sorption surfaces are mutually independent and identical; (c) the rate of VOC adsorption on the surface is proportional to the concentration in the bulk air and the rate of VOC desorption from the surface is proportional to the mass of VOC adsorbed on the surface. As shown in Figure 1(a), the VOC adsorbed by the test specimen is denoted as  $M(t)$  ( $\text{mg}/\text{m}^2$ ) and the VOC adsorbed by the chamber wall as  $M_1(t)$  ( $\text{mg}/\text{m}^2$ ).

With the above assumptions, the rate of VOC mass changes of the test specimen and the chamber walls can be described as:

$$\frac{dM(t)}{dt} = k_a C_a(t) - k_d M(t) \quad (1)$$

$$\frac{dM_1(t)}{dt} = k_{a1} C_a(t) - k_{d1} M_1(t) \quad (2)$$

where  $k_a C_a(t)$  = the VOC adsorption rate from the bulk air to the specimen surface  
 $k_d M(t)$  = the VOC desorption rate from the specimen surface to the bulk air  
 $k_{a1} C_a(t)$  = the VOC adsorption rate from the bulk air to the chamber wall surface  
 $k_{d1} M_1(t)$  = the VOC desorption rate from the chamber wall surface to the bulk air

Assuming perfect mixing of VOCs in the chamber, the mass change rate of each VOC in the test chamber can be described by the following Langmuir model (An et al. 1999):

$$V \frac{dC_a(t)}{dt} = QC_{in}(t) - QC_a(t) - k_a C_a(t)A + k_d M(t)A - k_{a1} C_a(t)A_1 + k_{d1} M_1(t)A_1 \quad (3)$$

with the following initial conditions:

$$C_a = 0, \quad \text{at } t=0 \quad (4)$$

$$M = 0, \quad \text{at } t=0 \quad (5)$$

$$M_1 = 0, \quad \text{at } t=0 \quad (6)$$

With these initial conditions, the  $k_a$  and  $k_d$  can be determined by fitting Equations (1), (2), and (3) to the measured VOC concentration as a function of time from the adsorption and/or desorption periods. The equilibrium coefficient  $k_e$ , used to represent the sink strength of VOC, is defined as the ratio of the adsorption coefficient and the desorption coefficient ( $k_e = k_a/k_d$ ).

### The Diffusion Model

The diffusion model was developed with the following assumptions: (a) The material is homogeneous; (b) The surface sorption is an instantaneous process and is always at equilibrium; (c) The material is so thin that VOC diffusion in the material can be assumed to be one dimensional; and (d) Fick's law applies to VOC diffusion in the material, and an effective diffusion coefficient may be assumed.

If the thickness of the test specimen is  $L_m$  and the VOC concentration in the material is  $C_m(x,t)$  (Figure 1(b)), which is a function of location  $x$  and time  $t$ , the diffusion process can be described by Fick's second law,

$$\frac{\partial C_m(x,t)}{\partial t} = D_m \cdot \frac{\partial^2 C_m(x,t)}{\partial x^2} \quad (7)$$

According to Henry's law and assumption (b), the equilibrium condition at the material-air interface can be described by:

$$C_m(0,t) = K_{ma} \cdot C_a(t) \quad (8)$$

If the test specimen has a zero mass flux on the bottom surface,

$$\left. \frac{\partial C_m(x, t)}{\partial x} \right|_{x=L_m} = 0 \quad (9)$$

and according to the mass balance in the chamber, we have the diffusion model as,

$$V \cdot \frac{dC_a(t)}{dt} = Q \cdot C_{in}(t) + D_m \cdot A \left. \frac{\partial C_m(x, t)}{\partial x} \right|_{x=0} - Q \cdot C_a(t) \quad (10)$$

The initial conditions are:

$$C_a(0)=0 \quad (11)$$

$$C_m(x,0)=0 \quad (12)$$

In analogy to a heat transfer problem, Little et al. (1996) obtained the analytic solution to the above diffusion equation, which can be used to fit the experimental data for the determination of model parameters  $K_{ma}$  and  $D_m$ .

## METHODS OF EVALUATION

The present study uses the statistical tools recommended by ASTM D5157 (1997) to evaluate the two models.

### ASTM Method

ASTM D5157 (1997) “Standard Guide for Statistical Evaluation of Indoor Air Quality Models” recommends several statistical indices such as: correlation coefficient (R), regression slope (b), regression intercept (a), normalized mean square error (NMSE), and fractional bias (FB). Considering the potential measurement uncertainties, ASTM D5157 recommends the following values as generally indicative of adequate model performance:

- (1)  $R > 0.9$
- (2)  $0.75 < b < 1.25$
- (3)  $a < 25\%$  of the average measured concentration
- (4)  $NMSE < 0.25$
- (5)  $FB < 0.25$

In addition to these quantitative indices, a qualitative indication of the model performance is a comparison of  $C_p$  (predicted concentrations) and  $C_o$  (measured concentrations) over time. This comparison will indicate not only the general extent of the agreement between the  $C_p$  and  $C_o$  but also the specific areas of disagreement.

### Selection of Sorption Data to Validate the Models

The next step to validate the sorption model is to select suitable sorption data. Strictly speaking, the data used for model evaluation process should be independent of the data used to develop the model. However, due to large variations among materials in different categories and even among materials in the same category, e.g. carpet, model parameters

obtained for one test material may not be able to be used for other material bearing the same name. In addition, due to lacking of standard in the test, it is very difficult to compare the test results from one researcher with those from another. For example, although the materials and most VOCs tested in this project are similar to those tested by An et al. (1999), the test results were still very different because of the differences in the materials, test conditions, and operators. Therefore, it is difficult, sometimes almost impossible, to find two independent sets of test data for model evaluation. The sorption tests in ASHRAE RP-1097 (Zhang et al. 2002b) were for two periods, the adsorption period and the desorption period. We can use the test data from the adsorption period to estimate the model parameters and then use these parameters to predict desorption. The predicted results can then be compared with the test data in the desorption period. This implies that the model can be used for both adsorption and desorption periods, which is a commonly used assumption. Note that this method is not the ultimate validation way, but serves as a way of comparing the model performance.

In this study, Four sets of test data from ASHRAE RP-1097 (Zhang et al. 2002b) have been selected to evaluate the linear Langmuir and diffusion models:

- (1) The sorption data of dodecane on painted drywall (reference condition, 192 hrs)
- (2) The sorption data of dodecane on ceiling tile (reference condition, 192 hrs)
- (3) The sorption data of dodecane on carpet (long-term reference condition, 2112 hrs)
- (4) The sorption data of dodecane on carpet (high velocity condition, 504 hrs)

Dodecane instead of other compounds was used because it had the strongest sink strength on all materials among the tested compounds. The long-term carpet test data and the high velocity carpet test data were selected to include both short and long term test scenarios for the carpet.

In addition, the effects of environmental conditions on the model coefficients are also studied to determine if these effects can be properly reflected consistently in the change of the model parameters.

## **RESULTS AND DISCUSSION**

With the test data, this section will report the evaluation results for the linear Langmuir and diffusion models, and discuss the impacts of environmental parameters, such as air temperature, relative humidity, and air velocity, on the sorption.

### **The Linear Langmuir Model**

#### **a) Evaluation of the model by the goodness of curve-fitting**

Table 2 shows the adsorption coefficient  $k_a$  and equilibrium coefficient  $k_e$  calculated by fitting the linear Langmuir model to the experimental data under reference condition for the painted drywall, ceiling tile, and carpet respectively, together with their uncertainties from curve-fitting denoted by  $\delta_{k_a}$  and  $\delta_{k_e}$ . The table also lists the corresponding statistical indices such as correlation coefficient (R), regression slope (b), regression

intercept (a), normalized mean square error (NMSE) and fractional bias (FB) for each regression. It was found that those calculated statistical parameters are well within the range recommended by ASTM D5157. In addition, the best-fit curves using the linear Langmuir model were also plotted during data analysis process for qualitative evaluation purpose as ASTM D5157 recommends. Those figures were not presented here due to the limited space available for the paper, but they can be found in the final report for ASHRAE RP-1097 (Zhang et al. 2001). The figures show that the fittings are generally good. It means that the linear Langmuir model is a reasonable representation of the sorption process for the painted drywall, ceiling tile, and carpet. However, comparing among different VOCs and different materials, the R, b, a, NMSE, and FB for the sorption of dodecane on carpet are much worse than those for the sorption of other VOCs on carpet or those for the sorption of all test VOCs on the painted drywall and ceiling tile. It indicates that the linear Langmuir model may not be the most suitable for modeling the sorption process of dodecane on carpet, which is a typical diffusion-controlled process (Little et al. 1996), although it satisfies the ASTM D5157 criteria.

#### **b) Evaluation of the model by predicting both the adsorption and desorption periods**

Table 3 lists the model parameters,  $k_a$  and  $k_e$ , obtained by fitting the linear Langmuir model to the adsorption data. For comparison, the table also shows the  $k_a$  and  $k_e$  obtained by fitting the linear Langmuir model to the data from both the adsorption and desorption periods. For the sorption of dodecane on the painted drywall and ceiling tile, considering the uncertainties involved in the regression, the  $k_a$  and  $k_e$  obtained from the adsorption data are very close to those obtained from the whole test data.

The  $k_a$  and  $k_e$  from the adsorption period were then used in the linear Langmuir model to predict the concentration change over the whole test period (both the adsorption and desorption periods). Figures 2 through 5 illustrates that the predicted dodecane concentration is in reasonable agreement with the experimental data for different building materials under both short-term and long-term testing conditions. The agreement is further confirmed by the good values of the statistical parameters as shown in Table 3.

For the dodecane sorption on carpet, the estimated  $k_a$  in the short-term test and  $k_e$  in the long-term test for the adsorption period are different from those from the whole test data, which is for both adsorption and desorption periods. This difference leads to a notable discrepancy between the predicted dodecane concentration and the experimental data as shown in Figures 4 and 5. In fact, the whole period curve-fitting is not as good as for the painted drywall and ceiling tile, which implies the inadequacy of the linear Langmuir model for the carpet.

#### **c) Effects of environmental conditions on sorption**

This investigation has obtained the sorption data for six different VOCs (EB, BZA, DEC, DCB, UND, and DOD) on three materials (the painted drywall, ceiling tile, and carpet) under six different environmental conditions (Table 1). This paper selectively shows in Table 4 the  $k_a$  and  $k_e$  by fitting the linear Langmuir model to the whole period sorption data of ethylbenzene under the six environmental conditions and in Table 5 for the six

VOCs under different temperatures. The tables also list statistical indices. The statistical indices for different VOCs and different environmental conditions are well within the range recommended by ASTM D5157. Due to the large amount of data obtained from this study, it can be very confusing to study the effects of the environmental conditions by studying the change of  $k_e$  under different environmental condition for each of the six VOCs. In addition, individual data can be of little value unless they can be summarized into a general correlation with the physical properties of the VOCs. Therefore, to effectively summarize the experimental results and also to maximally eliminate the random errors from data analysis, the correlation between the equilibrium coefficient  $k_e$  and the vapor pressure (VP) of the VOCs for the six environmental conditions have been studied, as previous studies recommended (An et al. 1999). Figures 6 and 7 show that the equilibrium constant ( $k_e$ ) is linearly correlated with the inverse of the vapor pressure. Table 6 lists the regression coefficient  $g$  and the correlation coefficients  $R$ , which are close to 1 and indicate that the correlation  $k_e=y/VP$  is valid. The results are for the ceiling tile and carpet. The data for painted drywall are not included because the sorption effect of the painted drywall is small and the impact of the environmental conditions is not significant. From Table 6, we can study the effects of the environmental conditions on  $k_e$  in a much simpler way by studying the effects of the environmental conditions on the regression coefficient  $y$ .

The regression coefficient  $y$  for the ceiling tile decreases with the increase of temperature, essentially indicating that the equilibrium coefficient decreases with the increase of temperature. The result confirms the trend found by Tichenor et al. (1991) and Goss et al. (1997). Nevertheless, the confirmation is not very conclusive, because of the limited data available (only three points). On the other hand, the regression coefficient  $y$  does not have consistent relationship with temperature for the carpet. It may indicate that the linear Langmuir model cannot fully capture the sorption process of VOCs on the carpet.

Table 6 also shows that the  $y$  for the ceiling tile decreases slightly with the increase of relative humidity. The water vapor molecules may have competed for sorption with the VOCs. Therefore, the sorption of VOCs is smaller under high humidity condition while stronger under low humidity condition. The result is consistent with that found by Goss et al. (1997). However, the  $y$  for carpet does not have a consistent relationship with relative humidity either. The reason may be the same as that for the temperature effect discussed above.

It can be observed from Table 6 that the regression coefficient  $y$  for ceiling tiles decreases slightly with the increase of air velocity. The result may be explained by the thinner boundary layer at the high velocity condition, causing less VOCs to be adhered to the material surface. The same trend can be found for the carpet. The reason may be the same as that for ceiling tiles. However, more data are needed to develop a sound conclusion.

#### **d) Evaluation of the model assumptions**

The above analyses show that the linear Langmuir model may not be a good model for the carpet. The linear Langmuir model assumes that the sorption happens only on the surface of the material, which may not always be true in reality, especially for porous building materials, such as carpet. As one would expect, given enough time, the VOC adsorbed on the surface of the material would diffuse into the interior of the material. The linear Langmuir model essentially assumes a uniform distribution of VOC in the source, and thus could not account for the diffusion process in which concentration gradient is inevitable.

### **The Diffusion Model**

#### **a) Evaluation of the model by the goodness of curve-fitting**

Table 7 showed the calculated statistical indices for reference environmental conditions for the three materials using the diffusion model. Those calculated statistical indices are well within the range recommended by ASTM D5157. In addition, the best-fit curves using the diffusion model were also plotted during data analysis process for qualitative evaluation. The fittings were generally good. It means that the diffusion model is again a reasonable representation of the sorption process.

#### **b) Evaluation of the model by predicting both the adsorption and desorption periods**

Table 8 lists the model parameters  $D_m$  and  $K_{ma}$  obtained by fitting the diffusion model to the adsorption data, together with their uncertainties from curve-fitting denoted by  $\delta(D_m)$  and  $\delta(K_{ma})$ . For comparison, the table lists also the  $D_m$  and  $K_{ma}$  obtained by fitting to the whole period data. We can see that for the sorption of dodecane on the painted drywall, ceiling tile and carpet, the  $D_m$  and  $K_{ma}$  obtained from the adsorption data are very close to those from the whole test data. The corresponding statistical indices are very good as well.

The obtained model parameters  $D_m$  and  $K_{ma}$  for the absorption period were then used in the diffusion model to predict the concentration change over the whole test period. Figures 2 through 5 show the comparison between the experimental data and the predicted dodecane concentration using the diffusion model. The agreement is rather good.

#### **c) Effects of environmental conditions on sorption**

With the sorption data of the six VOCs on the three building materials under the six different environmental conditions, Tables 9 and 10 report some of the diffusion coefficient  $D_m$  and partition coefficient  $K_{ma}$  obtained by fitting the diffusion model to the data together with the statistical indices. The indices are again well within the range recommended by ASTM D5157. Similar to the analyses for the linear Langmuir model, the relationship between  $K_{ma}$  and VP and the relationship between  $D_m$  and MW for the carpet are used to summarize the effects of different environmental conditions on sorption. Table 11 lists the results from the correlation study. The general high correlation coefficients R indicate that the correlation  $K_{ma}=g/VP^h$  and  $D_m=h-g*MW$  are valid. However, because both of the two correlations involve two regression coefficients,

g and h, it is very difficult to study the effects of environmental conditions on  $K_{ma}$  and  $D_m$  by only using the few parameters listed in Table 11. Therefore, Figures 8 and 9 are drawn to graphically show the correlation of  $K_{ma}$  and V, and the correlation of  $D_m$  and MW, respectively. The effects of the environmental conditions on  $K_{ma}$  and  $D_m$  can be revealed by studying Figures 8 and 9. For simplicity, regression coefficients g and h are not used in the following discussion; however, they can still be of great value in providing basic physical property information for future modeling work.

Figure 8 shows that partition coefficient,  $K_{ma}$ , decreases consistently with the increase of temperature. It is reasonable because the molecular movement under high temperature conditions is much more intense than that under low temperature conditions. The high temperature reduces the attraction force between the VOC molecules and the surface materials. As a result, the  $K_{ma}$ , which represents the ratio of the VOC concentration in the material phase to the VOC concentration in the air phase at the air-material interface, is lower under a higher temperature. Figure 9 also shows that the diffusion coefficient,  $D_m$ , is large when the temperature is high. Compared with the linear Langmuir model, which gives inconsistent effect of temperature on the sorption by the carpet, the diffusion model seems better to capture the temperature effects.

From Figure 8 and Figure 9, it can be observed that the effects of relative humidity on the partition and diffusion coefficients are not consistent throughout the relative humidity conditions tested. It may be due to the experimental and regression uncertainty or to the inadequacy of the diffusion model in modeling the effects of relative humidity, which requires further investigations.

For low vapor pressure compounds (VP less than about 0.8 mm Hg), higher air velocity decreases the partition coefficient, while for high vapor pressure compounds (VP larger than about 0.8 mm Hg) the higher air velocity appears to increase the partition coefficient slightly. The diffusion model does not consider the mass transfer resistance through the boundary layer over the material surface. The model assumes that this resistance through the boundary layer is significantly smaller than that within the material. However, for VOCs with a low vapor pressure, the boundary layer effect could have been relatively large compared to the VOCs with a high vapor pressure. Figure 9 also shows an increase of diffusion coefficient due to a higher velocity, as one would not have expected. This again could be resulted from the defect of the diffusion model and regression procedure in accounting for the mass transfer resistance across the boundary layer. Further investigations on this effect are needed.

#### **d) Evaluation of the model assumptions**

Our investigation further finds that two of the five assumptions used in the diffusion model may not always be satisfied in reality:

First, the homogeneous assumption may fail. For example, the carpet, consisting of fiber layer and backing, is not a strictly homogeneous material. In addition, the painted drywall, consisting of the surface painting and the interior gypsum board, is neither a homogeneous material.

Second, the assumption that the surface sorption is an instantaneous process and is always at equilibrium may not be true in some cases. If the partition coefficient is small, the assumption should not have any problem because the time scale to exchange VOCs at the interface will be very small. However if the partition coefficient is large, that assumption may pose a problem. For example, when the concentration is changing very fast, the time scale to exchange VOCs at the interface and to regain the surface equilibrium may be longer than the time scale of the concentration change in the air.

## CONCLUSIONS

Based on the evaluations of the linear Langmuir model and the diffusion model for sorption, the following conclusions can be made:

1. The linear Langmuir model is suitable for sorption on materials with moderate sink effect process where the surface effect is dominant, such as the painted dry wall and ceiling tile. The model may not work well for the long-term sorption process, especially internal-diffusion is strong, such as dodecane sorption on carpet, because the model cannot take the diffusion process into account.
2. The diffusion model can capture the long-term sorption process of VOCs on the ceiling tile and carpet reasonably well. The model can predict strong and long-term sink effect process, such as internal-diffusion dominated processes. For the painted drywall, the diffusion model may not be good because of its weak sink effect.
3. This investigation studied six different environmental conditions (air temperature, relative humidity, and velocity) on VOC sorption. The results show clearly the impact of the environmental conditions on the model parameters. The changes of the model parameters do not always follow the trend of the environmental conditions. Further research is needed to fully understand the mechanism.

## NOMENCLATURE

a	Regression intercept	$k_d$	Desorption coefficient of the test specimen (m/h)
A	Specimen surface area ( $m^2$ )	$k_{d1}$	Desorption coefficient of the chamber wall (m/h)
$A_1$	Chamber wall surface area ( $m^2$ )	$k_e$	Equilibrium coefficient, $mg/m^2 / mg/m^3$
b	Regression slope	$K_{ma}$	Material-air partition coefficient (-)
$C_a(t)$	VOC concentration in the bulk air at time t ( $mg/m^3$ )	$M(t)$	VOC mass adsorbed per unit sink surface area at time t ( $mg/m^2$ )
$C_{in}(t)$	Inlet VOC concentration at time t ( $mg/m^3$ )	$M_1(t)$	VOC mass adsorbed per unit chamber wall surface area at time t ( $mg/m^2$ )

$C_{m(x,t)}$	VOC concentration in the sink material at location $x$ and time $t$ ( $\text{mg}/\text{m}^3$ )	MW	Molecular weight
$C_o$	Observed VOC concentration	NMSE	Normalized mean square error
$C_p$	Predicted VOC concentration	Q	The supply air flow rate for the chamber ( $\text{m}^3/\text{h}$ )
$D_m$	Diffusion coefficient ( $\text{m}^2/\text{s}$ )	R	Correlation coefficient
FB	Fractional bias	$t_a$	Adsorption test time (h)
g	Regression coefficient	t	Test time (h)
h	Regression coefficient	V	Chamber volume ( $\text{m}^3$ ), excluding the volume of the test specimen
$k_a$	Adsorption coefficient of the test specimen (m/h)	VP	Vapor pressure
$k_{a1}$	Adsorption coefficient of the chamber wall (m/h)	x	Location in the material
		y	Regression coefficient

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Table 1. Environmental conditions tested

Case design	Temperature (°C)	Relative Humidity (%)	Air Velocity (m/s)
Reference test condition (Ref.)	23.0	50	0.05
High temperature condition (High T)	35.0	50	0.05
Low temperature condition (Low T)	10.5	50	0.05
Low relative humidity condition (Low RH)	23.0	25	0.05
High relative humidity condition (High RH)	23.0	80	0.05
High velocity condition (High V)	23.0	50	0.62

Table 2. The  $k_a$  and  $k_e$  of VOCs for the painted drywall under the reference condition

VOCs	$k_a$ (m/h)	$\delta_{k_a}$	$k_e$ (m)	$\delta_{k_e}$	$k_d$ (h <sup>-1</sup> )	R	b	a	NMSE	FB
Painted drywall										
EB	0.037	0.001	1.092	0.591	0.034	0.9984	1.0355	-0.0218	0.0044	-0.0099
BZA	0.04	0.001	2.733	1.247	0.015	0.9981	1.0018	-0.0118	0.0039	-0.0238
DEC	0.032	0.026	0.045	0.055	0.715	0.9978	0.9726	0	0.0053	-0.0277
DCB	0.039	0.001	3.546	1.716	0.011	0.9981	1.0081	-0.0091	0.0037	-0.0114
UND	0.039	0	3.757	1.98	0.01	0.9982	1.0313	-0.0173	0.0043	-0.0052
DOD	0.038	0	7.713	5.772	0.005	0.9976	1.0096	-0.0064	0.0043	-0.0042
Ceiling tile										
EB	0.057	0.072	0.036	0.053	1.594	0.9965	0.9812	0.0131	0.0067	0.0089
BZA	0.365	0.003	3.032	0.449	0.12	0.9933	0.9562	0.0011	0.0119	-0.0423
DEC	0.3	0.017	0.499	0.084	0.601	0.9965	0.9856	0.0111	0.006	0.0092
DCB	0.3	0.011	0.67	0.094	0.448	0.9969	0.9742	0.0126	0.0053	0.0012
UND	0.301	0.004	1.697	0.252	0.178	0.9953	0.9762	0.0099	0.007	-0.0025
DOD	0.515	0.003	4.543	0.475	0.113	0.9932	0.9696	0.0033	0.0086	-0.0233
Carpet										
EB	0.193	0.003	1.117	0.138	0.173	0.9985	0.9802	0.0109	0.003	0.0033
BZA	0.539	0.008	3.08*	0.577	0.175	0.9847	0.9806	-0.0068	0.0309	-0.0347
DEC	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
DCB	0.577	0.001	10.05	0.925	0.057	0.9936	0.9732	-0.0109	0.0135	-0.052
UND	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
DOD	0.573	0	55.63	5.047	0.01	0.9816	0.9338	-0.005	0.0235	-0.0803

EB – Ethylbenzene, BZA – Benzaldehyde, DEC – Decane, DCB – 1,4-dichlorobenzene, UND – Undecane, DOD – Dodecane

Table 3. Comparison between parameters estimated from the adsorption period with parameters estimated from the whole test period for dodecane

VOCs	$k_a$ (m/h)	$\delta_{k_a}$	$k_e$ (m)	$\delta_{k_e}$	$k_d$ (h <sup>-1</sup> )	R	b	a	NMSE	FB
PD (AP)	0.05	0.01	3.800	1.705	0.014	0.997	0.965	0.024	0.006	0.017
PD (WP)	0.04	0.001	7.713	5.772	0.005	0.998	1.010	-0.006	0.004	-0.004
CT (AP)	0.48	0.045	5.566	0.484	0.087	0.993	0.985	0.015	0.008	0.017
CT (WP)	0.52	0.003	4.543	0.475	0.113	0.993	0.970	0.003	0.009	-0.023
CPs (AP)	1.21	0.119	48.79	2.891	0.025	0.976	0.924	0.053	0.020	0.059
CPs (WP)	0.80	0.003	48.15	3.34	0.017	0.978	1.042	-0.037	0.022	-0.055
CP (AP)	0.52	0.043	80.98	7.505	0.007	0.981	0.961	0.050	0.019	0.067
CP (WP)	0.57	0.001	55.62	5.047	0.010	0.982	0.934	-0.005	0.024	-0.080

AP- adsorption period; WP-whole period; PD-painted drywall; CT- ceiling tile; CP- carpet; s-short term test

Table 4. The  $k_a$  and  $k_e$  of ethylbenzene for the carpet under different conditions

VOCs	$k_a$ (m/h)	$\delta_{k_a}$	$k_e$ (m)	$\delta_{k_e}$	$k_d$ (h <sup>-1</sup> )	R	b	a	NMSE	FB
Ref.	0.193	0.003	1.117	0.138	0.173	0.9985	0.9802	0.0109	0.003	0.0033
Low RH	0.198	0.001	2.07	0.24	0.095	0.9984	0.9802	-0.0001	0.0038	-0.0203
High RH	0.196	0.002	1.955	0.295	0.1	0.9978	0.9637	0.0088	0.005	-0.0178
Low T	0.106	0.004	0.378	0.065	0.281	0.9991	0.9804	0.0055	0.0019	-0.0086
High T	0.197	0.002	1.551	0.218	0.127	0.9985	0.976	-0.0054	0.0047	-0.0371
High V	0.195	0.002	1.577	0.186	0.124	0.9985	0.9777	0.0086	0.0031	-0.0036

Table 5. The  $k_a$  and  $k_e$  of different VOCs for the carpet under different temperatures

VOC	Temperature	$k_a$ (m/h)	$\delta_{k_a}$	$k_e$ (m)	$\delta_{k_e}$	$k_d$ (h <sup>-1</sup> )	R	b	a	NMSE	FB
EB	Low T	0.106	0.004	0.378	0.065	0.281	0.9991	0.9804	0.0055	0.0019	-0.0086
	Ref.	0.193	0.003	1.117	0.138	0.173	0.9985	0.9802	0.0109	0.003	0.0033
	High T	0.197	0.002	1.551	0.218	0.127	0.9985	0.976	-0.0054	0.0047	-0.0371
BZA	Low T	0.397	0.002	6.212	1.018	0.064	0.9877	0.9439	-0.0176	0.0285	-0.0992
	Ref.	0.539	0.008	3.08*	0.577	0.175	0.9847	0.9806	-0.0068	0.0309	-0.0347
	High T	0.546	0.003	5.273	0.585	0.104	0.995	0.9532	-0.0126	0.0158	-0.0795
DEC	Low T	0.189	0.003	1.154	0.176	0.164	0.9981	0.9655	0.0058	0.0044	-0.023
	Ref.	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
	High T	0.452	0.004	3.358	0.463	0.135	0.9949	0.9462	-0.0059	0.0157	-0.07
DCB	Low T	0.222	0.001	11.25	2.07	0.02	0.9852	0.9923	-0.0215	0.0225	-0.0553
	Ref.	0.577	0.001	10.05	0.925	0.057	0.9936	0.9732	-0.0109	0.0135	-0.052
	High T	0.569	0.002	6.997	0.665	0.081	0.9953	0.9801	-0.0251	0.0146	-0.0825
UND	Low T	0.21	0.001	6.935	1.137	0.03	0.9917	0.9862	-0.0174	0.0142	-0.0517
	Ref.	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
	High T	0.354	0.001	16.01	1.842	0.022	0.9933	1.0133	-0.04	0.0175	-0.0888
DOD	Low T	0.406	0.001	27.65	3.562	0.015	0.985	1.0759	-0.0679	0.0315	-0.0883
	Ref.	0.573	0	55.63	5.047	0.01	0.9816	0.9338	-0.005	0.0235	-0.0803
	High T	0.725	0.001	42.97	3.983	0.017	0.9893	1.1571	-0.0769	0.0257	-0.046

EB – Ethylbenzene, BZA – Benzaldehyde, DEC – Decane, DCB – 1,4-dichlorobenzene, UND – Undecane, DOD – Dodecane

Table 6. Correlation between the  $k_e$  and VP for the ceiling tile and carpet ( $k_e=y/VP$ )

Conditions	Ceiling tile		Carpet	
	y	R	y	R
Ref.	1.1293	0.9996	13.3394	0.9877
Low RH	1.2535	0.9993	14.5583	0.9946
High RH	1.0027	0.9812	17.6955	0.9944
Low T	3.0136	0.9994	6.8159	0.9601
High T	0.6195	0.9886	10.444	0.9942
High V	0.9337	0.9989	12.019	0.9957

Table 7. The  $D_m$  and  $K_{ma}$  of VOCs for the painted drywall, ceiling tile, and carpet under the reference condition

VOCs	$D_m$ ( $m^2/s^2$ )	$\delta(D_m)$	$K_{ma}$	$\delta(K_{ma})$	R	b	a	NMSE	FB
Painted drywall									
EB	7.14E-10	2.75E-11	37.5	9.65	0.9969	0.9991	0.0056	0.0057	0.0107
BZA	3.88E-10	3.5E-12	123.9	29.25	0.9961	1.0047	0.0122	0.0075	0.0303
DEC	4.51E-10	2.6E-11	55	22.4	0.9967	1.0094	0.0057	0.0066	0.0213
DCB	5.51E-10	4.5E-12	70.4	24.15	0.9968	1.0200	0.0052	0.0070	0.0306
UND	4.31E-10	7E-12	80	26.6	0.9961	1.0135	0.0053	0.0077	0.0245
DOD	3.23E-10	4E-12	176.7	36.6	0.9955	1.0019	0.0127	0.0082	0.0289
Ceiling tile									
EB	1.80E-09	6E-11	16.0	8.4	0.9978	1.0166	-0.0045	0.0046	0.0071
BZA	7.97E-10	1.2E-11	327.6	27.85	0.9944	1.0206	0.012	0.01	0.0464
DEC	1.50E-09	5E-12	64.1	7.45	0.9961	1.0209	-0.0075	0.0072	0.0049
DCB	1.17E-09	5E-12	97.0	9.75	0.9966	1.0188	-0.0032	0.0062	0.0119
UND	2.08E-09	5E-12	162.8	12.75	0.9959	1.028	-0.0053	0.007	0.0165
DOD	9.62E-10	6.5E-12	475.6	19.8	0.9932	1.0089	0.0081	0.0085	0.0265
Carpet									
EB	2.43E-10	5E-13	204.0	21.05	0.9981	1.024	-0.009	0.0044	0.0055
BZA	1.11E-10	3.08E-11	865.0	169.5	0.9825	0.9849	0.0295	0.0331	0.0482
DEC	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
DCB	1.36E-10	2.5E-12	1643	95.8	0.9907	1.0098	0.0231	0.0178	0.0586
UND	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
DOD	1.18E-11	8E-13	15345	537	0.9649	1.0014	0.0067	0.031	0.0159

Table 8. Comparison between parameters estimated from adsorption period with parameters estimated from whole period for dodecane

VOCs	$D_m$ ( $m^2/s^2$ )	$\delta(D_m)$	$K_{ma}$	$\delta(K_{ma})$	R	b	a	NMSE	FB
PD (AP)	3.27E-10	5.30E-12	181.1	176.1	0.995	0.999	0.014	0.008	0.028
PD (WP)	3.23E-10	7.20E-12	176.7	73.1	0.995	1.002	0.013	0.008	0.029
CT (AP)	8.03E-10	3.76E-11	518.3	98.2	0.993	0.994	0.012	0.008	0.021
CT (WP)	9.62E-10	1.23E-11	475.6	39.6	0.993	1.009	0.008	0.009	0.027
CPs (AP)	6.90E-11	1.37E-11	7827	516.6	0.992	1.008	0.001	0.006	0.011
CPs (WP)	6.46E-11	8.55E-12	7973	1340	0.993	1.015	-0.003	0.005	0.007
CP (AP)	1.65E-11	2.95E-12	13720	3773	0.956	0.983	0.023	0.038	0.032
CP (WP)	1.18E-11	1.60E-12	15345	1074	0.965	1.001	0.007	0.031	0.016

Table 9. The  $D_m$  and  $K_{ma}$  of ethylbenzene for the carpet under different conditions

VOCs	$D_m$ ( $m/s^2$ )	$\delta(D_m)$	$K_{ma}$	$\delta(K_{ma})$	R	b	a	NMSE	FB
Ref.	2.43E-10	5E-13	204	21.05	0.9981	1.024	-0.009	0.0044	0.0055
Low RH	5.85E-10	1.35E-11	220.4	25.15	0.9982	1.0368	-0.008	0.0053	0.0196
High RH	4.81E-10	1.5E-12	240.7	25.9	0.9987	1.0451	-0.008	0.0048	0.027
Low T	6.20E-11	2.5E-13	278.4	23.2	0.9992	1.0026	-0.001	0.0013	0.002
High T	6.97E-10	3E-12	108.8	24.7	0.995	1.065	-0.012	0.0156	0.0363
High V	6.16E-10	1E-12	212.5	13.05	0.9986	1.0259	-0.007	0.0035	0.0113

Table 10. The  $D_m$  and  $K_{ma}$  of different VOCs for the carpet under different temperatures

VOC	Temperature	$D_m$ ( $m/s^2$ )	$\delta(D_m)$	$K_{ma}$	$\delta(K_{ma})$	R	b	a	NMSE	FB
EB	Low T	6.20E-11	2.5E-13	278.4	23.2	0.9992	1.0026	-0.001	0.0013	0.002
	Ref.	2.43E-10	5E-13	204	21.05	0.9981	1.024	-0.009	0.0044	0.0055
	High T	6.97E-10	3E-12	108.8	24.7	0.995	1.065	-0.012	0.0156	0.0363
BZA	Low T	1.65E-11	1.1E-12	3414	170.6	0.9974	1.0173	0.0072	0.0047	0.0325
	Ref.*	1.11E-10	3.08E-11	865	169.5	0.9825	0.9849	0.0295	0.0331	0.0482
	High T	4.35E-10	3.5E-12	782.5	63.75	0.988	1.0324	0.0181	0.0248	0.0724
DCB	Low T	3.39E-11	1.15E-12	2718	72.6	0.9987	1.0077	0.0037	0.0019	0.0155
	Ref.	1.36E-10	2.5E-12	1643	95.8	0.9907	1.0098	0.0231	0.0178	0.0586
	High T	5.20E-10	3.5E-12	871.4	80.3	0.9878	1.036	0.0184	0.0255	0.0766
UND	Low T	5.92E-12	7.35E-13	4976	234.8	0.9991	1.0066	-0.001	0.0012	0.0037
	Ref.	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
	High T	9.55E-11	4.45E-12	2112	113.4	0.9827	1.0238	0.0218	0.0274	0.0745
DOD	Low T	4.06E-12	8.65E-13	16800	1292	0.9894	0.984	0.0141	0.0112	0.0171
	Ref.	1.18E-11	8E-13	15345	537	0.9649	1.0014	0.0067	0.031	0.0159
	High T	5.62E-11	7.5E-13	5995	82	0.9302	0.9607	0.0282	0.06	0.0343

\* The results may not be very accurate due to the inconstant inlet conditions.

Table 11. Correlation for the carpet ( $K_{ma}=g/VP^{**}h$ ,  $D_m=h-g*MW$ )

Conditions	$K_{ma}$ and VP			$D_m$ and MW		
	g	h	R	g	h	R
Ref.	1672.5	1.6	0.9976	3.5E-12	6.23E-10	0.982
Low RH	2184.2	1.2	0.9986	9.26E-12	1.56E-09	0.984
High RH	2400.7	1.2	0.9966	7.64E-12	1.28E-09	0.984
Low T	3311.6	1.2	0.9966	9.71E-13	1.71E-10	0.949
High T	1238.3	1.1	0.997	1.02E-11	1.8E-09	0.947
High V	1865	1	0.9975	9.02E-12	1.59E-09	0.965

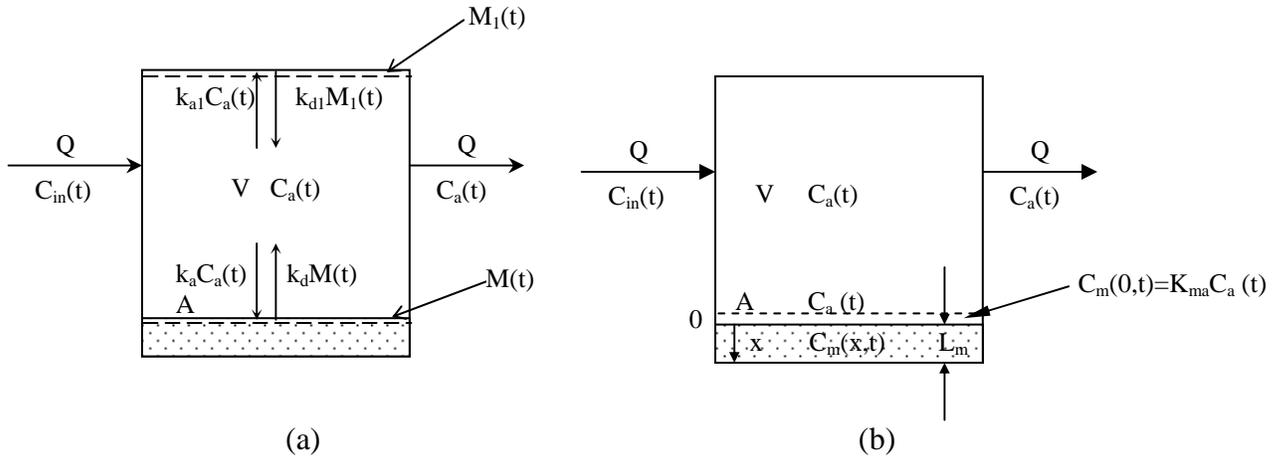


Figure 1. Schematic of sorption test using a small-scale chamber (a) for the linear Langmuir model and (b) for the diffusion model

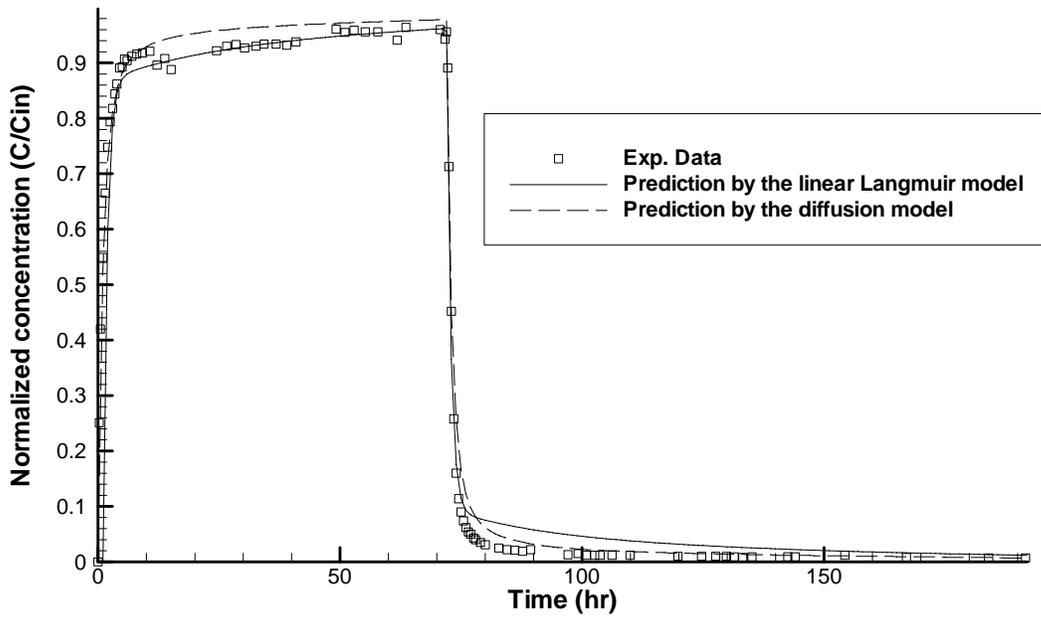


Figure 2. Comparison of the predicted dodecane concentration using the linear Langmuir and diffusion models with the experimental sorption data for the painted drywall

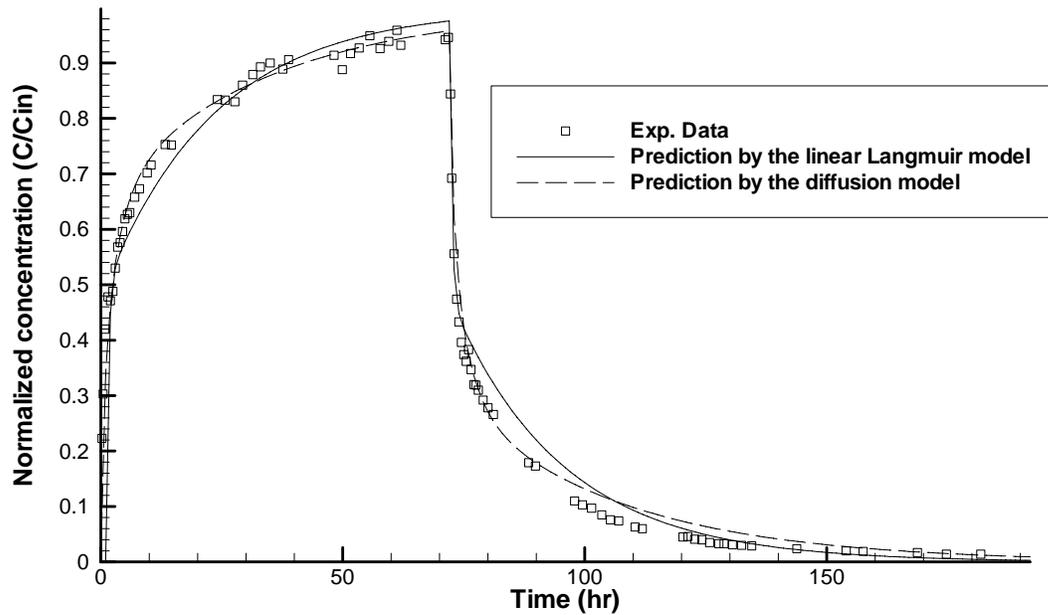


Figure 3. Comparison of the predicted dodecane concentration using the linear Langmuir and diffusion models with the experimental sorption data for the ceiling tile

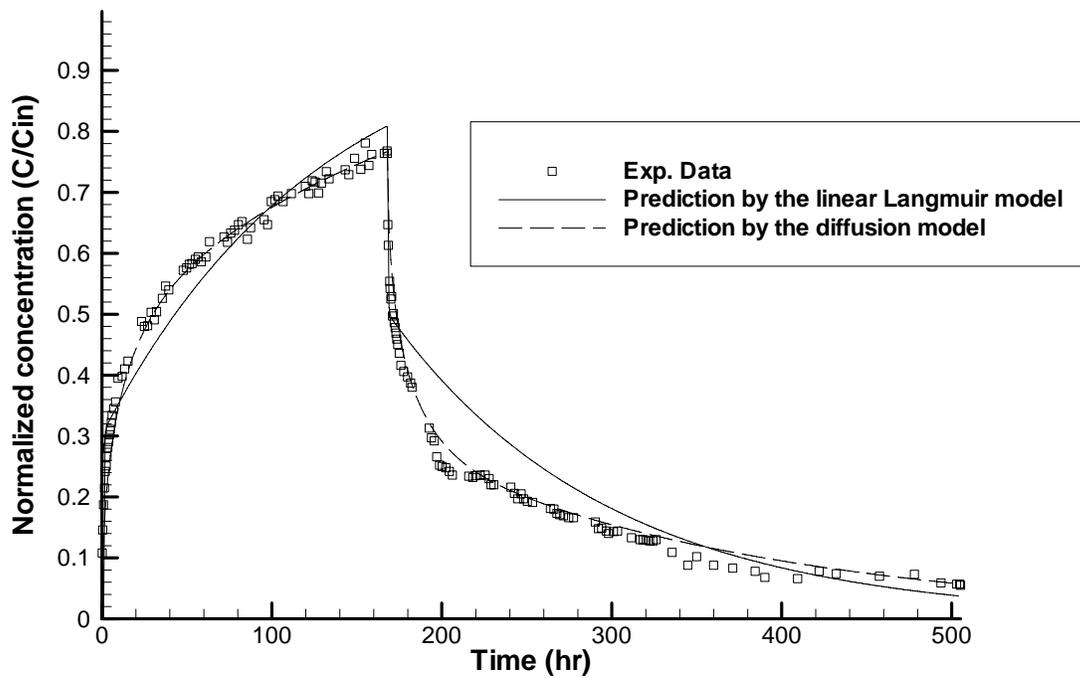


Figure 4. Comparison of the predicted dodecane concentration using the linear Langmuir and diffusion models with the experimental sorption data for the carpet

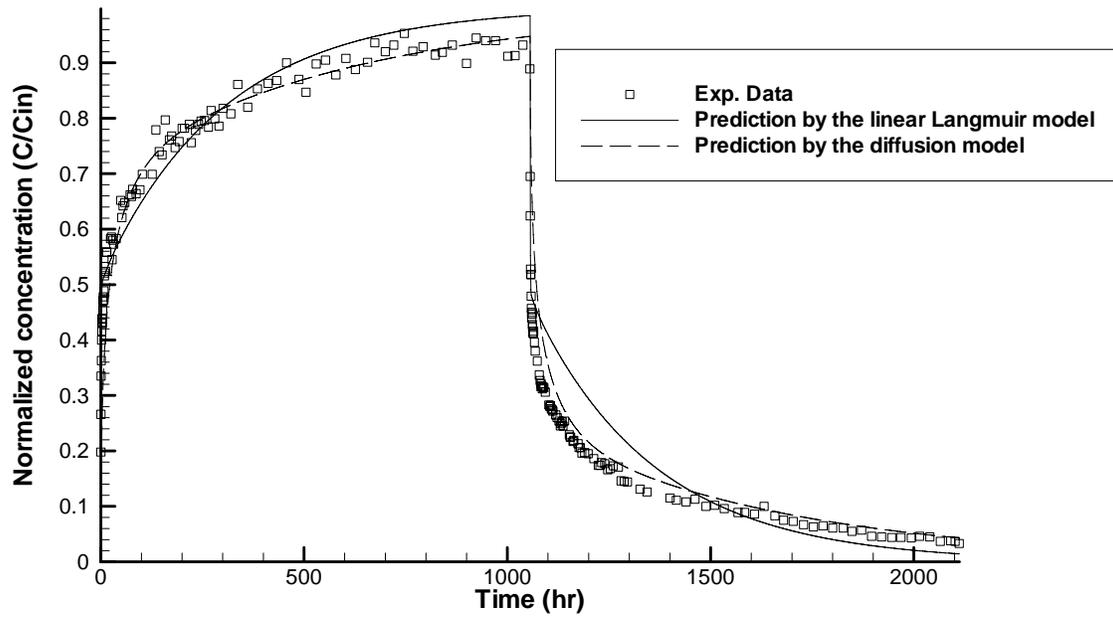


Figure 5. Comparison of the predicted dodecane concentration using the linear Langmuir and diffusion models with the long-term experimental sorption data for the carpet

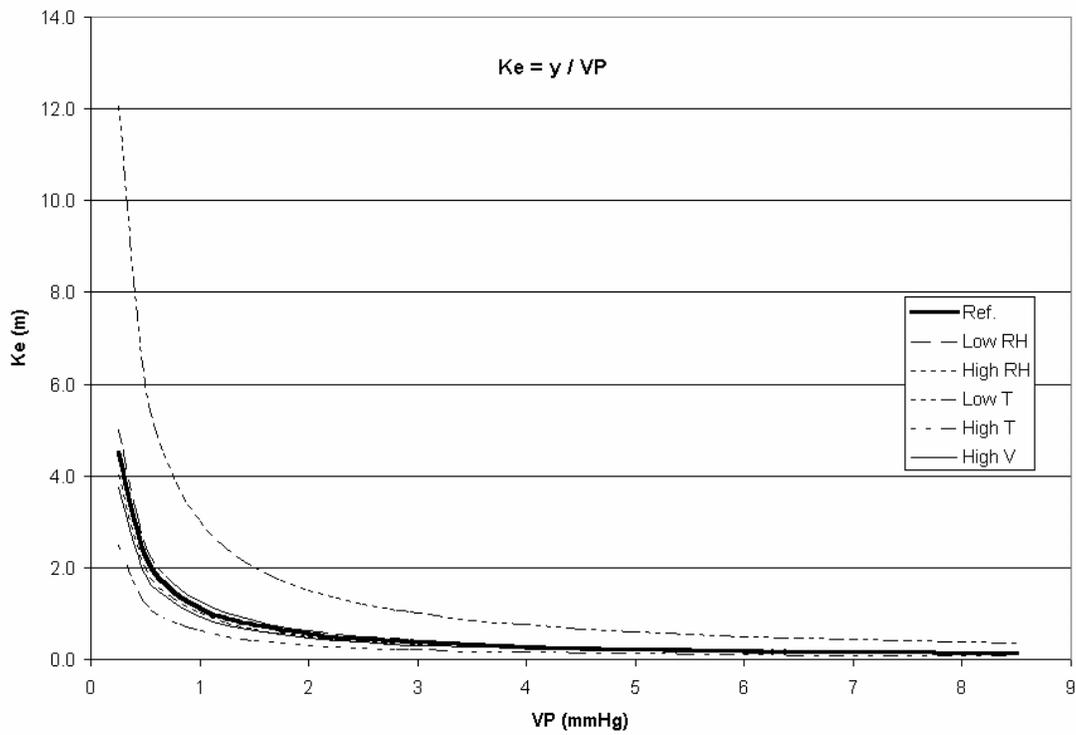


Figure 6. Relationship between the  $k_e$  and VP for the ceiling tiles

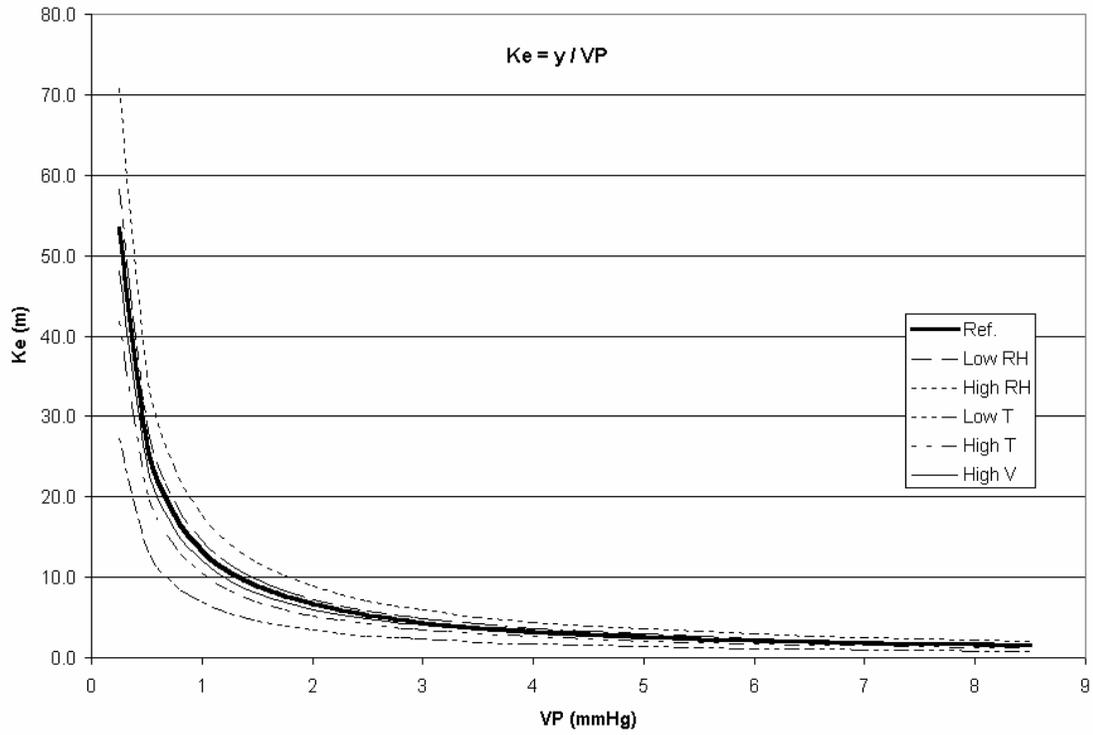


Figure 7. Relationship between the  $k_e$  and VP for the carpet

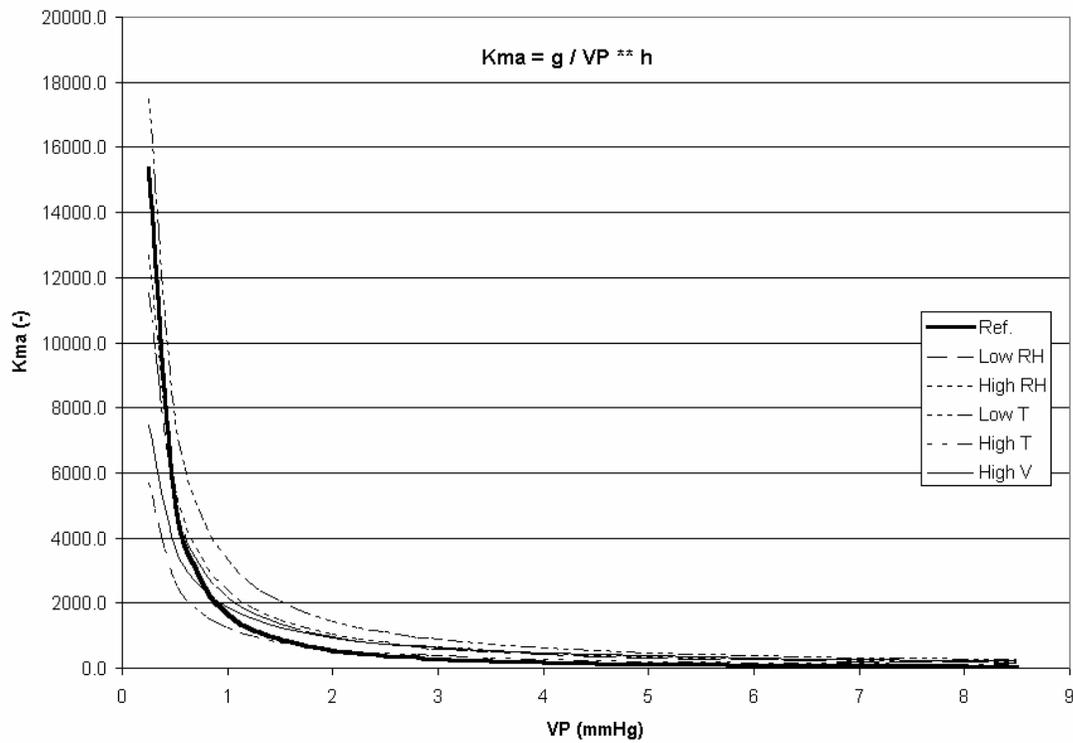


Figure 8. Relationship between the  $K_{ma}$  and VP for the carpet

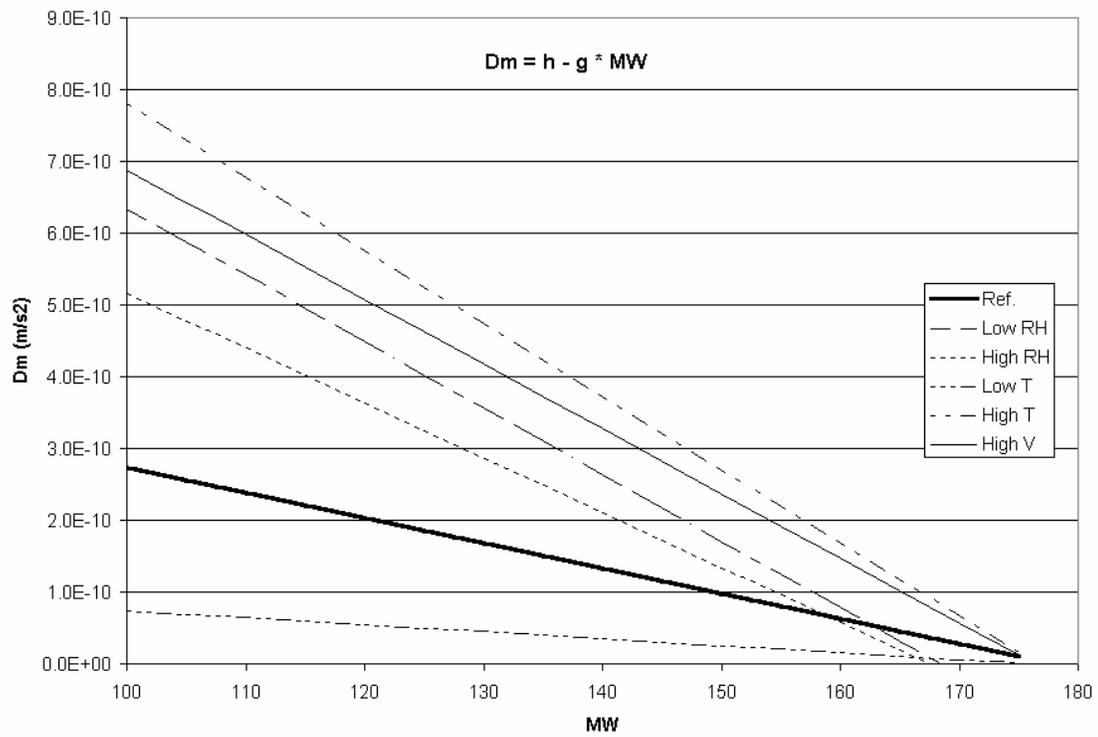


Figure 9. Relationship between the  $D_m$  and MW for the carpet