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SORPTIVE INTERACTIONS BETWEEN VOCS AND INDOOR MATERIALS

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Abstract

A study was completed with various materials (carpet, gypsum board, upholstery, vinyl and wood flooring, acoustic tiles, and fruit) that were exposed to eight gaseous VOCs (isopropanol, MTBE, cyclohexane, toluene, ethylbenzene, tetrachloroethene, 1,2-dichlorobenzene, and 1,2,4-trichlorobenzene) in electro-polished stainless-steel chambers. Dynamic responses in VOC concentrations were used to determine linear adsorption and desorption rate coefficients and equilibrium partition coefficients. A linear adsorption/desorption model was used to effectively describe the interactions between VOCs and indoor surface materials for short-term source events (10 h). Relationships between sorption parameters and chemical vapor pressure and octanol-air partition coefficient were observed. Carpet was identified as the most significant sorptive sink for non-polar VOCs. Virgin gypsum board was observed to be a significant sink for highly polar VOCs. Sorptive interactions between non-polar VOCs and indoor materials were not affected by variations in relative humidity. However, increases in relative humidity were observed to increase the degree of sorption of isopropanol to carpet.

Key words: sorptive sinks, volatile organic compounds, indoor air, vapor pressure, octanol-air partition coefficient

Practical Implications

Linear adsorption/desorption coefficients and equilibrium partition coefficients are provided for a large number of volatile organic compounds (VOCs) and indoor materials. These sorption parameters can be used by modelers to predict the impacts of sorptive materials on indoor air quality, and on occupant exposures to VOCs. The experimental results presented herein clearly

demonstrate the relative sorption capacities of various indoor materials, the importance of carpet as a sorptive sink for non-polar VOCs, and the importance of virgin gypsum board for polar VOCs. Such information may be valuable to architects and building designers who wish to minimize or maximize sorptive interactions as a means of influencing indoor air quality. Finally, results of this study indicate a significant potential for estimating fundamental sorption parameters based on chemical properties such as vapor pressure or octanol-air partition coefficient, a process that could streamline future screening assessments of sorptive interactions for chemicals in which experimental data are lacking in the published literature.

Introduction

Adsorptive materials may lead to reductions in peak concentrations of volatile organic compounds (VOCs), and hence reductions in occupant exposure to VOCs during transient source events. However, sorptive materials may also act as re-emitting sources, thus increasing VOC retention times in indoor environments (Sparks *et al.*, 1991). Sorptive materials may also serve as VOC "reservoirs", leading to dermal or oral exposures upon direct contact with the material.

Several authors have used either static or dynamic (flow-through) chamber experiments to determine equilibrium partition coefficients or sorption rate coefficients for gaseous chemicals and indoor materials. Tichenor *et al.* (1991) studied five common materials (carpet, wallboard, ceiling tile, pillow, and glass) and two chemicals (tetrachloroethene and ethylbenzene). Colombo *et al.* (1993) considered two sorption processes (fast and slow) for three materials (carpet, gypsum board, and blown vinyl) and eight chemicals (tetrachloroethene, α -pinene, 1,2,4-trimethylbenzene, 2-butoxyethanol, *n*-decane, 1,4-dichlorobenzene, 2-ethylhexanol, and *n*-dodecane). van der Wal *et al.* (1998) used an empirical model to determine equilibrium partition

coefficients between six materials (nylon and wool carpet, particle board, wallpaper, curtain, and stainless steel) and ten chemicals (toluene, *m*- & *p*-xylene, mesitylene, *n*-decane, *n*-undecane, 2-ethylhexanol, tetrachloroethene, limonene, ethylene glycol monobutylether, and 2,2,4-methyl-1,3-pentanediol diisobutyrate). Jørgensen and Bjørseth (1999) studied two carpets (nylon and wool) and two chemicals (toluene and α -pinene).

Despite past efforts to quantify the importance of sorptive sinks, and related parameter estimation for sorption models, there have been only limited attempts to study sorption parameters within the context of adsorbate properties. An *et al.* (1999) showed that the equilibrium partition coefficient should be inversely proportional to chemical vapor pressure to the first power for mono-layer sorption defined by Langmuir theory and ideal gas conditions. They provided experimental data for five VOCs and four materials that were consistent with such an inverse relationship. Van der Wal *et al.* (1998) presented screening results for 10 chemicals and several indoor materials, and also observed an inverse relationship between the extent of adsorption and adsorbate vapor pressure. However, relationships between kinetic parameters (adsorption and desorption coefficients) and chemical properties have not been reported in the published literature. Such information might be valuable for ascertaining whether surface interactions or mass transfer phenomena limit sorption kinetics. For example, a strong correlation between sorption kinetic parameters and adsorbate properties would suggest that surface interactions dominate the rate of adsorption or desorption. Conversely, a weak correlation between sorption kinetic parameters and chemical properties would suggest that mass transfer to the adsorbent surface, or diffusion within a porous material, are the processes that limit the sorption process. The latter phenomenon would, theoretically, provide a relationship

between molecular diffusion coefficients and sorptive interactions, e.g., as opposed to vapor pressure and sorptive interactions.

The results presented in this paper are intended to expand the existing data and knowledge bases associated with the sorptive interaction of VOCs and indoor materials, and serve as a follow-up to a recent paper focused entirely on sorptive interactions between VOCs and new carpet (Won *et al.*, 2000). Adsorption and desorption parameters for a combination of fifteen common indoor surface materials and eight chemicals were determined and are presented herein

Background

The most widely used model for predicting sorptive interactions between gaseous chemicals and indoor materials is given by Equations 1 and 2, which define mass balances on the headspace of an inert and well-mixed chamber and a sorptive material placed within that chamber, respectively.

$$V \frac{dC_g}{dt} = Q_g C_{g,in} - Q_g C_g - k_a C_g A + k_d M^n A \quad (1)$$

$$\frac{dM}{dt} = k_a C_g - k_d M^n \quad (2)$$

Here, C_g is the VOC concentration in chamber air (mg/m^3), $C_{g,in}$ is the VOC concentration in inlet air (mg/m^3), V is the chamber volume (m^3), Q_g is the air flow rate through the chamber (m^3/h), A is the sink area (m^2), k_a is the adsorption rate coefficient (m/h), k_d is the desorption rate coefficient ($1/\text{h}$ if $n = 1$), M is the mass collected on the sink per unit area (mg/m^2), and n is a constant that accounts for non-linearities in the desorption process (-).

The area (A) is typically assumed to be the horizontally projected area of a material surface, i.e., as opposed to the true area that accounts for interior pores and irregularities

(roughness) of exposed surfaces. For all intents and purposes, increased surface areas due to surface irregularities and internal pores, as well as bulk mass transport and diffusive transport processes, are implicitly "lumped" into the adsorption and desorption coefficients. Furthermore, "n" is typically assumed to equal unity, consistent with an assumption that a linear equilibrium relationship exists between M and C_g at the low concentrations often observed in non-industrial indoor environments. This assumption allows for the material/air equilibrium partition coefficient (K_{eq}) for a specific VOC to be defined by the ratio k_a/k_d . Thus, knowledge of any two of these three parameters defines the complete set of three equilibrium and kinetic parameters. For example, if k_a and k_d are known, K_{eq} can be determined and used to estimate the equilibrium mass loading on materials for a given indoor concentration. Conversely, if K_{eq} and either k_a or k_d are known, the second kinetic parameter can be determined and used to model the dynamic sorptive interaction between indoor materials and gaseous contaminants.

Tichenor *et al.* (1991) and Jørgensen and Bjørseth (1999) employed Equations 1 and 2 for the case of $n = 1$. Analytical solutions for C_g and M were used in conjunction with data from small chamber experiments to back-calculate k_a and k_d . Values of K_{eq} were estimated as the ratio k_a/k_d . Tichenor *et al.* (1991) noted that Equations 1 and 2 are appropriate for relatively flat, smooth surfaces, e.g., wallboard, but may be inappropriate for complex surfaces such as carpet systems and other porous materials. Diffusion-controlled and hybrid (sorption and diffusion) models have been proposed for the latter materials (Little and Hodgson, 1996; Dunn and Chen, 1993), and may be more appropriate than Equations 1 and 2 when relevant data are available. This is particularly true for longer periods of sorptive interaction and for long-term re-emission from the sorptive material.

Experiments were completed over relatively short time periods (18 hours) and precluded evaluations based on advanced models, e.g., diffusion or hybrid models. However, as with recent work by van der Wal *et al.* (1998) and Jørgensen and Bjørseth (1999), the experimental protocols described herein allowed for a rapid screening of the relative importance of sorption for several VOCs and materials. Furthermore, experimental results were used to back-calculate k_a and k_d , and to subsequently estimate K_{eq} , for a large number of chemical and material combinations.

Methodology

The experimental system consisted of four 50-L electro-polished stainless steel chambers arranged in parallel (Figure 1). During each experiment, one of the four chambers was used as a blank (no material added). A syringe pump was used to deliver a mixture of target VOCs into a manifold, where the chemicals were volatilized into an air stream that was split evenly for delivery to each chamber. Exhaust from each chamber was directed to a valve that was programmed to allow for sequential sampling from each chamber. Samples were directed to an on-line gas chromatography system (SRI 8610C) equipped with a flame ionization detector (GC/FID). All transfer lines in the system were made of either TeflonTM or stainless-steel.

Each experiment lasted 18 hours, and included a 10-hour adsorption stage (with chemical injection) and an 8-hour desorption stage (no chemical injection). Equations 1 and 2 and concentration (C_g) profiles for the adsorption stage were used along with a best-fit, regression analysis using Marquardt's method to solve for k_a and k_d . The resulting sorption parameters were used to compare predicted and measured desorption stage concentration profiles.

Sorptive materials included three carpets, two carpet pads (cushions), three types of gypsum board (virgin, painted, wallpapered), vinyl and wood flooring (maple plank with polyurethane coating), ceiling (acoustic) tile, fiberglass shower stall, upholstery (100% cotton), and apples (unwashed). The cut edges and reverse side of each specimen were sealed with sodium silicate and allowed to dry prior to each experiment. The three carpet specimens were all tufted with polypropylene backing. Two of the carpet specimens (carpet 1 and carpet 3) consisted of nylon cut-pile fibers, while the third (carpet 2) was comprised of 90% olefin/10% nylon loop-pile fibers. Carpet fibers were treated with either Stainmaster™ (carpet 1) or Scotchgard™ (carpets 2 and 3) at the manufacturer. Two carpet pads were used, each comprised of bonded polyurethane. Differences in the sorptive capacities of each pad were small and are hereafter neglected.

Target VOCs were selected based on a broad range of vapor pressures and octanol-air partition coefficients, and not necessarily on their frequency of occurrence or magnitude of concentration in indoor environments. However, MTBE, toluene, and ethylbenzene are constituents of gasoline, and the latter two compounds, along with cyclohexane, are also found in many adhesives and consumer products. As such, these compounds are often observed in indoor environments. Tetrachloroethene is a common dry-cleaning agent and a constituent of some consumer products. As such, it is also observed in many residential dwellings. *o*-Dichlorobenzene is a reasonable surrogate for *p*-dichlorobenzene, a common moth repellent and air “freshener” that is found at elevated levels in buildings where such products are employed. 1,2,4-Trichlorobenzene was added as a chemical that borders on being a semi-volatile organic compound (SVOC). Isopropanol was selected to represent highly polar VOCs. Chemical vapor pressure ranged from 46 to 33,000 Pa and octanol-air partition coefficients, calculated as the ratio of octanol-water partition coefficient and Henry’s law constant, ranged from 97 to 19,000 $\text{m}^3_{\text{air}}/\text{m}^3_{\text{octanol}}$. Preliminary experiments indicated that multi-component effects were statistically insignificant (Won *et al.*, 2000). Thus, subsequent experiments included all eight VOCs.

Standard experimental conditions included inlet gas concentrations ranging from 6 to 15 mg/m³, 0% final relative humidity, a temperature of 24 - 25 °C, and an air exchange rate of 0.5 air changes per hour. Three different classes of inlet concentrations (6-15, 12-30, and 37–102 mg/m³) (2.5, 5, and 15 ppm) were studied for each VOC in the presence of carpet 1 with padding. In all cases, the inlet concentrations had no observable effect on sorption parameters, suggesting that, although higher than observed in most indoor environments, concentrations in chambers were low enough to exhibit a linear relationship between concentration in air and mass on the adsorbent material. Air exchange rates of 0.5, 2.1 and 3.2/h were also used with carpet 1 and padding. There were no apparent effects of air exchange rate on k_a , suggesting that mass transfer from air to the material surface was not a limiting factor in the sorption process. Small reductions in k_d were observed as the air exchange rate increased for 1,2-dichlorobenzene and 1,2,4-trichlorobenzene. However, the effects were generally small relative to those influenced by chemical and material properties and will not be considered further in this paper.

Relative humidity (RH) was always in the range of 50 to 70% at the beginning of each experiment. Inlet gas conditions were adjusted to allow for establishment of constant RH by the sixth hour of each experiment. Final values of 0%, 50% and 80% RH were tested for six different materials.

Results

Normalized concentration profiles (gas concentration in chamber divided by inlet gas concentration) for tetrachloroethene are presented in Figure 2. One set of curves corresponds to the reference (empty) chamber, and includes measured data and a dashed line that corresponds to a theoretical well-mixed reactor at the experimental air exchange rate of 0.5 per hour. The

second set of curves corresponds to a chamber containing carpet 1 with an underlying pad. Open circles depict measured data. The solid line corresponds to model predictions based on values of k_a and k_d that were determined during the adsorption stage (first ten hours). Similar plots were developed for every combination of VOC and material.

Data for the reference chamber compared favorably with an assumed well-mixed and inert chamber. This was true for all VOCs other than 1,2,4-trichlorobenzene, which generally exhibited some level of sorption to the experimental and/or analytical systems. The extent of tetrachloroethene sorption to carpet 1 with padding is clear, as over 40% of the inlet mass sorbed to the material during the adsorption stage. Furthermore, values of k_a and k_d determined from the adsorption stage led to good agreement between predicted and measured desorption profiles. Desorption stage data also illustrate that sorptive sinks can increase chemical retention times in an indoor environment. This is reflected by higher gas concentrations in the material chamber than in the reference chamber after hour 12.

The value of the coefficient of multiple determination (R^2) from nonlinear regression analyses was 1.0 for all chemicals in the reference chamber and very close to unity for all experiments in the material chamber. The value of R^2 was as low as 0.97 for 1,2,4-trichlorobenzene.

Summary of Sorption Parameters

A summary of the average and standard deviation of sorption parameters is provided in Tables 2 (k_a and k_d) and 3 (K_{eq}). For reasons of brevity, standard deviations are not provided for k_a and k_d . In nearly all cases, variations associated with relative humidity, inlet gas concentration, and air exchange rate were used in the averaging process. The one exception was for isopropanol, for

which only 0% RH data were used in the averaging process. Variabilities can be expressed in terms of a coefficient of variation (CV = standard deviation divided by the arithmetic mean) for those VOC/material combinations with three or more data points. Over all experimental conditions, the mean values of CV were 0.42, 0.54, and 0.32 for k_a , k_d and K_{eq} , respectively. With virgin gypsum board excluded, the mean values of CV were 0.33, 0.45 and 0.31, respectively.

Due to differences in test chemicals and material properties, it is difficult to compare sorption parameters with those reported previously. Compared to the findings of Tichenor *et al.* (1991), the best agreement was for tetrachloroethene and carpet, with their k_a within 25% (lower) of the average values obtained in this study for two nylon carpets. Their value of k_d for tetrachloroethene and gypsum board was only 30% greater than the average value obtained in this study. Other parameters were generally within an order of magnitude of those obtained for this study. Tichenor *et al.* (1991) also reported a K_{eq} of 0.97 m for tetrachloroethene and carpet. The range of K_{eq} for tetrachloroethene and carpet in this study was 0.36 m to 0.97 m. A value of $K_{eq} = 0.08$ m reported by van der Wal *et al.* (1998) for tetrachloroethene and virgin gypsum board was in excellent agreement with the average value of 0.09 m observed in this study. Jørgensen and Bjørseth (1999) reported a value of $k_a = 0.422$ m/h, $k_d = 0.674$ /h, and $K_{eq} = 0.626$ m for toluene and nylon carpet. Their values of k_a and K_{eq} were four and three times greater than that of carpet 1 in this study, respectively. However, their value of $k_d = 0.674$ /h exhibited excellent agreement with values of 0.56 /h and 0.65 /h for carpet 1 and carpet 3, respectively, in this study.

Effects of Sorptive Materials

As shown in Tables 2 and 3, the extent of sorption is highly dependent on adsorbent (material) characteristics. Example concentration profiles for 1,2-dichlorobenzene are presented in Figure 3 for fifteen materials. Sorption capacities for non-polar VOCs were greatest for carpet and carpet/pad systems followed by gypsum board and vinyl flooring. However, virgin gypsum board exhibited the greatest extent of sorption for polar VOCs (isopropanol and MTBE). Figure 4 provides concentration profiles for isopropanol exposed to each of five materials. The observations presented in this paper are consistent with those presented by Meininghaus *et al.* (1999), who reported that polar compounds, e.g., *tert* butyl acetate, sorbed and/or diffused to gypsum board to a greater than did non-polar compounds.

Interestingly, apples were observed to sorb both 1,2-dichlorobenzene and 1,2,4-trichlorobenzene, presumably to the waxy film attached to the apple skin. These results are novel and suggest that foodstuff which is left exposed to airborne VOCs (on counter tops or within cupboards) may become contaminated and later serve as sources for ingestion exposure to those compounds.

The importance of understanding sorption kinetics, as opposed to simply equilibrium sorption conditions, is illustrated by the findings presented in Tables 1 and 2 for virgin and painted gypsum board. With the exception of isopropanol, which exhibited significant sorptive interaction with virgin gypsum board, the equilibrium partition coefficients for each chemical were similar for both virgin and painted gypsum board (Table 1). One might interpret these results to suggest that both types of gypsum board will have a similar effect on indoor concentrations of non-polar VOCs. However, virgin gypsum board generally exhibited higher adsorption and desorption coefficients when compared with painted gypsum board, and would thus be expected to reach an equilibrium condition more rapidly, have a greater impact on

reductions in airborne VOC concentrations for short-term source events, and provide for less chemical retention time on the material surface, and in indoor air, than would painted gypsum board.

An additional discussion of the role of carpet components as sinks for non-polar VOCs was presented elsewhere by the authors (Won *et al.*, 2000). Selective results are presented herein for comparative purposes.

Effects of Chemical Properties of VOCs

For a given material, the level of sorption was observed to be extremely sensitive to chemical properties. Chemical property effects are illustrated in Figure 5, which depicts concentration profiles for eight chemicals in the presence of virgin gypsum board. The greatest amount of sorption was observed for isopropanol, presumably due to polar-polar interactions between isopropanol and gypsum board (calcium sulfate). MTBE, toluene, and tetrachloroethene exhibited only a small amount of sorption to virgin gypsum board as well as other materials.

In general, the extent of sorption to a specific material is inversely related to vapor pressure (Kephelopoulos *et al.*, 1996; van der Wal *et al.*, 1998; An *et al.*, 1999). As such, correlations between vapor pressure and sorption parameters were examined in this study. Analysis of these relationships was facilitated by classifying VOCs into two groups and using the most appropriate group for each material. Significant experimental difficulty was encountered for 1,2,4-trichlorobenzene, which appeared to be sorbed to the experimental and/or analytical systems. Thus, group A consisted of all VOCs minus 1,2,4-trichlorobenzene. Group B consisted of group A minus MTBE, cyclohexane, and isopropanol. These three chemicals exhibited little to no sorptive interaction with several test materials, and were thus omitted from group A. They were

included in group B for materials in which the extent of sorption was sufficient to back-calculate sorption parameters. Thus, groups A and B generally contain four and seven data points, respectively.

Coefficients for the linear regression between $-\ln(\text{vapor pressure})$ and $\ln(K_{eq})$ are summarized in Figure 6. The median R^2 value for all K_{eq} analyses was 0.95. The slope of the logarithmic relationship between K_{eq} and vapor pressure fell within a relatively narrow range (0.5 to 0.87 and, mostly, 0.63 to 0.87). However, values of the slope are slightly less than the value of unity derived theoretically based on fundamental thermodynamic principles and $n = 1$ by An *et al.* (1999). Figure 6 also suggests that it may be possible to group some materials. For example, carpets with padding (underlying bonded urethane cushion) appeared to exhibit a similar level of sorption. On the other hand, grouping appears less desirable for carpet itself, i.e., without an underlying cushion. The importance of bonded urethane carpet cushion as a sorptive material was discussed in detail by Won *et al.* (2000).

Figure 7 summarizes the results from the linear regression between $-\ln(\text{vapor pressure})$ and $\ln(k_a)$. The relationship between k_a and vapor pressure was not as good as that between K_{eq} and vapor pressure. For several materials with low R^2 for the $-\ln(\text{vapor pressure})/\ln(k_a)$ relationship, including carpet1/pad, carpet3, virgin gypsum board, painted gypsum board, and vinyl flooring, the linear regression between $-\ln(\text{vapor pressure})$ and $\ln(k_d)$ exhibited improved R^2 values (Figure 8).

A correlation was also observed between octanol-air partition coefficient (K_{oa}) and sorption parameters. Linear relationships between K_{oa} ($L_{air}/L_{octanol}$) and K_{eq} were obtained (Figure 9). Values of R^2 indicate a strong linear relationship between K_{oa} and K_{eq} . Linear regression was also completed for K_{oa} and k_a (Figure 10). Sorption to all materials except carpet 1/pad 1

exhibited a strong linear relationship between K_{oa} and k_a . The relationship between K_{oa} and k_a is most reflective of the last step in the sorption process, i.e., reaction between chemical and material, as opposed to bulk mass transfer from air to a material or diffusion to/within the material. Interestingly, no relationship was obtained between K_{oa} and k_d , although k_d can be estimated based on K_{eq} and k_a . However, it should be emphasized that there is a large gap between the last two data points in Figure 9, and it is recommended that additional experiments using chemicals with K_{oa} in the range of 5,000 to 20,000 $L_{air}/L_{octanol}$ be completed to confirm the linear relationship between K_{oa} and K_{eq} .

The relationships described above indicate that it is possible to relate chemical properties to fundamental properties of the sorption process. This finding is significant in so much as it suggests the possibility of being able to reasonably model sorptive interactions for VOCs that have not been tested in laboratory chambers. However, because the relationships have not explicitly accounted for material properties, it may not be legitimate to extrapolate them to material specimens that differ significantly from those used in this study. This caveat is particularly important for carpet due to the fact that the results described in this paper implicitly “lump” non-horizontal surface area effects into sorption parameters, and different brands of carpet can have significantly different fiber and backing areas. Nevertheless, the results suggest that carpet can serve as a major sink for VOCs, and that relationships between sorption parameters and chemical properties are possible for specific brands of carpet, or more generally for carpet if actual surface areas are taken into account. A more detailed analysis of carpet results, including effects of carpet material differences and components was presented by Won *et al.* (2000).

Effects of Relative Humidity

With a couple of significant exceptions, relative humidity (RH) had no observable effect on sorption parameters. An example is given in Figure 11 for ethylbenzene and painted gypsum board. One exception occurred for virgin gypsum board, for which K_{eq} generally decreased as RH increased, particularly between RH profiles that approached 0% and 50%. For this change in RH, the decrease in K_{eq} varied from 33% to 58% with an average of 45%. Figure 12 provides an example for virgin gypsum board and 1,2-dichlorobenzene. It is possible that polar-polar attractions between water molecules and gypsum board reduced the sorption capacity of the gypsum board for VOCs. The maximum value of K_{eq} was for isopropanol, a polar VOC (K_{eq} = 7.2 m at 0% final RH; 3.6 m at 50% final RH; 3.2 m at 80% final RH). No sorption was observed for cyclohexane on virgin gypsum board for any RH, or for tetrachloroethene or ethylbenzene at 80% RH. Interestingly, there was no consistent trend between RH and either k_a or k_d for any of the VOCs.

Other than for virgin gypsum board, isopropanol was the only VOC that was significantly influenced by RH. This was particularly true for carpet with padding (Figure 13), for which K_{eq} actually increased with increasing RH (0.68 m at 0% final RH; 1.1 m at 50% final RH; 1.4 m at 80% final RH). It is conceivable that this was due to the absorption of isopropanol into water that condensed in the pores of the urethane padding or to the carpet surface. The solubility of isopropanol is 26 times greater than that of the second most soluble target VOC (MTBE), and it has a much lower Henry's law constant than any of the other VOCs. The value of K_{eq} for isopropanol increased dramatically with increasing RH for painted gypsum board (0.20 m at 0% final RH to 1.4 m at 50% final RH). Sorption of isopropanol was only observed at RH = 80% for vinyl flooring and upholstery.

The findings associated with non-polar compounds agree with those reported by Colombo *et al.* (1993). However, Colombo *et al.* (1993) concluded that the sorption of both *n*-decane (non-polar) and 2-butoxyethanol (polar) on carpet was not influenced by relative humidity, the latter being in contrast to the findings of this study for isopropanol. It is not possible to ascertain why the degree of sorption of isopropanol increased with increasing relative humidity in this study, and why the same was not true for 2-butoxyethanol in the study by Colombo *et al.* (1993). However, in this study, the positive relationship between isopropanol sorption and relative humidity occurred for a carpet system that included an underlying carpet cushion. Colombo *et al.* (1993) did not include an underlying cushion in their work. As stated above, any water condensation in the pores of the urethane carpet cushion could enhance the removal of isopropanol by absorption, as opposed to adsorption. This hypothesis requires additional study before it is properly addressed.

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Table 1. Physico-chemical Properties of Surrogate Chemicals

Characteristics	MTBE ^j	CH ^k	IP ^l	TOL ^k	PCE ^k	EB ^k	DCB ^k	TCB ^k
Formula	C ₅ H ₁₂ O	C ₆ H ₁₂	C ₃ H ₈ O	C ₇ H ₈	C ₂ Cl ₄	C ₈ H ₁₀	C ₆ H ₄ Cl ₂	C ₆ H ₃ Cl ₃
MW ^a	88.2	84.2	60.1	92.1	165.8	106.2	147.0	181.5
P ^o ^b	3.9E+4	1.3E+4	4.3E+3	3.9E+3	2.5E+3	1.3E+3	2.0E+2	4.6E+1
K _{ow} ^c	15.8	2754.2	0.692	489.8	758.6	1412.5	2398.8	4466.8
K _{oa} ^d	9.7E+1	3.8E+2	2.0E+3	1.8E+3	6.7E+2	4.3E+3	1.9E+4	1.9E+4
H _c ^e	0.02	7.2	0.0055	0.3	1.1	0.3	0.1	0.2
T _b ^f	55.0	80.7	82.4	110.6	121.0	136.2	180.0	213.0
C _w ^g	4.3E+1	6.08E-2	7.6E+2 ⁱ	5.2E-1	1.5E-1	1.7E-1	9.3E-2	8.5E-2
Φ ^h	-	1.070	-2.810	0.502	-0.453	0.839	0.031	-

^a MW: molecular weight. ^b P^o: vapor pressure at 25 °C (Pa).

^c K_{ow}: octanol-water partition coefficient at 25°C (m³_{water}/m³_{octanol}).

^d K_{oa}: octanol-air partition coefficient at 25°C; estimated by K_{ow}/H_c (m³_{air}/m³_{octanol}).

^e H_c: Henry's law constant at 25 °C (m³_{water}/m³_{air}), ^f T_b: boiling point (°C); ^g C_w: water solubility (kg/m³).

^h Φ: polarizability index from Nirmalakhandan and Speece (1988).

ⁱ Estimated from 1/C_w = 1.113 log K_{ow} - 0.926 in Lyman *et al.* (1982).

^j Buckley *et al.* (1997) except boiling points & H_c, ^k Schwarzenbach *et al.* (1993); ^l Verschueren (1996).

Table 2. Summary of Average Adsorption and Desorption Coefficients (k_a/k_d)

Material	n_e	Chemical							
		MTBE	CH	IP	TOL	PCE	EB	DCB	TCB
Cp1	9	ns	ns	-	0.11 / 0.56	0.17 / 0.47	0.30 / 0.62	0.52 / 0.25	0.58 / 0.10
Cp2	2	nc	nc	-	0.26 / 0.44	0.31 / 0.32	0.41 / 0.34	0.80 / 0.17	0.91 / 0.13
Cp3	1	nc	ns	-	0.18 / 0.65	0.16 / 0.42	0.17 / 0.37	0.43 / 0.21	0.49 / 0.16
Cp1.p	10	0.76 / 4.9	0.39 / 1.7	0.75 / 1.1	0.49 / 0.29	0.44 / 0.25	0.48 / 0.15	0.60 / 0.08	1.5 / 0.46
Cp2.p	2	0.10 / 0.45	0.10 / 0.67	0.36 / 1.2	0.42 / 0.23	0.45 / 0.22	0.49 / 0.15	0.96 / 0.15	2.1 / 0.36
Cp3.p	2	0.10 / 0.69	0.10 / 0.60	0.27 / 0.47	0.23 / 0.16	0.23 / 0.17	0.29 / 0.14	0.62 / 0.13	1.4 / 0.42
G.v	5	0.46 / 1.6	ns	0.79 / 0.11	0.21 / 1.7	0.12 / 1.1	0.21 / 0.87	0.54 / 0.49	0.68 / 0.32
G.p	4	0.07 / 0.12	0.01 / 0.18	0.08 / 0.24	0.10 / 0.60	0.06 / 0.45	0.07 / 0.27	0.26 / 0.25	0.50 / 0.29
G.wp	1	nc	ns	-	0.04 / 0.12	0.09 / 0.50	0.11 / 0.19	0.54 / 0.24	1.1 / 0.28
FL.v	3	ns	ns	nc	0.09 / 0.66	0.07 / 0.39	0.06 / 0.22	0.23 / 0.13	0.53 / 0.17
FL.w	1	nc	ns	nc	ns	ns	0.01 / 0.01	0.09 / 0.74	0.09 / 0.60
Uphol	4	ns	ns	nc	ns	ns	ns	2.0 / 10	1.8 / 3.2
Ceil	2	0.01 / 0.34	ns	nc	0.01 / 0.03	0.01 / 0.17	0.09 / 1.0	0.48 / 0.73	0.63 / 0.52
SS.fg	4	ns	ns	nc	ns	ns	ns	ns	2.2 / 7.8
App	1	ns	ns	nc	0.02 / 0.18	0.01 / 0.05	0.07 / 0.72	0.32 / 0.62	4.8 / 3.8

k_a in m/h. k_d in 1/h. Values are averages of " n_e " experiments. "ns" = no sorption. "nc" = little sorption with indeterminate sorption parameters (no convergence). "-" = failure of quality assurance protocols relative to variations in inlet concentrations. CpX = carpet X. CpX.p = carpet X with padding. G.v = virgin gypsum board. G.p = painted gypsum board. G.wp = wallpapered gypsum board. FL.v = vinyl flooring. FL.w = wood flooring. Uphol = upholstery. Ceil = ceiling (acoustic) tile. SS.fg = fiberglass shower stall. App = apples.

Table 3. Summary of Equilibrium Partition Coefficients (K_{eq}) (Average \pm Standard Deviation)

Material	n_e	Chemical							
		MTBE	CH	IP	TOL	PCE	EB	DCB	TCB
Cp1	9	ns	ns	-	0.22 \pm 0.07	0.36 \pm 0.09	0.46 \pm 0.13	2.1 \pm 1.5	5.9
Cp2	2	nc	nc	-	0.6 \pm 0.02	0.97 \pm 0.002	1.2 \pm 0.05	4.7 \pm 0.3	7.8 \pm 3
Cp3	1	nc	ns	-	0.28	0.38	0.46	2.0	3.1
Cp1.p	10	0.15 \pm 0.03	0.24 \pm 0.05	0.78 \pm 0.2	1.7 \pm 0.18	1.76 \pm 0.2	3.3 \pm 0.4	8.0 \pm 3	4.9 \pm 3
Cp2.p	2	0.22 \pm 0.04	0.15 \pm 0.02	0.29 \pm 0.03	1.9 \pm 0.1	2.1 \pm 0.1	3.4 \pm 0.4	6.6 \pm 0.5	6.1 \pm 0.8
Cp3.p	2	0.14 \pm 0.01	0.16 \pm 0.01	0.57 \pm 0.06	1.5 \pm 0.1	1.4 \pm 0.08	2.1 \pm 0.07	4.9 \pm 0.8	3.5 \pm 0.5
G.v	5	0.35 \pm 0.2	ns	7.2	0.12 \pm 0.04	0.2 \pm 0.09	0.27 \pm 0.09	1.2 \pm 0.5	2.4 \pm 0.7
G.p	4	0.45	0.054 \pm 0.02	0.20	0.18 \pm 0.04	0.18 \pm 0.1	0.28 \pm 0.03	1.0 \pm 0.4	1.8 \pm 0.4
G.wp	1	nc	ns	-	0.34	0.17	0.58	2.3	3.9
FL.v	3	ns	ns	nc	0.14 \pm 0.01	0.19 \pm 0.05	0.58 \pm 0.5	1.8 \pm 0.7	3.5 \pm 0.1
FL.w	1	nc	ns	nc	ns	ns	0.63	0.13	0.15
Uphol	4	ns	ns	nc	ns	ns	ns	0.19 \pm 0.0	0.55 \pm 0.05
Ceil.	2	0.06	ns	nc	0.25	0.088 \pm 0.1	0.10 \pm 0.01	0.68 \pm 0.1	1.2 \pm 0.1
SS.fg	4	ns	ns	nc	ns	ns	ns	ns	0.33 \pm 0.15
App	1	ns	ns	nc	0.061	0.12	0.10	0.52	1.3

K_{eq} in m. Values are averages of " n_e " experiments. "ns" = no sorption. "nc" = little sorption with indeterminate sorption parameters (no convergence). "-" = failure of quality assurance protocols relative to variations in inlet concentrations. CpX = carpet X. CpX.p = carpet X with padding. G.v = virgin gypsum board. G.p = painted gypsum board. G.wp = wallpapered gypsum board. FL.v = vinyl flooring. FL.w = wood flooring. Uphol = upholstery. Ceil = ceiling (acoustic) tile. SS.fg = fiberglass shower stall. App = apples.

Figure Captions:

Figure 1. Major Components of Experimental System

Figure 2. Example Concentration Profiles (tetrachloroethene)

Figure 3. Effects of Materials on Sorption (1,2-dichlorobenzene)

Figure 4. Effects of Materials on Sorption (isopropanol)

Figure 5. Effects of Chemical Properties on Sorption (virgin gypsum board)

Figure 6. Linear Relationship between $-\ln(\text{vapor pressure})$ and $\ln(K_{eq})$ ($K_{eq} = m$; vapor pressure = Pa)

Figure 7. Linear Relationship between $-\ln(\text{vapor pressure})$ and $\ln(K_{eq})$ ($k_a = m/h$; vapor pressure = Pa)

Figure 8. Linear Relationship between $-\ln(\text{vapor pressure})$ and $\ln(k_d)$ ($k_d = 1/h$; vapor pressure = Pa)

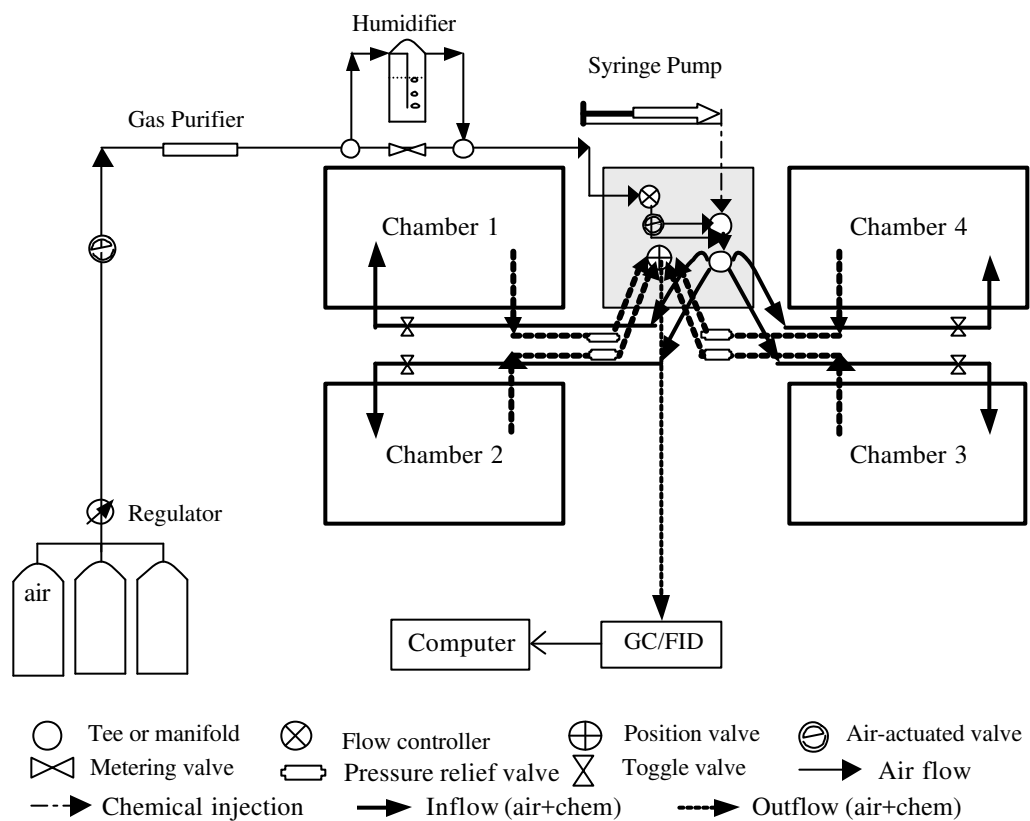
Figure 9. Linear Relationship between Octanol-air partition coefficient (K_{oa}) and K_{eq} ($K_{eq} = m$; $K_{oa} = m^3_{\text{air}}/m^3_{\text{octanol}}$)

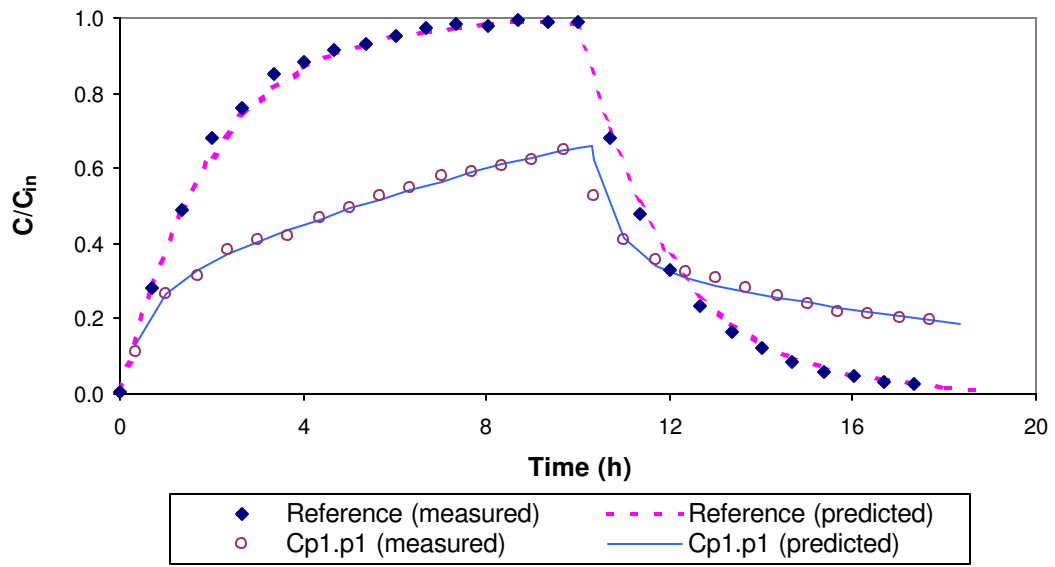
Figure 10. Linear Relationship between Octanol-air partition coefficient (K_{oa}) and k_a ($k_a =$
m/h; $K_{oa} = \text{m}^3_{\text{air}}/\text{m}^3_{\text{octanol}}$)

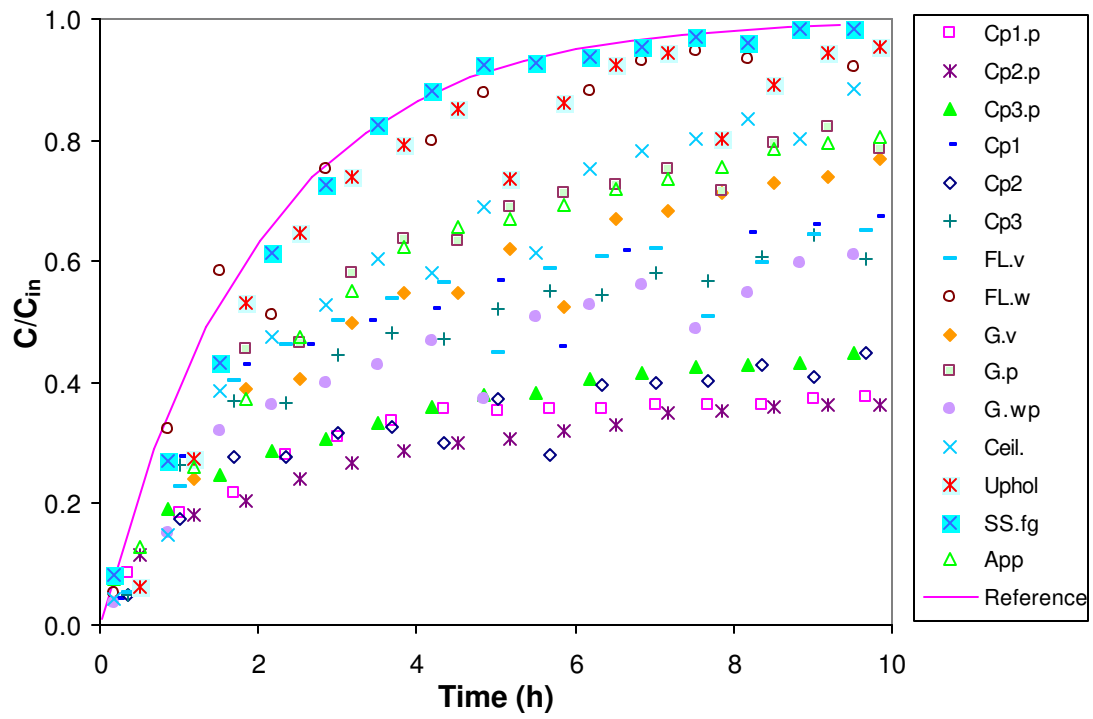
Figure 11. Effects of Relative Humidity on Sorption (ethylbenzene and painted gypsum board)

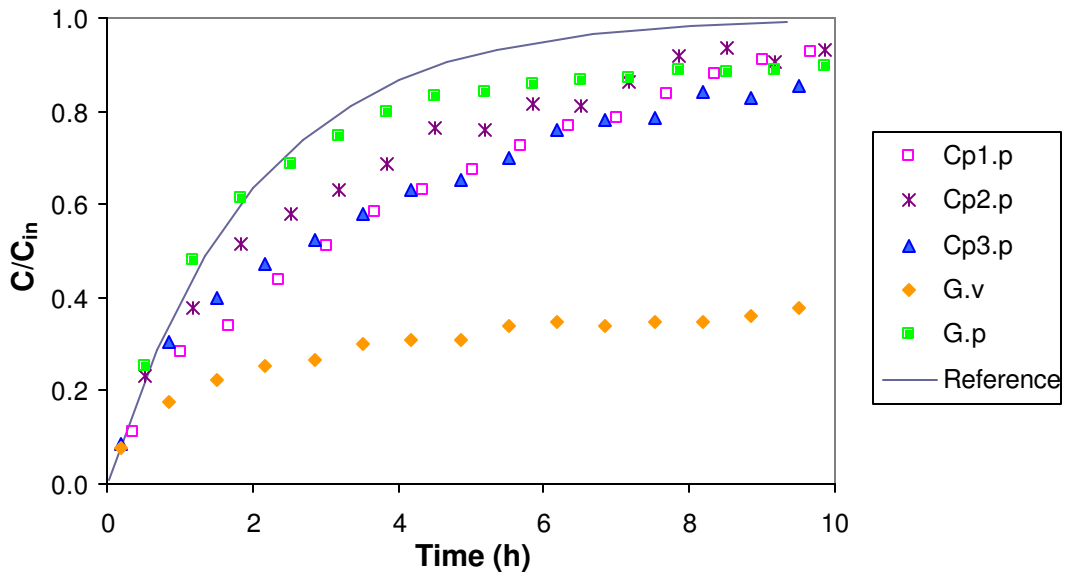
Figure 12. Effects of Relative Humidity on Sorption (1,2-dichlorobenzene and virgin gypsum board)

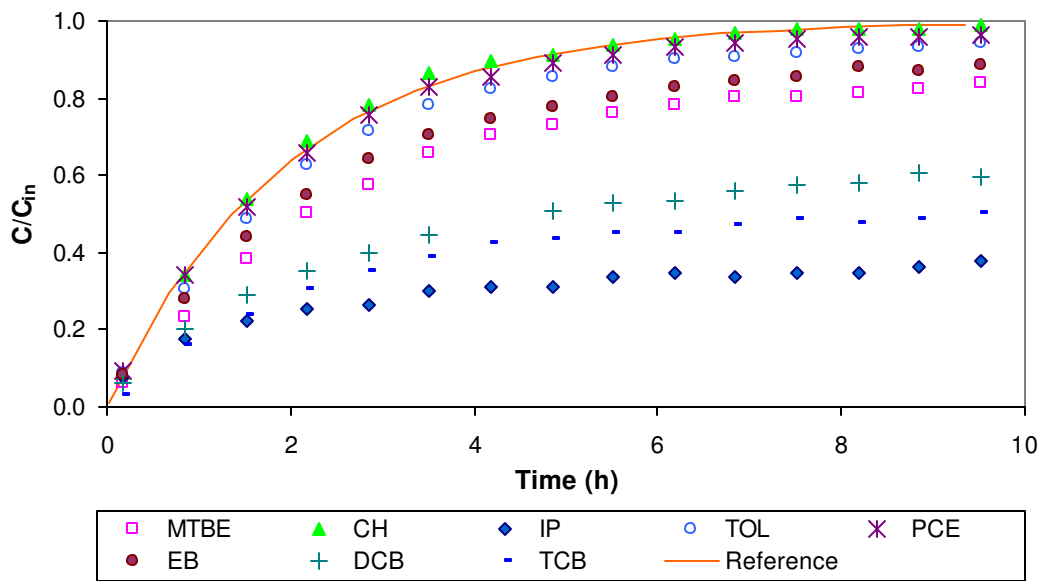
Figure 13. Effects of Relative Humidity on Sorption (isopropanol and carpet1/pad)

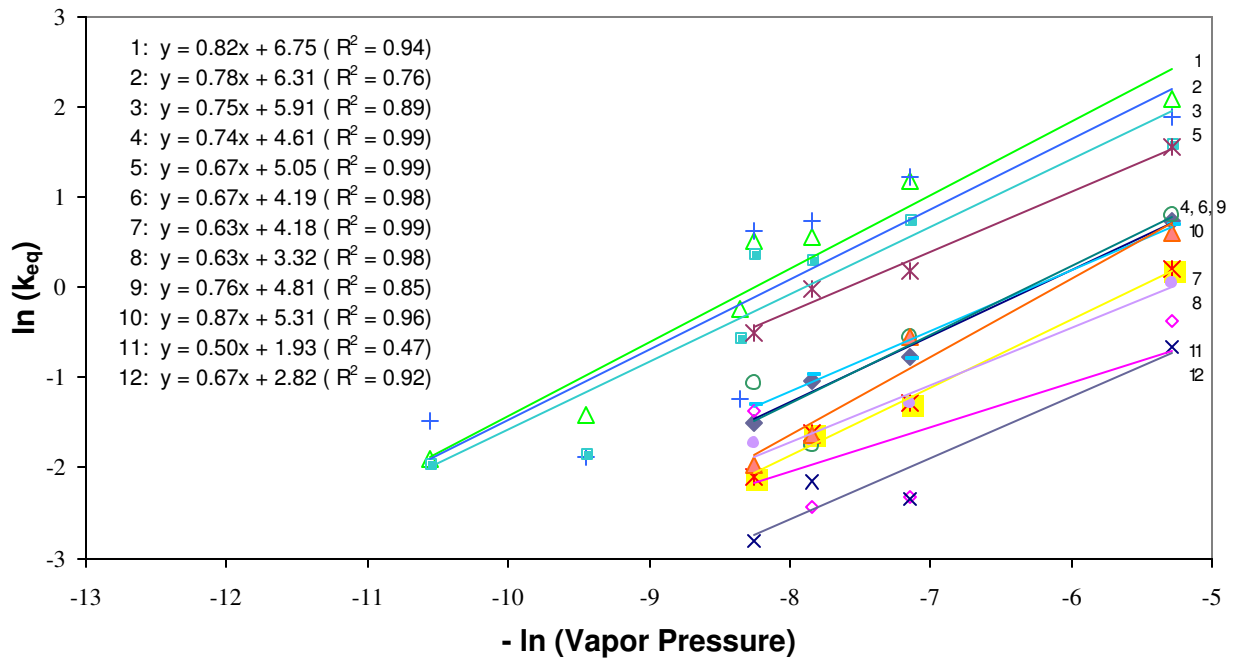




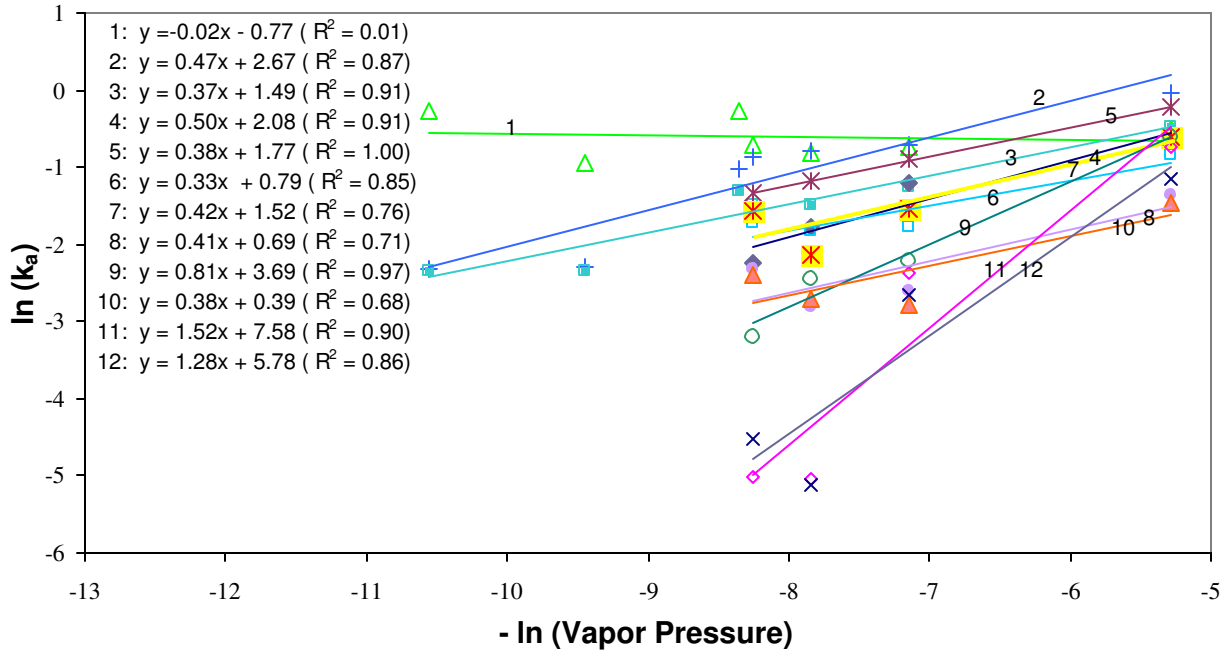








△ 1: carpet 1/padding	+ 2: carpet 2/padding	■ 3: carpet 3/padding
◆ 4: carpet 1	× 5: carpet 2	— 6: carpet 3
✕ 7: virgin gypsum board	● 8: painted gypsum board	○ 9: wall-papered gypsum board
▲ 10: vinyl flooring	◇ 11: ceiling tile	× 12: apples



△ 1: carpet 1/padding	+ 2: carpet 2/padding	■ 3: carpet 3/padding
◆ 4: carpet 1	× 5: carpet 2	□ 6: carpet 3
⊠ 7: virgin gypsum board	● 8: painted gypsum board	○ 9: wall-papered gypsum board
▲ 10: vinyl flooring	◇ 11: ceiling tile	× 12: apples

