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# EFFECT OF REVERSIBLE, DIFFUSION-CONTROLLED SINKS ON VOC CONCENTRATIONS IN BUILDINGS

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## ABSTRACT

This paper evaluates the impact of reversible, diffusion-controlled sinks on indoor air contaminant concentrations. Four typical scenarios are considered, each involving a variable mass flow rate entering a room containing an idealized sink with realistic properties. The four scenarios include a sinusoidal source, a double-exponential decaying source, an episodic introduction of a volatile compound, and a constant source with varying ventilation rates. Using a source/sink diffusion model developed in earlier work, the evolving indoor-air concentrations are predicted. A parametric study, with respect to the material/air partition coefficient (K), and the material-phase diffusion coefficient (D), shows that equilibrium dominates the source/sink effect for volatilities typical of a wide range of VOCs commonly found indoors. D only becomes important for low volatility compounds.

## INTRODUCTION

Diffusion is an important mechanism governing the source/sink behavior of certain indoor materials [1]. Although several empirical or semi-empirical models have been proposed to describe diffusion-controlled emission processes [2], predictions for conditions not covered by the experimental data are often uncertain, and such models provide little insight into the controlling mechanisms. Little et al. [3] developed a source model for predicting emissions from new carpets. An analytical solution was obtained assuming that the influent air was free of VOCs. Later, Little and Hodgson [1] extended the model to allow predictions to be made with a transient forcing function. This model permits the evaluation of the source/sink behavior of homogeneous, diffusion controlled indoor materials based solely on a knowledge of relevant properties such as the material-air partition coefficient (K) and the material-phase diffusion coefficient (D). This paper applies the sink model developed by Little and Hodgson [1] to cases where a room is subject to a time-varying contaminant source. Model predictions for four VOC source scenarios are demonstrated. Also, to gain insight into the underlying mechanisms, a parametric study is conducted with respect to the key model parameters, K and D.

## THE MODEL

Consider a room, which contains a homogeneous sink in the form of a slab. Transient diffusion through the slab can be described using the one-dimensional diffusion equation

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

where  $C(x, t)$  is the concentration of the contaminant in the slab,  $t$  is time, and  $x$  is distance from the base of the slab.

Equilibrium is assumed to hold between the VOC concentration in the surface layer of the slab and the indoor air, or

$$K = \frac{C|_{x=L}}{y} \quad (2)$$

where  $y$  is the air-phase concentration. Further assuming that the sink is initially free of contaminant, and that there is no flux through the base of the slab, the following analytical solution is obtained [1]

$$C(x, t) = 2 \frac{Q}{A \cdot K} \sum_{n=1}^{\infty} \left\{ \frac{\exp(-Dq_n^2 t) \cos(q_n x)}{[L(h - kq_n^2)^2 + q_n^2(L + k) + h] \cos(q_n L)} \cdot \int_0^t \exp(Dq_n^2 \tau) \cdot K \cdot y_{in}(\tau) d\tau \right\} \quad (3)$$

where

$$h = \frac{Q}{ADK} \quad (4)$$

and

$$k = \frac{V}{AK} \quad (5)$$

The  $q_n$ 's are the positive roots of

$$q_n \tan(q_n L) = h - kq_n^2 \quad (6)$$

$A$  is the exposed surface area of the slab,  $V$  the volume of well-mixed air within the room,  $Q$  the volumetric flow rate of air,  $L$  the thickness of the slab, and  $\tau$  is a dummy variable.

Once the source function,  $y_{in}(t)$  is defined, equation (3) can be used to predict the evolving contaminant concentration in the slab. The concentration of a VOC in the room at any time is obtained by first finding the concentration at the slab surface ( $x = L$ ) and then applying the equilibrium condition defined by equation (2).

## MODEL PARAMETERS

Styrene and naphthalene are used as example VOCs with a sink represented by a carpet with a 2mm Styrene Butadiene Rubber (SBR) backing. The surface area ( $A$ ) is assumed to be  $9 \text{ m}^2$  and the volume ( $V$ ) of the room is  $20 \text{ m}^3$ . A ventilation rate of 1 air change per hour is used, which results in a  $Q$  of  $20 \text{ m}^3/\text{h}$ . Values of  $K$  and  $D$  were estimated using appropriate correlation equations [4]. Values of  $K$  and  $D$  are 330 and  $1.6 \times 10^{-12} \text{ m}^2/\text{s}$  for SBR-styrene, and 270,000 and  $1.6 \times 10^{-12} \text{ m}^2/\text{s}$  for SBR-naphthalene, respectively.

## RESULTS AND DISCUSSION

Four scenarios are now considered. In each case, air enters a single room either from the outside or from a connected room. The concentration or the flow rate of the air entering the room varies as a function of time. The previously described model is used to predict the resulting contaminant concentration within the target room, a calculation that implicitly includes the effect of the hypothetical sink. The VOCs used in the calculations (styrene and naphthalene) cover a wide range in volatility and illustrate the impact of this parameter on the predicted concentrations.

### Scenario 1

The first scenario involves a constant  $Q$  and a sinusoidal variation in concentration. A practical example of this type of source are pollutants, such as benzene, resulting from motor vehicle exhaust in outdoor air in Los Angeles, California, as described by Harley and Cass [5]. The following source function was inferred from that data

$$y_{in}(t) = 10 \cdot \sin\left(\frac{\pi}{12}t\right) + 20 \quad (7)$$

Figure 1 compares the source concentration profile defined by equation (7) to that predicted using the model. For naphthalene, whose  $K$  value is orders of magnitude higher than that of styrene, a significant depression in concentration is evident. For both compounds, the indoor material shows alternating sink and source behavior. While the source concentration rises, the SBR functions as a sink (i.e.,  $y < y_{in}$ ), while on the down slope of the sinusoidal curve, the SBR acts as a source, (i.e.,  $y > y_{in}$ ). In both cases, the periodicity of the output function remains the same as that of the source despite a discernable lag time.

### Scenario 2

The second scenario again involves a constant  $Q$  but with a slowly depleting VOC source, such as a new carpet, in a connected room. The decaying source function was obtained from a double exponential relationship for emission of styrene from a carpet as reported by Hodgson et al. [6]

$$y_{in}(t) = 793 \cdot e^{-0.15t} + 139 \cdot e^{-0.022t} \quad (8)$$

Figure 2 plots the source function as well as the resulting concentrations predicted for styrene and naphthalene. The concentrations peak about four hours after initialization of the source and naphthalene is again substantially reduced as a result of the sink effect.

### Scenario 3

The third scenario simulates the intermittent use of a volatile consumer product such as an aerosol spray in the connected room. The air flow rate  $Q$  remains constant. It is assumed that the product is used twice a day (once at 9 a.m. and again at 1 p.m.), that initial values for both spikes are 500 ppb, and that the parameters for styrene are applicable. A mass balance yields the following source functions on a daily basis

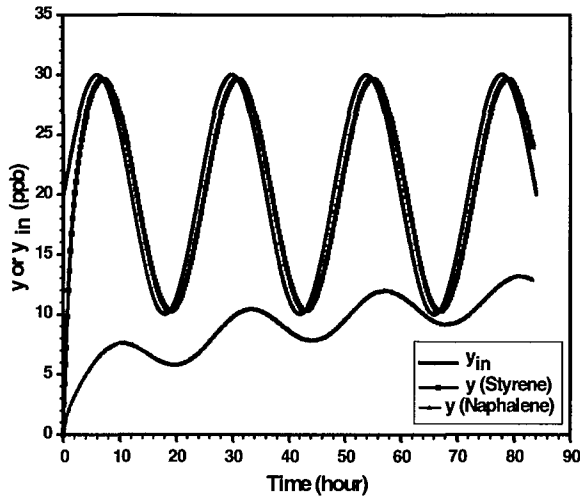


Figure 1. Sink effect on indoor VOC concentrations responding to a sinusoidal source.

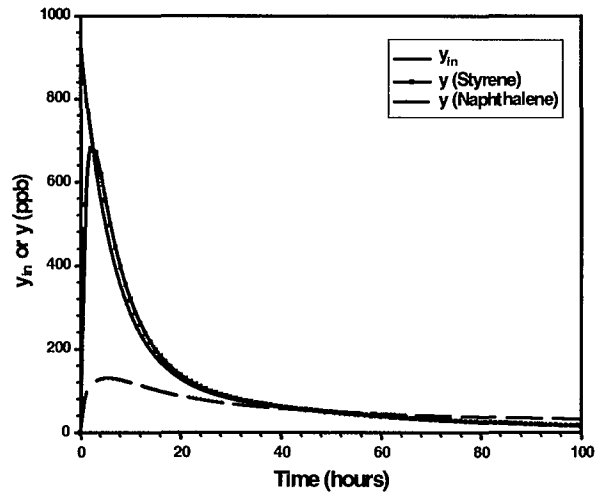


Figure 2. Sink effect on indoor VOC concentrations responding to a double-exponential decaying source.

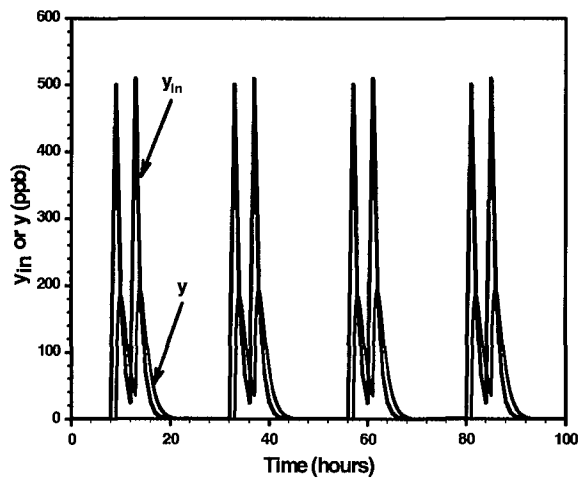


Figure 3. Sink effect on indoor concentrations following an episodic input of a volatile compound.

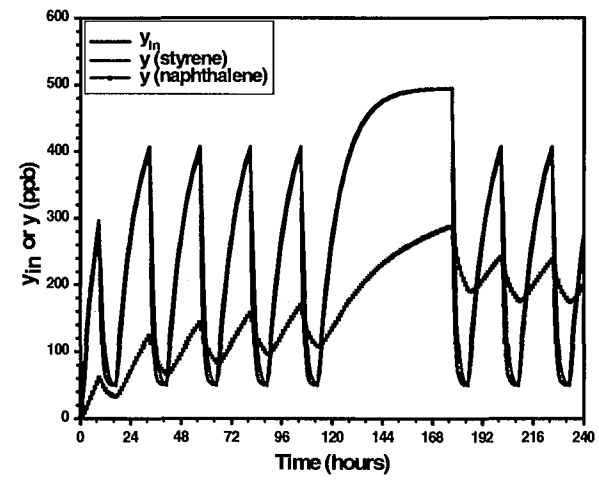


Figure 4. Effect of sink and daily change in ACH on indoor air concentrations responding to a constant source.

$$y_{in}(t) = 0 \quad 0 \leq t < 9 \quad (9)$$

$$y_{in}(t) = \frac{500}{e^{-9 \cdot \frac{Q}{V}}} \cdot e^{-\frac{Q}{V}t} \quad 9 \leq t < 13 \quad (10)$$

$$y_{in}(t) = \frac{500}{e^{-9 \cdot \frac{Q}{V}}} \cdot \left\{ e^{-\frac{Q}{V}(t-4)} + e^{-\frac{Q}{V}t} \right\} \quad 13 \leq t < 24 \quad (11)$$

where midnight is taken as the starting point. It is assumed that releases from the previous day will not affect the indoor air concentration on the following day. However, the impact of the first release is added to the second release on the same day as shown in equation (11). Figure 3 shows the transient concentrations induced by these releases with and without the sink effect.

#### Scenario 4

The fourth scenario utilizes an unspecified source emitting a VOC at a constant rate. A ventilation rate of 1.0 air changes per hour is assumed between 9 a.m. and 5 p.m. from Monday through Friday, while it is reduced to 0.1 air changes per hour during nights and weekends. A mass balance approach similar to that taken in scenario 3 is used to define the appropriate source functions. Figure 4 presents the concentration histories for styrene and naphthalene, respectively, in the presence the hypothetical sink.

#### Parametric analysis

The model allows the influence of the key parameters on the predicted concentrations to be examined. For illustrative purposes, a constant  $y_{in}$  of 500 ppb is considered in equation (3). Figures 5 and 6 provide plots of  $y(t)$  for values of  $D$  varying between  $0.01 \times 10^{-12}$  and  $100 \times 10^{-12} \text{ m}^2/\text{s}$ , while  $K$  is fixed at 1000 and 100,000, respectively. Figure 5 demonstrates that for a  $K$  value of  $\sim 1000$ , which is typical for several VOC/indoor material combinations, a variation in  $D$  does not alter the  $y(t)$  profiles considerably. However,  $D$  becomes important when  $K$  is large as shown in Figure 6.

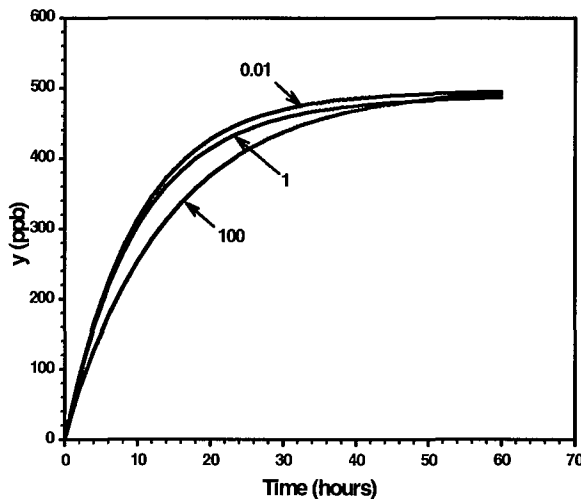


Figure 5. Plots of  $y(t)$  for  $D$  varying between  $0.01 \times 10^{-12}$  and  $100 \times 10^{-12} \text{ m}^2/\text{s}$  at a constant  $K$  of 1000 and  $y_{in}$  of 500 ppb.

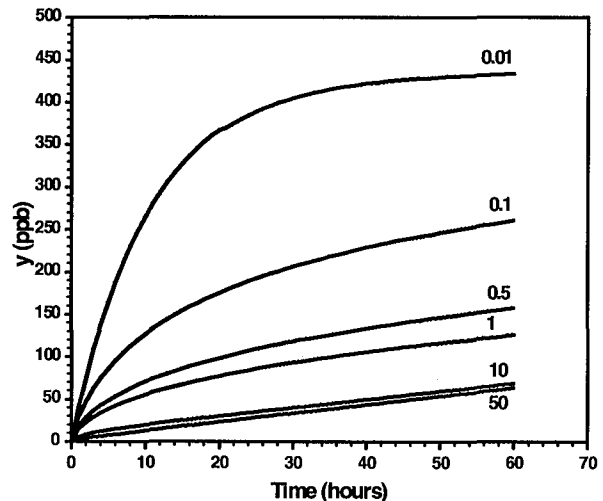


Figure 6. Plots of  $y(t)$  for  $D$  varying between  $0.01 \times 10^{-12}$  and  $50 \times 10^{-12} \text{ m}^2/\text{s}$  at constant  $K$  of 100,000 and  $y_{in}$  of 500 ppb.

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## REFERENCES

1. Little J. C. and Hodgson A. T. 1996. A strategy for characterizing homogeneous, diffusion-controlled, indoor sources and sinks. *Standard Technical Publication* 1287, American Society for Testing and Materials, 294-304.
2. Mathews T. G., Hawthorne A. R. and Thompson C. V. 1987. Formaldehyde sorption and desorption characteristics of gypsum wallboard. *Envir. Sci. Technol.*, 21, 629-634.
3. Little J. C., Hodgson A. T., and Gadgil A. J. 1994. Modeling emissions of volatile organic compounds from new carpets. *Atmospheric Environment* 28, 227-234.
4. Zhao D. Y., Cox S. C., and Little J. C. 1999. Source/sink characterization of homogeneous, diffusion-controlled building materials. Paper in preparation.
5. Harley R. A. and Cass G. R. 1994. Modeling the concentrations of gas-phase organic air pollutants: direct emissions and atmospheric formation. *Envir. Sci. & Technol.*, 28, 88-98.
6. Hodgson, A. T., Wooley, J. D. and Daisey, J. M. 1992. Volatile Organic Chemical Emissions from Carpets. Final report to the U.S. Consumer Product Safety Commission under Contract CPSC-IAG-90-1256. Lawrence Berkeley Laboratory Report LBL-31916.

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