

# Comparison of Data from an IAQ Test House with Predictions of an IAQ Computer Model

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## Abstract

*One of the objectives of EPA's indoor air quality (IAQ) program is to provide guidance on the impact of indoor sources on IAQ. A computer model, EXPOSURE, was developed to assist in this effort. EXPOSURE calculates pollutant concentration as a function of time for each room of the building. EXPOSURE includes effects of sources, sinks, room-to-room air movement, and air exchange with the outdoors. Several experiments designed to evaluate the impact of indoor sources on IAQ are described. Measured concentrations are compared with concentrations predicted by an IAQ model. The measured concentrations are in excellent agreement with the predictions. The model predictions and the experimental data demonstrate the importance of sinks in determining long-term IAQ.*

## Introduction

One of the objectives of EPA's indoor air quality (IAQ) program is to provide guidance on ways to reduce individual exposure to pollutants. An IAQ model for calculating pollutant concentrations from sources and individual exposure due to the sources was developed to support this objective. The model, called EXPOSURE, is based on the IAQ model INDOOR (Sparks, 1988). EXPOSURE calculates the pollutant concentration as a function of time for each room of the building. The calculated concentrations are used to predict individual exposure.

The concentration time curves predicted by EXPOSURE are compared with those measured in several IAQ test house experiments. This paper does not discuss the exposure predictions.

## The Model

There are numerous IAQ models designed for a wide range of purposes (McNall et al., 1985). Most of the models assume well mixed zones and are based on solution of mass balance equations. INDOOR was developed to provide an easy-to-use generally available IAQ model that allowed rapid analysis of the effects of a wide range of sources, sinks, air cleaners, and ventilation on indoor pollutant concentrations. EXPOSURE was developed to expand the ideas of INDOOR to allow analysis of effects of sources, sinks, air cleaners, and ventilation on individual exposure. EXPOSURE is a multi-zone mass balance model similar to many of the available IAQ

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models. The emphasis of this paper is on the comparison of the model predictions and experimental data so only a brief description of the model is presented here. See Sparks and Tucker (1990) or Sparks (1991) for more information on the model itself.

The model treats a building as a collection of well mixed rooms. A mass balance for room  $i$  of  $N$  rooms gives:

$$V_i \frac{dC_i}{dt} = C_a Q_{a,i} + \sum_{j=1, j \neq i}^{j=N} C_j Q_{j,i} - C_i Q_{i,a} - \sum_{j=1, j \neq i}^{j=N} C_i Q_{i,j} + S_i - R_i \quad (1)$$

where  $C_i$  is the concentration in room  $i$ ,  $C_a$  is the concentration outdoors,  $Q_{a,i}$  is the airflow from the outdoors into room  $i$ ,  $C_j$  is the concentration in room  $j$ ,  $Q_{j,i}$  is the airflow from room  $j$  into room  $i$ ,  $Q_{i,a}$  is the airflow from room  $i$  to the outdoors,  $Q_{i,j}$  is the airflow from room  $i$  into room  $j$ ,  $S_i$  is the source term for pollutants produced in room  $i$ , and  $R_i$  is the removal term for pollutants removed in room  $i$ , including those removed by sinks and air cleaners.

Equation 1 is one of a set of identical equations that must be solved simultaneously in a multiple room model. There are numerous methods for solving this set of equations. EXPOSURE uses a fast discrete time step algorithm developed by Yamamoto et al. (1988) to solve the series of equations. The algorithm is based on the assumption that, for sufficiently small time steps,  $dt$ , the source and sink terms and all neighboring concentrations are constant. The exact solution to Equation 1 can then be used to calculate the concentration at the end of the time step. The exact solution is:

$$C_i = C_i(t_0)e^{-L_i t} + \frac{P_i}{L_i} (1 - e^{-L_i t}) \quad (2)$$

where  $C_i(t_0)$  is the concentration in room  $i$  at time  $t_0$ ,  $t$  is some time greater than  $t_0$ ,  $L_i$  is

$$L_i = \frac{Q_{i,a} + Q_{i,h} + \sum_{j=1, j \neq i}^N Q_{i,j}}{V_i} \quad (3)$$

and  $P_i$  is given by:

$$P_i = \frac{I}{V_i} \left[ \sum_{j=1, j \neq i}^n Q_{j,i} C_j(t) + S_i - R_i + Q_{a,i} C_a + Q_{h,i} C_h \right] \quad (4)$$

where  $Q_{i,j}$  is the airflow from room  $i$  into room  $j$ ,  $Q_{j,i}$  is the airflow from room  $j$  into room  $i$ ,  $Q_{i,a}$  is the airflow from room  $i$  to the outdoors,  $Q_{a,i}$  is the airflow from the outdoors into room  $i$ ,  $Q_{i,h}$  is the airflow from room  $i$  into the HVAC system,  $Q_{h,i}$  is the airflow from the HVAC system into room  $i$ ,  $C_j(t)$  is the concentration in room  $j$  at time  $t$ ,  $C_a$  is the outdoor concentration, and  $C_h$  is the concentration in the HVAC system. Equation 2 is stable for all time steps and is accurate for sufficiently small time steps. (The size of the time step depends on how rapidly concentrations are changing. In most situations a time step between 0.05 and 0.2 hour provides good results.)

### Source Terms

The behavior of sources plays a major role in determining the indoor concentration as a function of time. Sources can be divided into a few idealized classes:

- long-term steady state sources such as moth crystals and air fresheners;
- on/off sources such as heaters;
- decaying or wet sources such as paints, waxes, and stains;
- burst sources such as aerosol products.

The decaying or wet sources are the most difficult source types to simulate both because the emission rates change with time and because there are usually emissions associated with applying the source. For exam-

ple, there are emissions due to the act of painting a wall and emissions due to the paint on the wall. Emissions due to the application of the source are termed application emissions. In many cases, the application emissions are much smaller than the long-term decaying emissions. Research is needed to better define the application phase emissions for many products.

Sources in EXPOSURE are represented by a first order decay equation of the form

$$ER = R_0 \text{EXP}(-kt) + R_A \text{ for } t \leq t_A \\ R_0 \text{EXP}(-kt) \text{ for } t > t_A \quad (5)$$

where ER is the emission rate,  $R_0$  is the initial emission rate,  $k$  is a decay constant,  $R_A$  is the application emission rate, and  $t_A$  is the application time. This source model treats the application phase as a steady state source of limited duration. This type of source term allows simulation of a wide range of source types. If the source is a steady state source,  $k$  is equal to zero. Application phase emissions may be associated with any type of source. The model allows sources to be turned on and off several times during a simulation. On/off sources are simulated by turning the source on and off at specified times. Burst sources are simulated by turning a source on for a very short time.

$R_0$  and  $k$  can be determined from chamber studies (Tichenor, 1989; ASTM, 1991). In many cases all of the emissions are accounted for by  $R_0$  and  $k$  as determined by chamber studies. However, there are sources, such as wood stain, paint, and floor wax, where significant emissions occur while the source is being applied. These application phase emissions are not accounted for by the chamber studies. The value of  $R_A$  can be estimated or at least bounded from large chamber studies, test house studies, mass balance analysis of small chamber studies, or other experiments.

There may also be emissions that are unaccounted for due to the time lag after the source is applied and before it is placed in

the chamber. If the time lag is short, these emissions can probably be neglected. However, if the time lag is long, then the emission rates must be corrected to account for the missed emissions.

Estimates of source terms for several sources are given in Table I. These data are based on experiments conducted in EPA's small chambers and in EPA's IAQ test house. Most of these data have been reported elsewhere, often as a range of values. The values given in Table I represent the best estimate of the emission rates from these sources based on analysis of both chamber emission tests and test house experiments. The major differences between the emission rates shown in Table I and those reported for small chambers are the decay constant for wood stain and the  $R_0$  reported for polyurethane.

The chamber data for wood stain provide a much higher value of  $k$  for wood stain than that found in test house experiments. Follow-up experiments on wood stain emission rates were conducted to verify the test house estimates of  $k$ . Wood samples were stained and the emission rates were determined by continuous monitoring of the weight loss from the wood. The value of  $k$  from these weight loss experiments was consistent with the  $k$  from the test house experiments and the value shown in Table I.

The value of  $R_0$  for polyurethane reported by Tichenor and Guo (1991) is based on waiting 1 hour after the sample was varnished before it was placed in the chamber. Thus their value of  $R_0$  is actually the emission rate at time  $t = 1$  hour, not time  $t = 0$  hours. The value in Table I was obtained by extrapolating the Tichenor and Guo value back to time  $t = 0$  hours.

The application phase emission rates given in Table I are rough estimates based on weight loss experiments and test house experiments. Note that the application phase emissions are much less than long-term emissions. The application time,  $t_A$ , is the time required to apply the source. Consider-

**Table 1** Selected total organic emission factors.

Source	$R_0$ mg/m <sup>2</sup> -h	k l/h	$R_A$ mg/m <sup>2</sup> -h	Fraction emitted	Reference
Wood stain	20,000	0.4	1,000	0.9*	Tichenor and Guo (1991)
Polyurethane	20,000	0.25	1,000	0.8*	Tichenor and Guo (1991)
Wood floor wax	20,000	6	1,000	1.0**	Tichenor and Guo (1991)
Moth cakes	14,000	0			Nelms et al. (1987)
Dry cleaned clothing	1.4	0.044			Tichenor et al. (1990a)

\* From weight loss experiments

\*\* From Tichenor and Guo (1991)

able additional work is necessary to quantify the application phase emission rates and to improve the model of the application phase emissions.

The emission rate data shown in Table 1 for wet sources also include the fraction of the total amount applied that is emitted. This information is needed to correct the emission rates for situations where the amount applied is different from the amount applied during the emission rate experiments. If the application phase emissions are neglected, the total amount of material emitted is the amount applied times the fraction emitted. This must equal  $R_0/k$ . Thus if the amount applied is different from that used in the chamber studies,  $R_0$ ,  $k$ , or both must be corrected. Research is necessary to determine how to make the necessary corrections. The best guidance that can be offered now is to keep  $k$  constant and change  $R_0$ . For example, in a test house experiment, floor wax was applied with an application of 17 g/m<sup>2</sup> compared with an application of 5 g/m<sup>2</sup> used in the chamber studies of Tichenor and Guo. The value of  $R_0$  used to model the wax experiment must be increased to account for the increased application. The application phase emissions are added to the corrected emissions.

### Sink Terms

Research in the EPA test house and in the small chamber laboratory has shown that sinks (i.e., surfaces that act to remove pollutants from the indoor air) play a major role

in determining indoor pollutant concentrations. These sinks may be reversible or irreversible. A reversible sink re-emits the material collected in it and an irreversible sink does not. The sink behavior depends on the pollutant and the nature of the sink. A sink may appear to be irreversible when the pollutant concentration is high and then become reversible when the pollutant concentration is low. Considerable research is necessary to define the behavior of sinks.

The sink model used in EXPOSURE is based on the research described by Tichenor et al. (1991):

$$R_s = k_a C A_{\text{sink}} - k_d M_s^n A_{\text{sink}} \quad (6)$$

where  $R_s$  is the rate to the sink (mass per unit time),  $k_a$  is the sink rate constant (length per time),  $C$  is the in-room pollutant concentration (mass per length cubed),  $A_{\text{sink}}$  is the area of the sink (length squared),  $k_d$  is the re-emission or desorption rate constant,  $M_s$  is the mass collected in the sink per unit area (mass per length square), and  $n$  is an exponent. This model is described by Tichenor et al. as the "Best Fit" model. When  $n = 1$ , the model becomes the Langmuir model presented by Tichenor et al.

The sink rate constant,  $k_a$ , is limited by the rate that pollutant molecules arrive at the surface of the sink. If we assume that transport of pollutant to the surface of the sink is due to diffusion (a reasonable assumption for the low turbulence situations common in indoor spaces where the large eddies keep the

pollutants well mixed in the room but do not disturb the boundary layer),  $k_a$  is the deposition velocity of pollutant molecules hitting the sink surface. Fuchs (1964) shows that the value of  $k_a$  can be calculated from gas kinetic theory as:

$$k_a = \sqrt{\frac{D}{\pi(1h)}} \quad (7)$$

where  $D$  is the diffusivity of the pollutant. Typical values of  $D$  for VOCs are between 0.02 and 0.1  $\text{m}^2/\text{h}$  resulting in typical values of  $k_a$  between 0.08 and 0.2  $\text{m}/\text{h}$ . Small chamber data reported by Tichenor et al. (1991) give  $k_a$  values from about 0.08 to 0.45  $\text{m}/\text{h}$ . While  $k_a$  can be estimated from properties of the pollutant,  $k_d$  and  $n$  must be determined experimentally. Tichenor et al. discuss the problems of determining  $k_d$  and  $n$  from small chamber data and indicate that the small chamber data for  $k_d$  for some pollutant/sink systems do not agree with values estimated from test house experiments.

Best estimates of the sink constants for various materials are given in Table 2. These are generalized sink rate terms and were the terms used in all the model verification studies.

**Table 2** Recommended values of sink constants.

Material	Pollutant	$k_a$ m/h	$k_d$ l/h	$n$
Carpet	General VOC, perchloroethylene	0.1	0.008	1
Carpet	p-dichlorobenzene	0.2	0.008	1
Painted walls and ceilings	General VOC and perchloroethylene	0.1	0.1	1
Painted walls and ceilings	p-dichlorobenzene	0.2	0.008	1

## Experiments

Considerable research has been conducted to verify the model and to validate the approach of using chamber emission factors to predict the pollution concentrations. The bulk of the verification experiments have been conducted in the EPA test house. The test house is a typical three-bedroom ranch style house. The house is unoccupied and unfurnished. The floor plan for the test house is shown in Figure 1.

The house has a natural gas central forced air heating and electric air conditioning system. The house is 11 years old and is well insulated. Exhaust fans are provided in the main bathroom and for the kitchen stove hood. These fans were not used in the experiments discussed below.

The walls between the kitchen and the den and the kitchen and the living room are

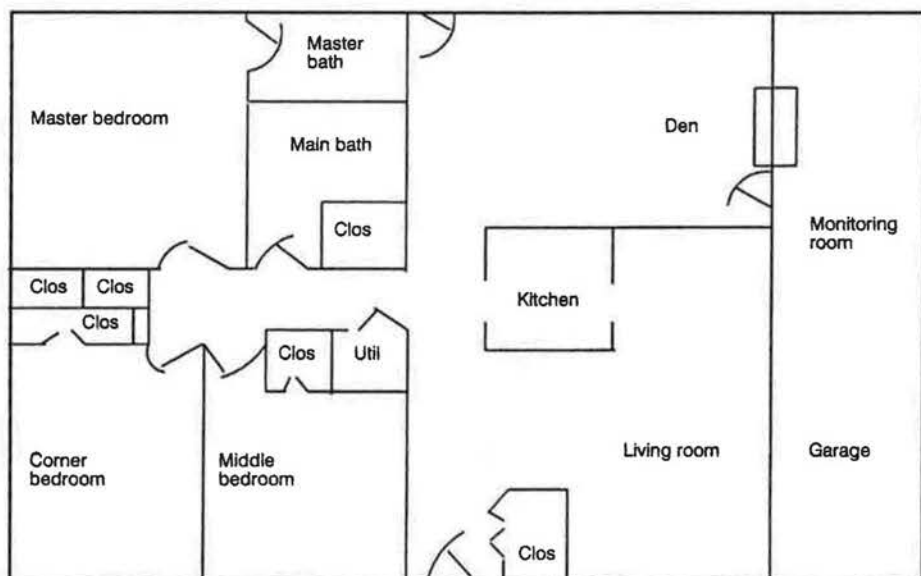


Fig. 1  
Floor plan  
of EPA IAQ  
house.

actually low counters that do not block airflow between the three spaces. Therefore these three rooms can be combined into one large room for modeling. Also the bedroom closets can be considered as part of the bedrooms. Thus for most situations the test house is modeled as a seven-room house. The important characteristics of the various rooms are given in Table 3. The HVAC airflows given in Table 3 are based on measurements made with a vane anemometer.

**Table 3** Model parameters for various rooms in the IAQ test house.

Room	Volume m <sup>3</sup>	Floor area m <sup>2</sup>	Wall area m <sup>2</sup>	HVAC flow m <sup>3</sup> /h
Den	150	63	81	830 (supply) 1760 (return)
Hall	12	5	2	125 (supply)
Middle bedroom	34	14	27	300 (supply)
Corner bedroom	42	18	36	60 (supply)
Master bedroom	10	4	8	120 (supply)
Master bath	12	5	7	

### Test House Airflows

A set of experiments to better define the test house airflows and to determine the reasonableness of the values used in the model were conducted. During these experiments the air handling system flows were measured. Flow visualization studies to determine the nature of the in-room and room-to-room mixing were conducted with neutral density balloons and with neutral density helium bubbles.

The first set of airflow measurements was taken in conjunction with experiments on the impact of moth cake on IAQ. The air conditioning vents in the middle bedroom were closed during these experiments. Thus the airflows for the moth cakes experiment were different from the airflows in other experiments where the air conditioning vents in all rooms were open. The flows for the moth cake experiments measured in the air handling system are shown in Table 4. The

HVAC airflows for other experiments are given in Table 3.

The airflows between rooms were measured. The model calculations are based on the assumption that the HVAC flow into all rooms, except the master bath, flows from the room into the hall. The HVAC flow into the master bathroom flows from the master bathroom into the master bedroom and then into the hall. The flow visualization studies showed that there were small mixing airflows on the order of 5-10 m<sup>3</sup>/h from the hall into the various rooms. These small airflows moved counter to the bulk airflow, driven by the HVAC flows, that moved from each room to the hall.

**Table 4** Measured airflows in test house for moth cake experiments.

Room	Measured airflow m <sup>3</sup> /h
Den	679
Middle bedroom	38
Corner bedroom	278
Master bedroom	280
Main bathroom	120
Master bathroom	280
Hall (HVAC return)	1510

When the moth cake experiment was modeled, it was necessary to assume that the flow from the corner bedroom closet (the location of the moth cakes) was much larger than expected. Therefore, hot wire anemometer measurements were made of the airflow velocities through the cracks under and around the closet door. These measurements showed that the airflow into and out of the closet was between 6 and 9 m<sup>3</sup>/h. This corresponds to a flow of about 2 to 5 closet volumes per hour (the closet volume is about 2 m<sup>3</sup>). This is the same value of the flow necessary to make the model predictions agree with the experimental data. The flow visualization experiments also indicated that there was a substantial airflow into and out of the corner bedroom closet even when the closet door

was closed. The visualization studies indicated that there was flow between the corner bedroom closet and the hallway and the corner bedroom closet and the master bedroom.

Tracer gas experiments were conducted to estimate the room-to-room airflows when the air handler was off. These experiments showed that the room-to-room airflows were of the same order as the room-to-room airflows with the air handler on. Model calculations show that the airflows would have to be reduced by a factor of five or more to significantly affect pollutant transport from room to room.

Blower door and tracer gas studies were conducted to determine the air exchange between the house and the outdoors. These experiments covered a wide range of conditions of house operation (e.g., air handler on/off, windows open/closed) and a range of temperature differences between indoors and outdoors. In addition to these air exchange specific measurements, air exchange measurements were routinely conducted as part of each experiment conducted in the test house. For most of the year the air exchange between the house and the outdoors ranges from 0.3 to 0.5 air changes per hour (ACH). For some experiments conducted in the spring, air exchange rates between 0.2 and 0.3 ACH were measured. The tracer gas data were used to develop a correlation between air exchange, ACH, the temperature difference between the indoors and outdoors,  $DT$ , and the wind speed,  $WS$ , measured at the test house:

$$ACH(\text{perhour}) = 0.2044 + 0.0124DT(^{\circ}c) + 0.0243WS(m/s) \quad (8)$$

This correlation was used to supplement tracer gas measurement.

Whenever possible, airflows within the house should be determined by direct observation instead of by tracer gas measurements. The use of tracer gas measurements introduces circular logic into the model verifica-

tion process. When tracer gas measurements are made, a model similar to the model being verified is used to estimate the airflows from the tracer concentration measurements. These airflows are then used in a model to estimate pollutant concentrations. Even though the models may not be identical, the basic assumptions used in the various models are essentially the same. The practice followed in the test house experiments is to make direct measurements whenever possible, especially when the values necessary to provide agreement between the model and the experimental data seem unusual, for example in the moth crystal experiment. It must be noted, however, that tracer gas experiments remain a valuable tool for estimating indoor to outdoor and room-to-room airflows. Additional house characterization tests were conducted and are reported by Jackson et al. (1987).

Five different sets of experiments are discussed below. The five experiments cover a wide range of sources. The experiments were conducted to determine the feasibility of using chamber emission data and the model to predict test house pollutant concentrations.

### Moth Cakes

Five moth cakes were placed in the corner bedroom closet of the test house. The moth cakes were laid on the shelves, providing an area for emission of 570 cm<sup>2</sup>. The air conditioning system operated continuously for the entire experiment. The test house temperature was maintained at 25°C. The relative humidity was 50 ± 10 % throughout the test. The p-dichlorobenzene emission rate from moth cakes as determined by Nelms et al. (1987) was 1.4 mg/cm<sup>2</sup>-h. The actual amount of p-dichlorobenzene emitted was determined by weighing the moth cakes before they were placed in the closet and after they were removed from the closet. The emission rate calculated from the weight loss was 1.36 mg/cm<sup>2</sup>-h. Input data for the moth cakes modeling are given in Table 5.

Concentrations of p-dichlorobenzene were measured in the closet, in the corner bedroom, in the master bedroom, and in the den. Two sets of p-dichlorobenzene measurements were made. One set of measurements was made by collecting samples in airtight syringes. The syringe samples were then injected directly into a gas chromatograph (GC) with an electron capture detector (ECD). The second set of samples was collected by adsorbing samples on Tenax. The Tenax was desorbed and the resulting gas was analyzed with the same GC/ECD system used to analyze the direct injection samples. The samples were collected once a day for 4 days. The first measurement was made 3 days after the moth cakes were placed in the closet. The moth cakes were removed from the closet after 10 days, and p-dichlorobenzene measurements were made for an additional 4 days (Clayton et al., 1988; Tichenor et al., 1990b).

The comparison of the model predictions

and the measured p-dichlorobenzene concentrations is given in Figure 2. The impact of the sinks on the p-dichlorobenzene concentration in the house is of special interest. A mass balance analysis of the p-dichlorobenzene test house data that neglects sinks can account for about 60% of the total mass emitted. This missing mass is the mass that is collected by the sinks (Tichenor et al., 1990b). The sinks reduce the concentration by about 50% during the time that the moth cakes are in the test house.

Re-emissions from the sinks cause a moderately high p-dichlorobenzene concentration in the test house for the entire experiment. In fact, p-dichlorobenzene was still detectable in the test house more than 2 years after the end of the experiment.

The experimental data and the model predictions show that the small chamber emission factors for p-dichlorobenzene can be used with the model to estimate p-dichlorobenzene concentrations in a building.

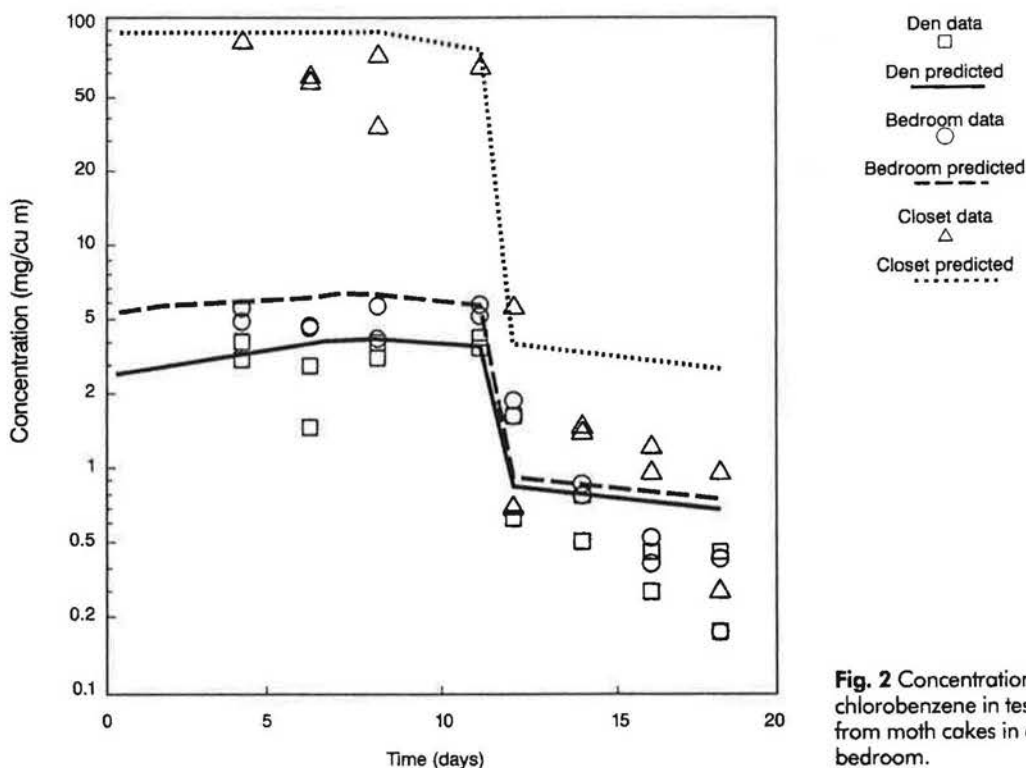


Fig. 2 Concentration of p-dichlorobenzene in test house from moth cakes in corner bedroom.



**Table 5** Model input for analysis of moth cake experiment.

Source strength = 1.4 mg/cm <sup>2</sup> -h (from Nelms et al., 1987)
Air exchange with outdoors = 0.35 ACH (SF <sub>6</sub> data)
Air exchange between closet and bedroom = 9 m <sup>3</sup> /h (hot wire measurement)
Air circulation due to air handling system is as measured (see Table 4)
Air exchange with outdoors is evenly divided between rooms.
Sink k <sub>c</sub> = 0.2 m/h
Sink k <sub>d</sub> = 0.008/h

### Kerosene Heater Experiments

The particulate emissions from two types of kerosene heater were evaluated in the test house. In each experiment the heater was placed in the den. The heater was operated with a window in the den open 5 cm. The particulate emission factors for use in the model were determined from large chamber studies (White et al., 1987). Particulate meas-

urements were made in the den, the master bedroom, and the corner bedroom. The samples were collected on Pallflex filters using 4 cfm (113 L/m) samplers. Filters were changed every 6 h and the total sampling time was 12 h. SF<sub>6</sub> measurements showed that the air exchange with the outdoors was 0.5 ACH. The sink rate constant was based on the deposition velocities for small particles calculated from Fuchs (1964). Room-to-room airflows were assumed to be as shown in Table 6. The comparison between measurements and experiments is shown in Table 7. The experimental data and sampling details for the kerosene heater experiments are reported in Jackson et al. (1988) and Tichenor et al. (1990b).

### Dry Cleaned Clothing

The impact of dry cleaned clothing on IAQ and possible mitigation options were evaluated in a series of experiments in the test

**Table 6** Room-to-room airflows used kerosene heater modeling, flows in m<sup>3</sup>/h.

From/to	Den	Hall	Middle bedroom	Corner bedroom	Master bedroom	Master bathroom	Main bathroom
Den		600	0	0	0	0	0
Hall	600		100	100	120	0	30
Middle bedroom	0	100		0	0	0	0
Corner bedroom	0	100	0		0	0	0
Master bedroom	0	120	0	0		30	0
Master bathroom	0	0	0	0	30		0
Main bathroom	0	30	0	0	0	0	

**Table 7** Comparison of predicted and measured particulate concentrations from kerosene heater experiments in test house.

Heater type	Location in house	Predicted $\mu\text{g}/\text{m}^3$	Measured $\mu\text{g}/\text{m}^3$	Std. dev. of measurements $\mu\text{g}/\text{m}^3$ (%)
Convective/Radiant	Den	60	68	17 (25)
	Master bedroom	52	38	20 (53)
Radiant/Radiant	Den	285	288	42 (15)
	Master bedroom	235	252	53 (21)

house. The clothing was taken to a commercial dry cleaner where it was dry cleaned along with the cleaner's normal business. The clothing was placed in a plastic bag per normal industry practice. The cleaned clothing was picked up from the cleaner as soon as possible after cleaning was completed and transported to the test house and hung in the closet of the corner bedroom and the closet doors were closed. The HVAC system was operated normally (i.e., in an on/off cycle determined by the need for air conditioning). A full description of the experiment is given by Tichenor et al. (1988).

The test series consisted of two experiments where the clothing was stored in the closet with the plastic bag off; one experiment where the clothing was stored in the closet with the plastic bag on; and one experiment where the clothing was aired out for 4 hours prior to being placed in the closet.

The source term for the dry cleaning experiment was determined from small chamber experiments. Test house concentrations were determined by collecting samples in gastight syringes. The samples were then immediately injected into a GC with an ECD. The GC was calibrated with liquid samples

over a range of perchloroethylene concentrations. The GC was calibrated every morning before any samples were taken, and its performance was checked every 3 h during the day by injecting two liquid perchloroethylene standards. The sample chromatograms had well defined and easily identifiable perchloroethylene peaks.

The air exchange rate between the house and the outdoors was determined on the first day of each test by use of SF<sub>6</sub> tracer gas.

Details of the chamber and test house experiments are given by Tichenor et al. (1990a).

A preliminary experiment was conducted to provide an estimate of the sink effect for the perchloroethylene. The sink experiment indicated that the sink was re-emitting. Small chamber experiments to better define the sink were conducted later (Tichenor et al., 1991). These experiments showed that there was a significant difference between the desorption rates for carpet and other surfaces in the test house. These differences in sink behavior were used in the modeling.

Because the source term was not steady and the sink was re-emitting, the dry cleaning experiment provided a more complicated test of the model than did the moth cakes

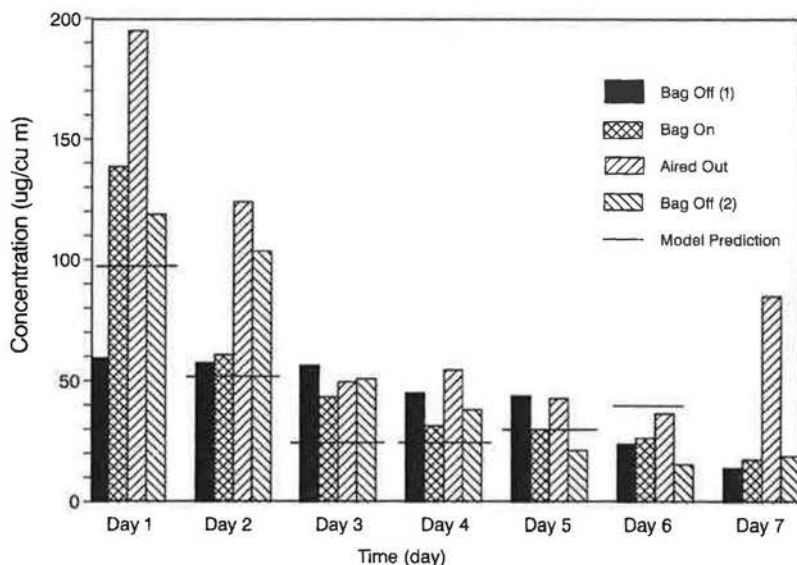


Fig. 3 Comparison of model predictions and measurements for dry cleaned clothing experiment.

and kerosene heater tests. The results of the comparison between the model and experimental data are shown in Figure 3.

Tichenor et al. (1990a) report that the variability between experiments is probably due to normal variations in the dry cleaning process. The model predictions are in fair agreement with the experimental data for these experiments. Uncertainty in the source emission rates is the major cause of uncertainty in the model analysis.

### Aerosol Spray Product

Because aerosol products are commonly used indoors and because the amount of material released by a single use of the product can be quite large, a series of experiments to determine the impact of aerosol product use on IAQ was conducted. An aerosol spot remover was chosen to represent the behavior of aerosol products. Note that the purpose of these experiments was to define the behavior of aerosol products typified by high release of material in a very short (a few seconds) time. Spot remover was selected as the aerosol product because of the ease of analyzing for perchloroethylene.

The chemical composition of the product was determined by GC analysis. The spot remover was 20% perchloroethylene. The amount of perchloroethylene emitted was determined by weighing the can before and after each use and the chemical composition information. The application time was less than 5 seconds. The spot remover was applied to a cloth to simulate actual use of the product.

In the experiment the spot remover containing perchloroethylene was used in the main bathroom and measurements of perchloroethylene made in the den, main bathroom, and master bedroom. Gas samples were obtained using gastight syringes. The syringe samples were then injected directly into the GC with ECD to determine the perchloroethylene concentration. As in previous experiments the GC was calibrated with liquid standards over a range of perchloroethylene concentrations daily and its performance was checked periodically.

Information on sinks developed in the small chambers was incorporated into the model for these experiments.

The results for the den are shown in Figure 4.

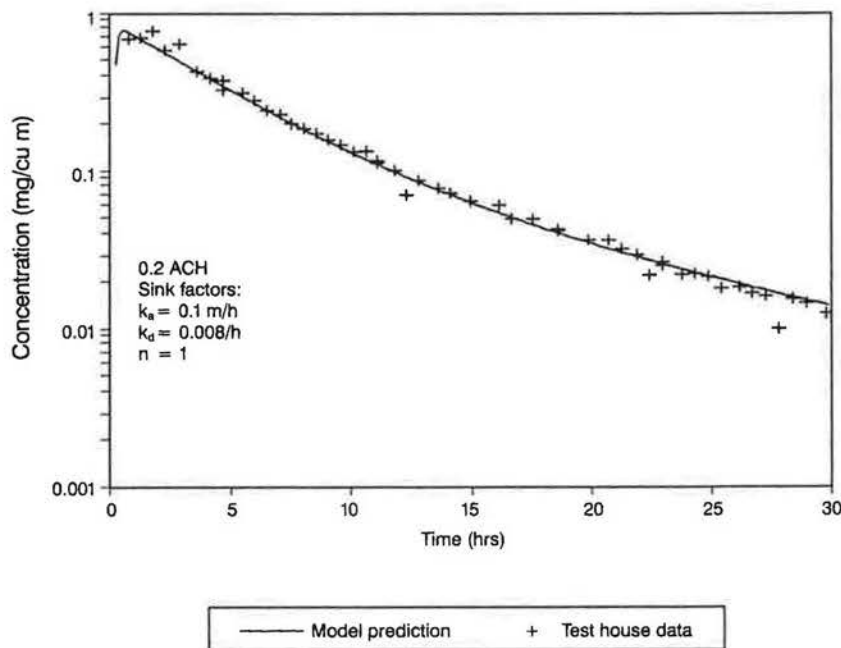


Fig. 4 Perchloroethylene concentration in den from use of spot remover in main bathroom.

## Wet Products

Wet products are defined as products with a high initial emission rate that rapidly decays. Stain, floor wax, and paint are examples of wet products.

A set of experiments was designed to determine the effects of various wet products on IAQ. For the experiment a 6 m<sup>2</sup> wood floor was stained with a wood stain, then varnished, and then waxed. Varnishing did not begin until the total VOC due to staining

had decayed to background. And waxing did not begin until the total VOC due to varnishing had decayed to background. The air handler system was on during this experiment and all windows were closed. The VOC concentration was determined using GC flame ionization detector (FID) analysis and is reported as toluene. Air exchange with the outdoors was determined with CO tracer gas measurements several times during the experiment. Inside and outdoor temperatures

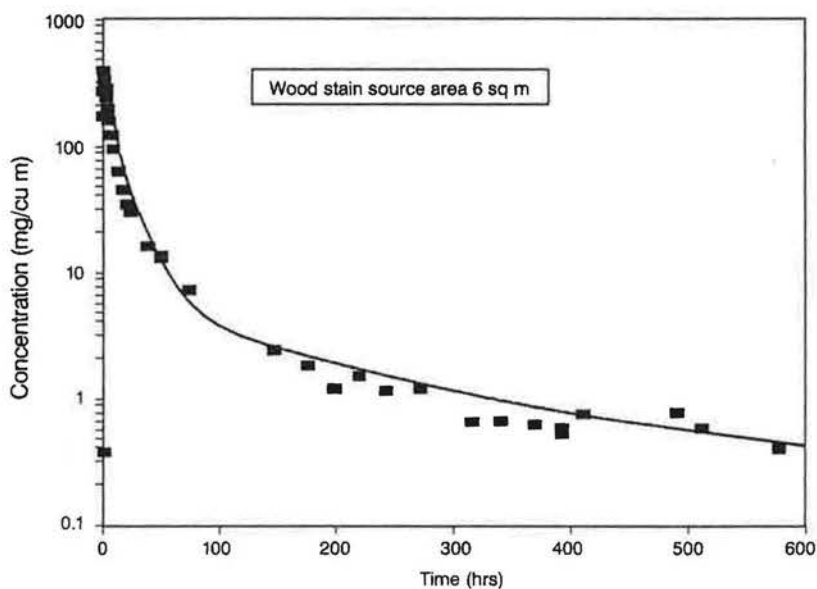


Fig. 5 Comparison of predictions and measurements of VOC concentration in den from use of wood stain.

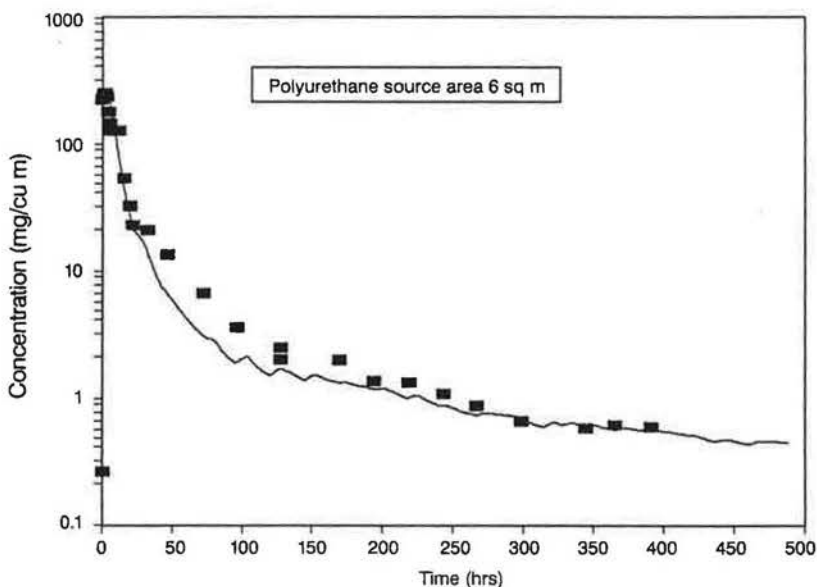


Fig. 6 Comparison of predictions and measurements of VOC concentration in den from use of polyurethane varnish.

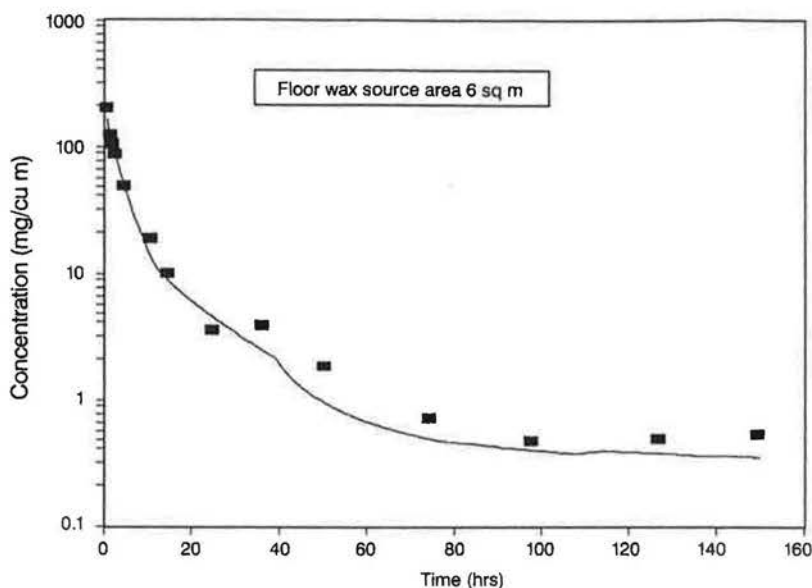


Fig. 7 Comparison of predictions and measurements of VOC concentration in den from use of wood floor wax.

and wind speed were monitored for these experiments. These data were used to calculate air exchange rates during periods when direct tracer gas measurements of air exchange were not made.

The emission rates for this experiment were calculated using the constants given in Table 1. The value of  $R_0$  was adjusted to account for different applications of product. The sink rate constants developed in chamber studies and previous test house studies were used in the modeling. The model calculations are based on hourly air exchange rates calculated from Equation 8. The results of the modeling for total hydrocarbons in the den for the three products are shown in Figures 5, 6, and 7. Predictions and measurements for other rooms are quite similar and are not shown. Note that the presence of the re-emitting sink causes concentrations to remain high for well over 14 days.

### Quantitative Comparison of Model and Data

Because there is little guidance in the technical literature on the evaluation of IAQ models, it seems reasonable to apply evaluation concepts from the outdoor air quality litera-

ture to evaluating EXPOSURE. These evaluation concepts include qualitative comparisons of fit between model predictions and data and quantitative statistical criteria. The comparisons between model predictions and experimental data shown in Figure 2 through 7 provide qualitative indications that EXPOSURE provides reasonable agreement with experimental data. The quantitative indications of how well the model fits the data are discussed in this section.

Several different methods of analyzing the agreement between the model predictions and experimental data are possible (Hanna, 1988). The first set of methods discussed below assess the general agreement between the model and the data. The second set of methods assess the possible bias in the model.

Three methods used to assess the general agreement between the model predictions and the experimental data are as follows.

The absolute value of the average fractional residual between the observed and predicted concentration; the correlation coefficient between observed and predicted concentration; and the normalized mean square error. Two methods used to assess the possible bias in the model are the normalized

or fractional bias and the bias based on the variance of the concentrations.

The absolute value of the average fractional residual between the measured or observed concentration,  $c_o$ , and the predicted concentration,  $c_p$ , is given by:

$$\frac{\sum_{i=1}^n \text{abs} \left[ \frac{C_{pi} - C_{oi}}{C_{oi}} \right]}{n} \quad (9)$$

The absolute value of the fractional residual gives a general sense of how well the model fits the data. The absolute value of the fractional residual for an ideal model would be of the same order as the experimental error in the data.

The correlation coefficient between observed concentration,  $c_o$ , and predicted concentration,  $c_p$  is given by:

$$\frac{\sum [(C_o - \bar{C}_o) \cdot (C_p - \bar{C}_p)]}{\sqrt{[\sum (C_o - \bar{C}_o)^2] \cdot [\sum (C_p - \bar{C}_p)^2]}} \quad (10)$$

The correlation coefficient ranges from -1 to 1, with 1 indicating a strong direct relationship, 0 indicating no relationship, and -1 indicating a strong inverse relationship.

The normalized mean square error (NMSE) is given by:

$$\frac{(\overline{C_p - C_o})^2}{(\bar{C}_o \cdot \bar{C}_p)} \quad (11)$$

The NMSE has a value of 0 when there is perfect agreement for all pairs of  $c_p$  and  $c_o$ , and tends toward higher values as  $c_p$  and  $c_o$  differ. For example, NMSE is near 0.2 for differences between  $c_p$  and  $c_o$  of 50%; NMSE is near 0.5 for differences of about 100%; and NMSE is near 8 for differences of an order of magnitude.

The least squares best fit regression line between  $c_p$  and  $c_o$  provides useful information on how well the model fits the data. The ideal line has a slope of 1, an intercept of 0, and a regression  $r^2$  of 1. The slope,  $b$ , of the line is given by:

$$b = \frac{\sum [(C_o - \bar{C}_o) \cdot (C_p - \bar{C}_p)]}{\sum [(C_o - \bar{C}_o)^2]} \quad (12)$$

and the intercept,  $a$ , is given by:

$$a = \bar{C}_p - b \cdot \bar{C}_o \quad (13)$$

The methods used to assess model bias are:

The normalized or fractional bias (FB) is given by:

$$\frac{2 \cdot (\bar{C}_p - \bar{C}_o)}{\bar{C}_p + \bar{C}_o} \quad (14)$$

FB ranges from -2 to 2 with a value of 0 indicating perfect agreement.

A similar index of bias (FS) based on the variance of the concentrations is given by:

$$\frac{2 \cdot (\sigma^2 C_p - \sigma^2 C_o)}{\sigma^2 C_p + \sigma^2 C_o} \quad (15)$$

The model verification statistics are given in Table 8. The statistics shown in Table 8 indicate that the model predictions are generally quite good. There is no indication of bias in the predictions. The predictions are highly correlated with the measurements; the slope of the regression line is close to 1 for all cases and the intercept is less than 10% of the average measured concentration for all cases. Except for the moth cake experiment the average absolute relative residual is less than 25% for all experiments. Also except for the moth cake experiment the maximum relative residual for all the experiments is 54%.

The large error for the moth cake experiment comes from three data points in the closet, both Tenax and direct injection data for day 6 and the Tenax data for day 8. There is no reason to reject these points, so they were used in the comparisons in Table 8.

A review of the residuals between predicted and measured concentrations for all the experiments indicates that the uncertainty in

**Table 8** Model verification statistics.

Experiment	Average absolute value of relative residual	Correlation coefficient	NMSE	FB	FS	Regression slope	Regression intercept	Regression $r^2$
Aerosol	0.1	0.99	0.05	0.093	0.22	0.9	0	0.98
Floor wax	0.17	0.96	0.19	-0.07	-0.28	1.04	-0.19	1.00
Moth cakes (all data)	0.47	0.97	0.57	0.23	0.22	1.2	0.54	0.89
Polyurethane	0.22	0.93	0.28	0.12	0.21	1.03	7.1	0.86
Wood stain	0.21	0.95	0.16	0.03	0.08	0.95	0	0.90

the source emission rate is probably the major source of error in the model predictions. The maximum residuals occur in the first few hours when the concentration is dominated by the source.

## Conclusions

Based on the qualitative and quantitative comparisons between model predictions and test house measurements, it appears that EXPOSURE does a good job of predicting indoor pollutant concentrations. The quality of the predictions provided by EXPOSURE, as is the case for any model, depends on the quality of the input data. Source emission data from chamber studies are adequate for modeling purposes.

Additional research on model verification for a wider range of sources and a wider range of indoor environments is planned. Experiments in multi-story and commercial buildings are planned as part of this effort.

## Model Availability

The model Sparks (1991), including disks for MS-DOS computers and the manual, is available from the National Technical Information Service (NTIS), in Springfield, VA.

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