RISK: Health, Safety & Environment (1990-2002)

Volume 11 | Number 2 Article 6

March 2000

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Introduction

The purpose of this research project was to determine the accuracy of a frequently used indoor air quality personal computer (IAQPC) model by comparing the measured airborne concentrations of a pesticide in a single residence building to those air concentrations predicted by the IAQPC model. A licensed pest control operator sub-slab injected "Equity®," a trade formulation of chlorpyrifos and propylene glycol manufactured by Dow Elanco Inc., under a Florida residence. This study modeled the active ingredient, chlorpyrifos. In the area of risk assessment and exposure estimation, models are frequently used to reconstruct past exposures, largely for litigation purposes. Although these models are often presented and relied upon for reconstructing various exposures, they have rarely been validated with field data.

Background

For this project, we used the newest version of three IAQPC models developed by the Environmental Protection Agency (EPA). These models are variations of the original, and were refined with each successive model. Historically, the multi-compartment model solves parabolic partial differential equations, such as the diffusion equation. The IAQPC model is an adaptation of an original multi-compartment model that predicted emission concentrations.[1] The purpose of these

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1 *See* Jan Christiansson, et al., *Emission Of VOC's From PVC Flooring — Model For Predicting The Time Dependent Emission Rates And Resulting Concentrations In The Indoor Air*, 2 Proc. of Indoor Air. 389 (1993).

multi-compartmental models is to predict, within a given room the emission concentration of volatile compounds from specified materials without having to carry out extensive field measurements.

Recently, a published study used this version of the IAQPC model to predict occupant exposures to volatile ingredients in insecticidal formulations.[2] The formulations were spread by broadcast sprays and perimeter-room (crack and crevice) insecticide applications in four unoccupied apartments in New Jersey. The study reported that the measured volatile organic compounds (VOC) concentrations were comparable to those predicted by the model for the broadcast application, apparently validating the IAQPC model. However, the model has never been tested for predictive accuracy in subterranean pesticide injection, as in this study.

The EPA Indoor Air Quality Model was used to simulate the concentrations of VOCs including xylene, methyl ethyl benzene, and cumene.[3] Based on this model, increased ventilation should have greatly decreased the VOC levels following the application of broadcast and aerosol fogger-type insecticides marketed for indoor applications. Yet, our field data did not support the predicted decrease in VOC concentrations with increased ventilation.[4]

Wright and Leidy performed several retrospective field measurement studies of the airborne and soil concentrations of chlorpyrifos in homes that were monitored up to eight years after the termiticide application.[5] Wright and Leidy showed that following application, air samples from treated houses sited on sandy soils had significantly elevated airborne concentrations of chlorpyrifos compared

2 *See* John A. Bukowski, et al., *Air Levels of Volatile Organic Compounds Following Indoor Application of an Emulsifiable Concentrate Insecticide*, 30 Envtl. Sci. Tech. 2543 (1996).

3 *See* John A. Bukowski & Leroy W. Meyer, *Simulated Air Levels of Volatile Organic Compounds Following Different Methods of Indoor Insecticide Application*, 29 Envtl. Sci.Tech. 673 (1995).

4 *See id.*

5 *See* C.G. Wright, R.B. Leidy & H.E. Dupree, Jr., *Chlorpyrifos in the Ambient Air of Houses Treated for Termites*, 40 Bull. Envtl. Contam. Tox. 561 (1988); C.G. Wright, R.B. Leidy & H.E. Dupree, Jr., *Chlorpyrifos in Air and Soil of Houses Four Years after Its Application for Termite Control*, 46 Bull. Envtl. Contam. Tox. 686 (1991); C.G. Wright, R.B. Leidy & H.E. Dupree, Jr., *Chlorpyrifos in Air and Soil of Houses Eight Years after Its Application for Termite Control*, 52 Bull. Envtl. Contam. Tox. 131 (1994).

to those sited on clay soils. According to Wright and Leidy, factors including room location, method of construction, temperature and relative humidity made no difference in the chlorpyrifos levels in ambient air inside the houses. Their conclusions about the relation between these factors and chlorpyrifos levels do not agree with the IAQPC model. Some of these factors are variables of the emission rate, which is an important input in this model. If the emission rate changes in the computer model then the predicted concentrations will vary.

Experimental Setup

Air Sampling Procedure for Chlorpyrifos

This project used OSHA Versatile Samplers (OVS-2) by SKC Inc. (catalog number 226-30-16) to collect chlorpyrifos air samples.[6] We calibrated the pumps before and after sampling with a Gillian Calibrator at one liter per minute (1 LPM). After sampling for approximately 500 minutes at a height of between 1.2 and 1.52 meters above floor level, we removed the samples, sealed each with plastic end caps and put them into a cooler containing dry ice. Each sample set contained seven air samples and two blanks, a "field" and a "laboratory" blank. The field blank was uncapped and recapped on site without any air drawn through the sample, and then traveled with the samples. The laboratory blank remained sealed at all times prior to analysis.

Recommended Air Volume and Sampling Time for Chlorpyrifos

This study used the National Institute of Occupational Safety and Health (NIOSH) Analytical Method 5600 for chlorpyrifos for its analyses, with the exception of using the more sensitive Electron Capture Detector (ECD) in place of the Flame Photometric Detector (FPD). Based on previous studies done by Wright and Leidy, about 0.1 $\mu g/m^3$ air concentration would be expected immediately after termiticide application. The ECD's limit of detection is 0.01 $\mu g/m^3$. Each sample in this study used air volume of approximately 500 liters.

The U.S. EPA IAQPC Model for Windows

The National Risk Management Research Laboratory prepared the IAQPC Model for the Office of Air and Radiation at Research Triangle Park. This computer program predicts the concentrations of

6 SKC Inc. Catalog.

chemicals found in indoor air environments over time. A file contains fixed information about the building (i.e., the number of rooms, the room dimensions, and the room arrangement). Scenariao files contain variable information, such as emission sources, sinks, air exchanges and room-to-room air flows.

This model operates on two major assumptions: First, the air in each *room* is assumed to be well mixed. This does not imply that all air within the building is uniformly mixed; concentrations may vary among rooms. Second, conservation of mass is assumed, meaning that the amount of air entering a room must equal the amount of air leaving the room and the amount of outdoor air entering the building must equal the amount of air leaving the building.

Also, the requires the following information: interior volume and area of the home; the ventilation rate of heating, ventilation, and air-conditioning (HVAC) system in each room; the number of rooms and their relative locations; overall exchange rates between indoor and outdoor air; initial, background pollutant concentrations in each room and outdoors; room-to-room air flows; number of specific air contaminant sources in the house and their locations; the emission rate and the decay constant of the specific air contaminant. Although most of this information may be accurately measured, the air exchange rate with outdoors, room-to-room air flows, number of specific air contaminant sources, and emission and decay constants are based on generally accepted assumptions or on other published data.

After measuring the interior dimensions of the home and determining the number of adjacent rooms (as specified in the IAQPC procedures manual), we calculated the overall air exchange rate using the carbon dioxide (CO_2) concentration decay method. We calculated the room-to-room air flows using a calibrated Alnor Flow Hood. The emission was entered in the model[7] as:

$$R(t) = R_0 \exp(-k_0\, t) + R_1 \exp(-k_1 t)$$

where $R(t)$ = the emission rate at time t, mg/h/m^2; k_0 = the first order decay constant, 1/hour; R_0 = the initial emission rate mg/h/m^2; and t = time, in hours.

[7] *See* Leslie Sparks, *Computer Model for Analysis of Indoor Air Pollutant Sources on Individual Exposures, Risk Version 1.0*, EPA Report EPA-600/R-96-037, U.S. EPA: Research Triangle Park, NC, 1996.

The test structure was 95% carpet over concrete slab. We obtained the emission rate and decay constant from the EPA,[8] making

$R(t) = 8.0 \exp(-0.02*t) + 0.7 \exp(-0.003*t)$.

Methodology for Measuring Air Exchange Rate

We used a CO_2 tracer gas method to determine residential home air exchange rates. We asked the occupants to leave in order to eliminate the human sources of CO_2. We next sampled the CO_2 concentrations outside of the house with a calibrated Q-Trak model 8551 CO_2 monitor manufactured by TSI, Incorporated. One hour after the residents left the building, we measured and recorded the CO_2 concentrations in each room.[9] To determine the effects of CO_2 generated by the person monitoring the CO_2 concentrations inside the residential home, we then monitored the CO_2 concentrations for 120 minutes following the entry of the monitor. No measurable effects were noted as a result of the CO_2 generated by the person monitoring the CO_2 concentrations. We then released CO_2 gas into the air conditioning's return register until CO_2 concentrations inside the house uniformly reached 2000 ppm. We set all fans and air handlers in the house for continuous operation to mix the CO_2 uniformly. After the CO_2 concentrations stabilized, we measured base line concentrations throughout the residence. For the next 120 minutes, we measured the concentrations every ten minutes, at locations shown in Figure 1. To calculate the air exchanges with outdoor air, we adjusted the CO_2 concentrations in each room to the fraction of the total volume of the house it occupied. After calculating the adjusted CO_2 concentrations, we used the decay method to calculate the air exchange rate,[10] using

$\ln C(\eta) = \ln C_0 - I\theta$

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8 Based on the emission rate of chlorpyrifos on carpet at 22°C and 50% relative humidity. Personal Communication with Leslie Sparks, Senior Chemical Engineer, U.S. EPA, National Risk Management Research Laboratory, Air Pollution Prevention and Control Division, Indoor Environment Mgmt. Branch, Research Triangle Park.

9 *See* Andrew Persily & W. Stuart Dols, The Relation of CO2 Concentration to Office Building Ventilation, Air Change Rate and Air-tightness in Buildings, 77-92 (Sherman, Ed., 1990); *see also* R. A. Grot, A Low-Cost Method for Measuring Air Infiltration Rates in a Large Sample of Dwellings, Building Air Change Rate and Infiltration Measurements, 50-59 (C. M. Hunt, J. C. King & H. R. Trechsel, Eds., 1980).

10 *See* S. A. Sherif et al., 1993 ASHRAE Handbook Fundamentals, I-P Edition (Am. Soc'y Heating, Refrigerating and Air Conditioning Engineers, Inc., 1993).

where I = Air exchange rate; C_0 = Initial concentration; $C(\eta)$= Tracer gas concentration at time η, and θ = Time

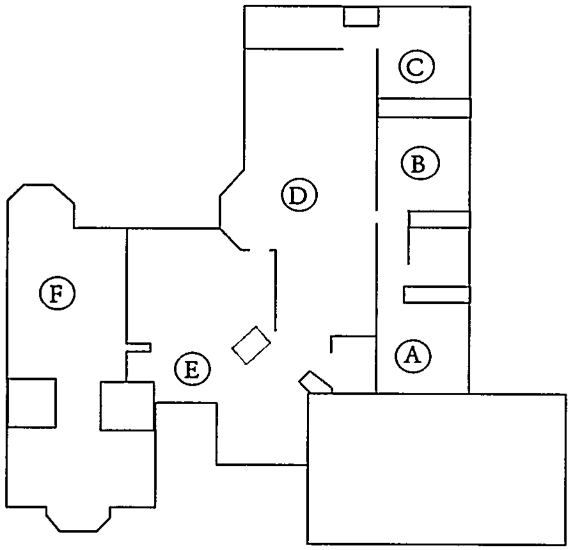
Statistics

To determine the significant differences between the field data and the computer model data, we used the paired sample t-test method. The level of significance: $\alpha = 0.05$.[11]

Description of Treated House and Termiticide Application

In February 1997, a subterranean chlorpyrifos treatment was applied to a one story, single family residence in Thonotosassa, Florida. See Figure 1.

Figure 1[12]
Where (CO_2) Concentrations Were Measured During Air Exchange Rate Determination



The house contained approximately 193m^2 (582m^3 volume) of living area, consisting of four bedrooms, three bathrooms, a living room and attached dining area, family room, kitchen, laundry room and two walk-in closets. Exterior sliding glass doors were located in three of four bedrooms, the living room and the family room. Except for the kitchen, each room had windows or sliding glass doors. These

[11] *See* Irwin R. Miller, John E. Freund & Richard Johnson, **Probability and Statistics For Engineers** (4th ed. 1990).

[12] A is Bedroom 1; B is Bedroom 2; C is Bedroom 3; D is the Family Room; E is the Living Room; and F is Bedroom 4.

accounted for about $53m^2$ of exterior walls. The house was furnished for normal occupancy, with ceiling and walls composed of drywall finished with paint and/or breathable wallpaper. The family room had a fireplace with a closed damper and closed glass doors at the front.

The HVAC system was a split system heat pump, with the evaporating coil in the attic. The house is served by eighteen supply registers and six return registers. During this study, we kept all windows closed, ran the HVAC fan at constant speed and minimized traffic in and out of the house. We conducted air measurements in the four bedrooms, the family room and the living room.

This house had a slab on compacted "yellow sand" built-up grade foundation with footers deeper than one foot. In accordance with the EPA-registered label for the pesticide, Equity®[13], a dilute solution was applied at a rate of four gallons per ten linear feet. Holes were drilled around the perimeter to form a continuous termiticide perimeter barrier. These holes were spaced at 0.6 meter intervals, approximately 0.4 meters deep to reach compacted sand behind the block footer. After the background sampling, a licensed pest control operator applied approximately 130 gallons of a 1% chlorpyrifos solution.

Discussion

Table 1 details the measured airtflows of each room. The outdoor sampler was located about one meter from the outer wall of the house. Table 2 and Figure 2 show that the outdoor chlorpyrifos concentration was highest, 0.416 $\mu g/m^3$, during termiticide application. During each termiticide injection, some chlorpyrifos was spilled on the ground between and around the holes. This could account for elevated outdoor concentration near the house as measured during application. Evaporation from the treated gravel around the perimeter and from spills, plus the 48 hour delay to plug the holes probably account for the 0.178 $\mu g/m^3$ outdoor concentration 24 hours post-application.

[13] *See* Dow Elanco, Material Safety Data Sheet: Equity Termiticide (Sept. 24, 1996).

Table 1
Air Flows of the Rooms

Room I.D.	*Supply (m^3/h)*	*Return (m^3/h)*	*Difference*
Bedroom 1(A)	194	43	150
Hallway 1	0	1154	-1154
Bathroom 1	61	NR	61
Bedroom 2 (B)	202	157	44
Bedroom 3 (C)	169	98	71
Bathroom 2	62	NR	62
Family room(D)	787	NR	787
Kitchen	354	NR	354
Laundry room	100	NR	100
Living room (E)	545	848	-303
Bedroom 4 (F)	646	NR	646
Hallway 2	0	233	-233
Closet 1	48	NR	48
Closet 2	43	NR	43
Bathroom 3	152	NR	152

NR = No return air vent was located in that room

Table 2
Summary of Chlorpyrifos Air Concentrations (μg/m3)

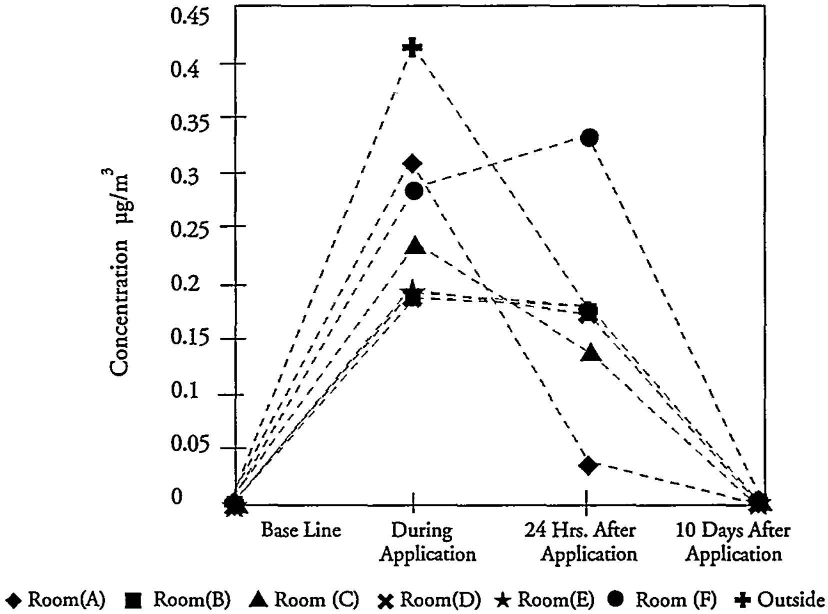
	Room A	*Room B*	*Room C*	*Room D*	*Room E*	*Room F*	*Outdoors*
Time				Concentration (mg/m^3)			
Pre-Application	ND	ND	ND	ND	ND	ND	ND
During App.	0.312	0.185	0.234	0.192	0.195	0.284	0.416
24 Hrs. After App.	0.042	0.172	0.141	0.175	0.168	0.331	0.178
10 Days After App.	ND	ND	ND	ND	ND	ND	ND

ND = None Detected: below level of detection, which was 0.01 ug/m^3

As shown in Table 2 and Figure 2, the highest concentration of chlorpyrifos during application was 0.312 $\mu g/m^3$ in room A. Interestingly, it also had the lowest interior concentration of 0.042 $\mu g/m^3$ at 24 hours after the application; this rapid decrease is probably due to the much higher supply air than return air flow, which produced a slight positive pressure relative to the exterior and under slab areas.

Room F had the highest concentration at 24 hours after the application of the termiticide. This is probably due to the small pool of pesticide that was on the floor after the application of chlorpyrifos in the master bedroom area, which seeped through a settle crack in the floor. Additionally, this room had the greatest area of pesticide injection exposure of any room in the house.

Figure 2
Concentration of Measured Chlorpyrifos in Each Room over Time



In the computer model, we made several assumptions:

- As mentioned above,[14] the chlorpyrifos emission rate was R(t) = 8.0 exp (-0.02*t) + 0.7 exp (-0.003*t).
- The area of applied termiticide equaled the area of the base block perimeter.
- No active sinks existed for removing chlorpyrifos as it was being released inside the house.

With regard to the second, however, the computer model focuses on the portion of the termiticide application area that can emit chlorpyrifos into the house interior. In this project, this area represents the cracks in the slab and at the expansion joints between that and the footer. There is no accurate and efficient way of measuring the area of the cracks in the slab, so it was assumed that the cracks cover 1% of the total floor area of the house (approximately 2.8m^2) and are evenly distributed around the perimeter and throughout the house.

14 *See supra* note 8.

Also, the model assumes a constant outdoor background concentration of chlorpyrifos. The environmental conditions such as barometric pressure, wind speed and direction, area of windows relative to the area of the walls, and age of the house can be accounted for in the air exchange calculation. This model, as do most, assumes a constant air exchange rate but does not accurately represent the conditions. As the barometric pressure, the wind direction or speed change, so will the air exchange rate. These variables, coupled with possible leakage of HVAC ducts, account for the discrepancy between the sum of the measured air flow exchange rates reported in Table 1 and the theoretical total exchange rate for the house of zero.

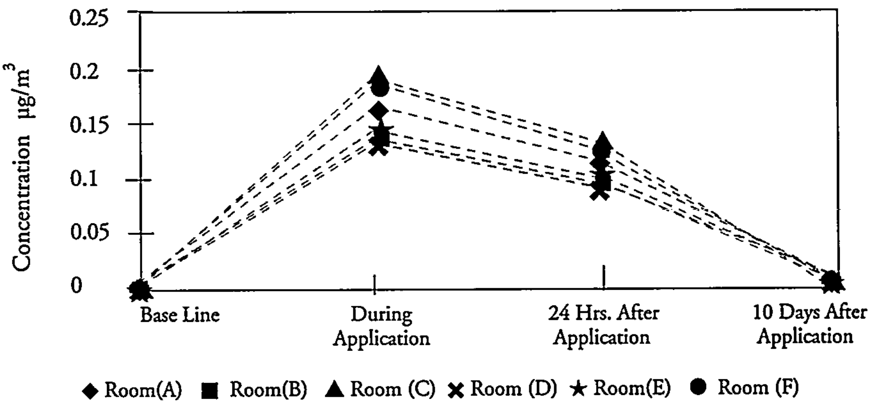
The cumulation of assumptions may contribute to the difference between the concentrations predicted by the IAQPC model and the field data. The concentrations derived by the IAQPC model (Table 3 and Figure 3) were based on a 0.31 air exchange rate per hour, a total termiticide application area of $2.8m^2$, the measured ventilation rate, the measured volume of the rooms, and an assumed chlorpyrifos emission rate from carpet at 22°C and 50% relative humidity. The computer model predicted the highest chlorpyrifos concentration of 0.031 $\mu g/m^3$ in room C compared with the highest field data concentration of 0.312 $\mu g/m^3$ in room A. Since the emission rate of chlorpyrifos in each room is treated as a constant, and the building has an air exchange rate per hour of 0.31, the determining factors for chlorpyrifos concentrations in each room were the area of the termiticide applied under the slab of each room, the ventilation of each room, and the volume of each room.

Table 3
Predicted Air Concentration for Chlorpyrifos by IAQPC Model ($\mu g/m^3$)

Time	Concentration (mg/m^3)*					
	Room A	*Room B*	*Room C*	*Room D*	*Room E*	*Room F*
During	0.026	0.022	0.031	0.021	0.023	0.029
24 Hrs.	0.018	0.015	0.021	0.015	0.016	0.020
10 Days	0.0011	0.0009	0.0014	0.0008	0.0007	0.0007

* Background level = 0 in all rooms.

Figure 3
Predicted Chlorpyrifos Concentration in Each Room over Time



Conclusions

As shown in Tables 4 and 5, the IAQPC computer model does not produce a statistically valid estimation of chlorpyrifos air concentrations inside the house during termiticide application, or at 24 hours after pesticide application for sub-slab injection treatment (Tables 4 and 5). Since both the predicted air concentrations and the field air sampling data fell below the limit of detection by ten days post-treatment, no valid comparison can be made at that point.

Table 4
Comparison of Field Air Concentrations (µg/m^3) with Modeled Estimates during Pesticide Application

	Field Data	*Model Data*	*Difference*
Room (A)	0.312	0.026	+0.286
Room (B)	0.185	0.022	+0.164
Room (C)	0.234	0.031	+0.203
Room (D)	0.192	0.021	+0.171
Room (E)	0.195	0.023	+0.172
Room (F)	0.284	0.029	+0.255
Mean Difference			+0.208
Standard Deviation			+0.051
Paired Sample T-test			±10.047

Table 5

Comparison of Field Air Concentrations (µg/m^3) with Modeled Estimates 24 Hours After Pesticide Application

	Field Data	*Model Data*	*Difference*
Bedroom 1 (A)	0.042	0.018	+0.024
Bedroom 2 (B)	0.172	0.015	+0.157
Bedroom 3 (C)	0.141	0.021	+0.119
Family room (D)	0.175	0.015	+0.160
Living room (E)	0.168	0.016	+0.150
Bedroom 4 (F)	0.331	0.020	+0.311
Mean Difference			+0.154
Standard Deviation			+0.092
Paired Sample T-test			±4.083

The IAQPC model has two major flaws. First, very few studies have reported the emission rates of different chemicals. Without knowledge of the emission rates of a chemical, the program is subject to major errors. Since there were no published data on the emission rate of chlorpyrifos at different conditions, the emission rate used in this study was developed by an in-house study conducted by the EPA. Second, this program does not consider the variation in air exchange rate per hour due to outdoor conditions, such as the barometric pressure, wind speed and direction, and area of windows relative to the area of the walls

Since this model failed accurately to predict the actual concentrations in the residence, we recommend caution in attempting to use these types of models in reconstructing past exposure events or predicting future possible exposures, particularly with sub-slab injection pesticide treatments.