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MODELING ENVIRONMENTAL TOBACCO SMOKE IN THE HOME USING TRANSFER FUNCTIONS

Wayne R. Ott
U.S. Environmental Protection Agency
Atmospheric Research and Exposure Assessment Laboratory and
Department of Statistics, Stanford University
Stanford, CA 94305

Neil E. Klepeis
Information Systems and Sciences, Inc.
4220 South Maryland Parkway, Suite 311
Las Vegas, NV 89119

Paul Switzer
Department of Statistics
Stanford University
Stanford, CA 94305

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ABSTRACT

This paper presents the theoretical and practical development of a multi-compartment indoor air quality model designed for predicting pollutant concentrations from environmental tobacco smoke (ETS) in the home. The model is developed using transfer functions for each compartment, thereby obtaining analytical solutions that can be expressed mathematically and do not require a computer. The input parameters to the model are the cigarette source emission rate, smoking activity patterns, room volumes, compartmental air exchange rates, and intercompartmental flow rates. Field experiments are conducted in an unoccupied home using a cigar and cigarettes as sources to evaluate the performance of the model, and real-time measurements are made in the home of carbon monoxide (CO), respirable suspended particles (RSP), and polycyclic aromatic hydrocarbons (PAH). The time series predicted from the equations by the model agree well with the concentration time series measured in the rooms of the home. The transfer function approach can be applied to any home simply by inspecting the floor plan and then writing the transfer functions by following simple rules. The experimental data show that the door and window positions in each room exert considerable influence on the pollutant concentrations observed in the home.

INTRODUCTION

Over a 24-hour period, people spend the greatest share of their time indoors at home. In a statewide survey of activity patterns[1], Californians over the age of 11 spent 63% of their time at home, 25% in other indoor locations (offices, stores, etc.), 7% in enclosed vehicles (buses, vans, automobiles, etc.), and only 5% outdoors. Many indoor sources of air pollution -- smoking, cooking, consumer products, gas appliances, building materials -- are found in homes. Despite the importance of the home microenvironment in contributing to one's total exposure to environmental pollutants, relatively few indoor air quality models have been applied to the home microenvironment and validated with experimental data from real homes.

This paper explores a multi-compartment indoor mass balance model that is adapted to a small, 2-bedroom home to predict the concentration time series from environmental tobacco smoke in various rooms. The home was temporarily unoccupied, allowing a variety of experiments to be conducted with different combinations of source locations, monitoring locations, door, and window positions. Transfer functions were used to predict the relationships among the time series of concentrations in different rooms, and the model's performance was evaluated using experimental time series data on carbon monoxide (CO), respirable suspended particles (RSP), and polycyclic aromatic hydrocarbons (PAH).

DEVELOPMENT OF AN INDOOR TIME SERIES MODEL

McKone[2] developed a three-compartment model to compute the 24-hour concentration history of Volatile Organic Compounds (VOCs) in the shower, bathroom, and remaining household volumes from tap water use. Wilks *et al.*[3] used an indoor model implemented on a personal computer to show that daily inhalation exposure for a person with a contaminated water supply could exceed the person's daily ingestion exposure from the same tap water. Axley and Lorenzetti[4] used a multi-compartment indoor air quality modeling system based on commercially available software. Sparks *et. al*[5] developed a multi-compartment computer model for a home and verified the model for VOC sources such as wood stain, varnish, and floor wax. Our approach is to develop the model for environmental tobacco smoke (ETS) in a home using a transfer function approach that yields analytical solutions and does not require a computer.

The mass balance model accounts for all the pollutant mass that either is emitted, deposited, or mixed into the interior air of an enclosed compartment (for example, a well-mixed room). Consider a four-room house in which "B" denotes the bedroom, "L" denotes the living room, "K" denotes the kitchen, and "P" denotes the porch (Figure 1). Here, the subscript "BL" denotes the bedroom-to-living room air movement, "LB" reflects living room-to-bedroom air movement, and "OB" denotes outdoors-to-living room air movement. Thus, the air flow rate from the bedroom to the living room is w_{BL} (volume of air per unit time, or L^3/T), and the reverse air flow rate is w_{LB}. The outdoors-to-bedroom air flow rate is w_{OB}, which reflects the air passing through the windows from outdoors or seeping through cracks in the walls. If the ambient air

has pollutant concentration x_o, then the quantity of pollutant carried into the bedroom from outdoors over time T will be the integral from $t = 0$ to $t = T$ of the product of the concentration and the outdoors-to-indoors flow rate, or the integral of $x_O w_{OB}$ over time T (mass per unit time).

Assume that the initial concentration in the room is $x_B = 0$ at time $t = 0$. Using the mass balance approach, each integral in Equation 1 is the total quantity of pollutant either entering or leaving the room's air from time $t = 0$ to time $t = T$. The sum of these quantities equals the amount of pollutant assumed to be present in the room at time T, or $x_B v_B$:

$$\int_0^T g\,dt + \int_0^T x_O w_{OB}\,dt + \int_0^T x_L w_{LB}\,dt - \int_0^T x_B w_{BO}\,dt - \int_0^T x_B w_{BL}\,dt - \int_0^T k_B x_B\,dt = x_B v_B \qquad (1)$$

Source (Cigarette)	Outdoor Infiltration	Living Room Infiltration	Outdoor Exfiltration	Living Room Exfiltration	Deposition Sink	Bedroom Contents

The first three integrals on the left side of this equation, each with positive signs, denote the quantity added to the room during period T. Of the three, the first integral is the quantity emitted from a source within the room at emission rate g; the second is the quantity entering from outdoors at concentration x_O and air flow rate w_{OB}; and the third is the quantity entering from the living room at concentration x_L and air flow rate w_{LB}. The fourth and fifth integrals, each with negative signs, denote the quantity of pollutant lost from the room's air to outdoor air (integral of $x_B w_{BO}$) and to the living room (integral of $x_B w_{BL}$). Finally, the sixth integral on the left-hand side (integral of $k_B x_B$) represents the amount of pollutant lost to "sinks" in the room (for example, the "plating out" of particles onto indoor surfaces). We assume that the deposition *rate* k_B is proportional to the concentration x_B; for pollutants such as CO that have no indoor sinks, $k_B = 0$. Setting the sum of the all integrals equal to the amount of pollutant present inside the room $x_B v_B$ (for bedroom volume v_B) implies that mixing takes place very rapidly causing the concentration x_B inside the room to be uniform (approximately everywhere the same at any time T).

Differentiating Equation 1 and rearranging terms, we obtain:

$$v_B \frac{dx_B}{dt} + x_B(w_{BO} + w_{BL} + k_B) = g + x_O w_{OB} + x_L w_{LB} \qquad (2)$$

Because the total air entering the bedroom must equal the total air leaving the bedroom -- that is, there is no compression or leakage -- we can substitute $w_{BO} + w_{BL} = w_{OB} + w_{LB}$ and then divide both sides of the equation by $w_{OB} + w_{LB} + k_B$ giving:

$$\left(\frac{v_B}{w_{OB} + w_{LB} + k_B}\right)\frac{dx_B}{dt} + x_B = \frac{g}{w_{OB} + w_{LB} + k_B} + x_O \frac{w_{OB}}{w_{OB} + w_{LB} + k_B} + x_L \frac{w_{LB}}{w_{OB} + w_{OL} + k_B} \qquad (3)$$

Using $X_B(s)$ to represent the Laplace transform[6] of the bedroom time series and $X_G(s)$ to represent the Laplace transform of the source term g, the ratio of the Laplace transforms $X_B(s)/X_G(s)$ is the system transfer function for the source emission rate g relative to the bedroom concentration x_B:

$$T_{GB}(s) = \frac{X_B(s)}{X_G(s)} = \frac{1}{v_B}\,\frac{1}{s + \phi_B} \qquad where \quad \phi_B = \frac{w_{OB} + w_{LB} + k_B}{v_B} \tag{4}$$

The living room has three air flow pathways: (1) to and from the bedroom; (2) to and from the outdoors; (3) and to and from the kitchen. If a similar mass-balance analysis is applied to the living room, then the transfer function for the bedroom to the living room is:

$$T_{BL}(s) = \frac{X_L(s)}{X_B(s)} = \frac{w_{BL}}{v_L}\,\frac{1}{s + \phi_L} \qquad where \quad \phi_L = \frac{w_{BL} + w_{OL} + w_{KL} + k_L}{v_L} \tag{5}$$

In general, the system transfer function from any external room A to any adjoining room B is written as follows:

$$T_{AB}(s) = \frac{X_B(s)}{X_A(s)} = \frac{w_{AB}}{v_B}\,\frac{1}{s + \phi_B} \qquad where \quad \phi_B = \frac{[sum\ of\ air\ flows\ into\ room] + k_B}{v_B} \tag{6}$$

Using the general form given by Equation (6), we can write the transfer function for the living room "L" to the kitchen "K" simply by inspection of Figure 1. For example, the sum of all the air flows into the kitchen is given by $w_{LK} + w_{OK} + w_{PK}$, yielding the following transfer function:

$$T_{LK}(s) = \frac{X_K(s)}{X_L(s)} = \frac{w_{LK}}{v_K}\,\frac{1}{s + \phi_K} \qquad where \quad \phi_K = \frac{w_{LK} + w_{OK} + w_{PK} + k_K}{v_K} \tag{7}$$

System transfer functions allow the analyst to predict the time series of concentrations in all the rooms of the house from the time series of the source $g = g(t)$ if its Laplace transform $G(s)$ is known. Application of these transform techniques to the house requires, of course, the values of the parameters w_{BL}, w_{OL}, v_L, etc., as well as the air exchange rate for each room. Even without the values of these parameters, the inverse Laplace transforms of a time series can be used to determine the general shapes of the concentration time series plots.

Consider a single cigarette smoked in the bedroom from time t = 0 to time t = 7 minutes and a residence time (reciprocal of the air exchange rate) of an hour or more. Using the delta function $\delta(t)$ as an idealized representation of a cigarette with total emissions of q_{cig} mg, the Laplace transform of the cigarette will be $X_G(s) = 1 \cdot q_{cig}$. For a single cigarette, therefore, the

Laplace transform of the bedroom concentration is the product of the cigarette's Laplace transform and the source-to-bedroom transfer function $T_{GB}(s)$ given by Equation 4:

$$X_B(s) = X_G(s)T_{GB}(s) = q_{cig}\frac{1}{v_B}\frac{1}{s+\phi_B} \tag{8}$$

Referring to a table of Laplace transforms[6], the concentration predicted in the bedroom as a function of time from the inverse Laplace transform is given by the following exponential function:

$$x(t) = \frac{q_{cig}}{v_B}e^{-\phi_B t} \qquad for \quad t \geq 0 \tag{9}$$

Similarly, the Laplace transform for the concentration predicted in the living room from a single cigarette smoked in the bedroom is given by the product of Equation 5 and Equation 8:

$$X_L(s) = X_B(s)T_{BL}(s) = X_G(s)T_{GB}(s)T_{BL}(s) = q_{cig}\frac{w_{BL}}{v_B v_L}\frac{1}{s+\phi_B}\frac{1}{s+\phi_L} \tag{10}$$

Referring to a table of inverse Laplace transforms[6], we find that the concentration time series predicted for the living room from the cigarette in the bedroom is given by:

$$x_B(t) = \frac{q_{cig}w_{BL}}{v_B v_L(\phi_L - \phi_B)}(e^{-\phi_B t} - e^{-\phi_L t}) \qquad for\ t \geq 0, \quad \phi_B \neq \phi_L \tag{11}$$

This function begins at the origin, since $x_B(0) = 0$. Differentiating Equation 11 and setting the result equal to zero shows that this function has a single mode x_{max} at time $t = t_{max}$:

$$x_{max} = \frac{q_{cig}w_{BL}}{v_B v_L(\phi_L - \phi_B)}\left(e^{\frac{\phi_B}{\phi_B-\phi_L}\ln(\phi_B/\phi_L)} - e^{\frac{\phi_L}{\phi_B-\phi_L}\ln(\phi_B/\phi_L)}\right) \qquad and \qquad t_{max} = \frac{\ln(\phi_B/\phi_L)}{\phi_B - \phi_L} \tag{12}$$

All the transfer functions for the compartments of a house are of the form in Equation 10; the denominators contain the products $(s+\phi_A)(s+\phi_B)$. Thus, all the solutions -- the time series in all rooms of the house -- will consist of the sums of exponential functions when the source is a single, relatively short "pulse" such as a cigarette. Representing the cigarette as a short pulse is an approximation; if the residence time is short relative to the duration of the cigarette, then the cigarette should be represented by a "rectangular" input function, as we have done elsewhere[7].

To evaluate whether these equations adequately predict the time series of concentrations for a cigarette smoked in an unoccupied home, over 40 experiments were conducted in a single-story, two-bedroom house with outside dimensions of 28 ft by 24 ft, or 672 ft^2 (62.5 m^2) on Partridge Ave. in Menlo Park, CA. The house was awaiting a new tenant, and we could vary the locations of the monitors and the door and window positions in a variety of configurations.

Spatial Variation within a Bedroom

An important assumption of the mass balance model (Equation 1) is that, for any time *t*, the room is sufficiently well-mixed to give nearly the same concentration at all locations. To evaluate this assumption, experiments were conducted at three widely spaced locations in the 907.5 ft^3 (25.7 m^3) bedroom: (1) near the floor in the corner of the room; (2) on a short step ladder 36" high in the center of the room; and (3) on a tall ladder 8.5" from the ceiling (Figure 2). CO concentrations were measured using a Langan L15 CO Personal Exposure Measurer[8] (Langan Products, San Francisco, CA). Wires ran from each CO sensor to a DataBear[8] data logger, and precision electronic operational amplifiers multiplied the signals by 10.0 to increase the sensitivity. CO concentrations in parts-per-ten-million (pptm) were logged at 30-second intervals.

Over a period of 16 hours, three Marlboro regular filter cigarettes were smoked in the center of the bedroom at a 36" height with the doors closed and one window partly open but covered with a shade. The first cigarette was smoked just after noon (12:46:30 pm) and lasted for 6 minutes and 30 seconds; the exponential decay of the CO concentrations from this cigarette was quite similar for all three locations and lasted approximately 4.25 hours until just before 5:00 pm (Figure 3). The second cigarette began approximately at 5:00 pm and lasted for 7 minutes and 16 seconds; it generated an exponential decay curve at each of the three locations, although the concentration at the corner floor was lower than the concentration time series at the center of the room or at the ceiling. Finally, a third Marlboro cigarette was smoked at 9:56 pm for 9-1/2 minutes, and its exponential decay was observed until 3:49 am. Each time series followed Equation 9. The air exchange rate was determined by subtracting the background concentration and taking the logarithms; the slope of the resulting straight line yielded approximately the same ventilatory air exchange rate of $\phi_v = 1.2$ air changes per hour (ach) at all locations.

The CO concentration time series, when averaged over each smoking episode, ranged from 3.88 pptm to 5.9 pptm, with an average for all episodes of 5.4 pptm (Table 1). The center of the room averaged about 1-1.2 pptm (21-23%) higher than the corner floor and about 0.7-1.3 pptm (19-33%) higher than the ceiling. One would expect a higher average concentration in the center, because the cigarette was smoked there within 12" of the CO monitor. It is unlikely that a person would spend several hours either at the two extreme locations -- the corner floor or the ceiling -- but would move about the room, so the person's average exposure would deviate by less than the 19-33% difference observed for the three locations. The average exposure of a person inside the room probably would be closer to the overall mean of 5.4 pptm.

Table 1. Average CO Concentration (pptm) Measured in the Bedroom at Three Locations after Smoking of Three Successive Marlboro Regular Filter Cigarettes				
Experiment No.	Corner Floor	Center of Room	Top of Ladder	Mean
1	5.62	6.81	5.90	6.11
2	5.18	6.30	5.61	5.70
3	4.19	5.16	3.88	4.41
Mean:	5.00	6.09	5.13	5.41

Baughman *et al.*[9] studied a chamber with 40 sampling points to determine how rapidly the concentrations at different points converge, and Mage and Ott[10], in reviewing their work, suggest three time phases: an α-period in which the source is emitting and the concentrations vary spatially, a β-period in which the source is off but the room is not well-mixed, and a γ-period in which the coefficient of variation across all points is less than 0.10. There are too few locations in the bedroom experiment to compute the coefficient of variation meaningfully, but Figure 3 shows that the concentration time series pattern after the cigarette ends are similar at the three locations. For a cigarette, the α-period is short relative to the other periods.

Our published cigarette smoking time series model[7] derives the the following expression for the average concentration over time T as a function of the average source strength $g(T)$, the instantaneous concentration $x(T)$, the volume v, and the air exchage rate ϕ:

$$\frac{Average\ of\ g(T)}{\phi v} - Average\ of\ x(T) = \frac{x(T)}{T\phi} \tag{13}$$

At the end of the exponential decay period, $x(T) \approx 0$ so that

$$\frac{Average\ of\ g(T)}{\phi v} \approx Average\ of\ x(T) \tag{14}$$

The product of the average source emissions and the time T gives the total emissions q_{cig}, so multiplying both sides of Equation 14 by T gives:

$$q_{cig} = [Average\ of\ g(T)]T = [Average\ of\ x(T)]T\phi v \tag{15}$$

Substituting the values of 5.41 pptm, ϕ = 1.2 air changes per hour (ach), v = 25.7 m^3, and the average experiment duration of 4.25 hours, we can compute the total source emissions for the cigarette experiment in the bedroom:

$$q_{cig} = (0.541\ ppm)\left(1.145\ \frac{mg}{m^3\text{-}ppm}\right)\left(1.2\ \frac{air\ change}{hr}\right)(4.25\ hr)\left(25.7\ \frac{m^3}{air\ change}\right) = 81.2\ mg$$

The resulting total CO emission of 81.2 mg is not too different from the total CO emission of 88 mg obtained by combining mainstream and sidestream smoke from Marlboro cigarettes from experiments in a chamber and an automobile and is similar to values reported in the literature.[7] Notice that, at time $t = 0$, the exponential function in Equation 9 gives $x(0) = q_{cig}/v_b = 81.2$ mg/25.7 $m^3 = 3.16$ mg/m^3 CO. This result converts to (3.16 mg/m^3)(1 ppm-m^3/1.147 mg)(10 pptm/ppm) = 27.6 pptm, which is very close to the peak concentration observed in Figure 3.

Concentrations in Two Rooms

In another experiment, the windows were closed, the door into the living room was opened, and three Kentucky reference cigarettes No. 2R1 were smoked one after another in the bedroom to obtain a strong source. RSP concentrations were measured (2-min averages) in the living room and center of the bedroom using a Model 8510 piezobalance (TSI, Inc., St. Paul, MN). The CO sensor on the tall ladder (location No. 3 in the bedroom) was moved into the living room from the bedroom, but the other two bedroom sensor locations were unchanged (Figure 2). PAH concentrations were measured at the corner floor location using a real-time PAH monitor (EcoChem Technologies, Inc., West Hills, CA) that has been used in other ETS experiments.[11]

Although the RSP concentrations for the two rooms initially diverge, they rapidly come together after 45 minutes and remain very similar for the next four hours (Figure 4). Thus, with the door between the two rooms open, the two rooms act almost as a single compartment. The RSP concentrations caused by the three research cigarettes were extremely high, reaching a peak of 5,500 µg/m^3 in the bedroom. Indeed, the levels were so high that the three investigators found it necessary to open a living room window at 4:00 pm, and the effect of opening this window in changing the air exchange rate is especially evident in the CO time series plots (Figure 5). Unlike CO, both RSP and PAH plate out on surfaces, and PAH therefore shows a more rapid decay than CO in the bedroom.

Concentrations in Three Rooms

To examine the relationships among the time series in three rooms, a cigar was smoked in the kitchen to serve as a strong source, and the resulting CO concentrations were measured in all three rooms. Long coaxial cables were extended into each room with Langan L15 CO sensors attached, and CO concentrations on all three channels were logged using a DataBear[8] data logger. As before, precision operational amplifiers multiplied the voltages by 10 to increase the

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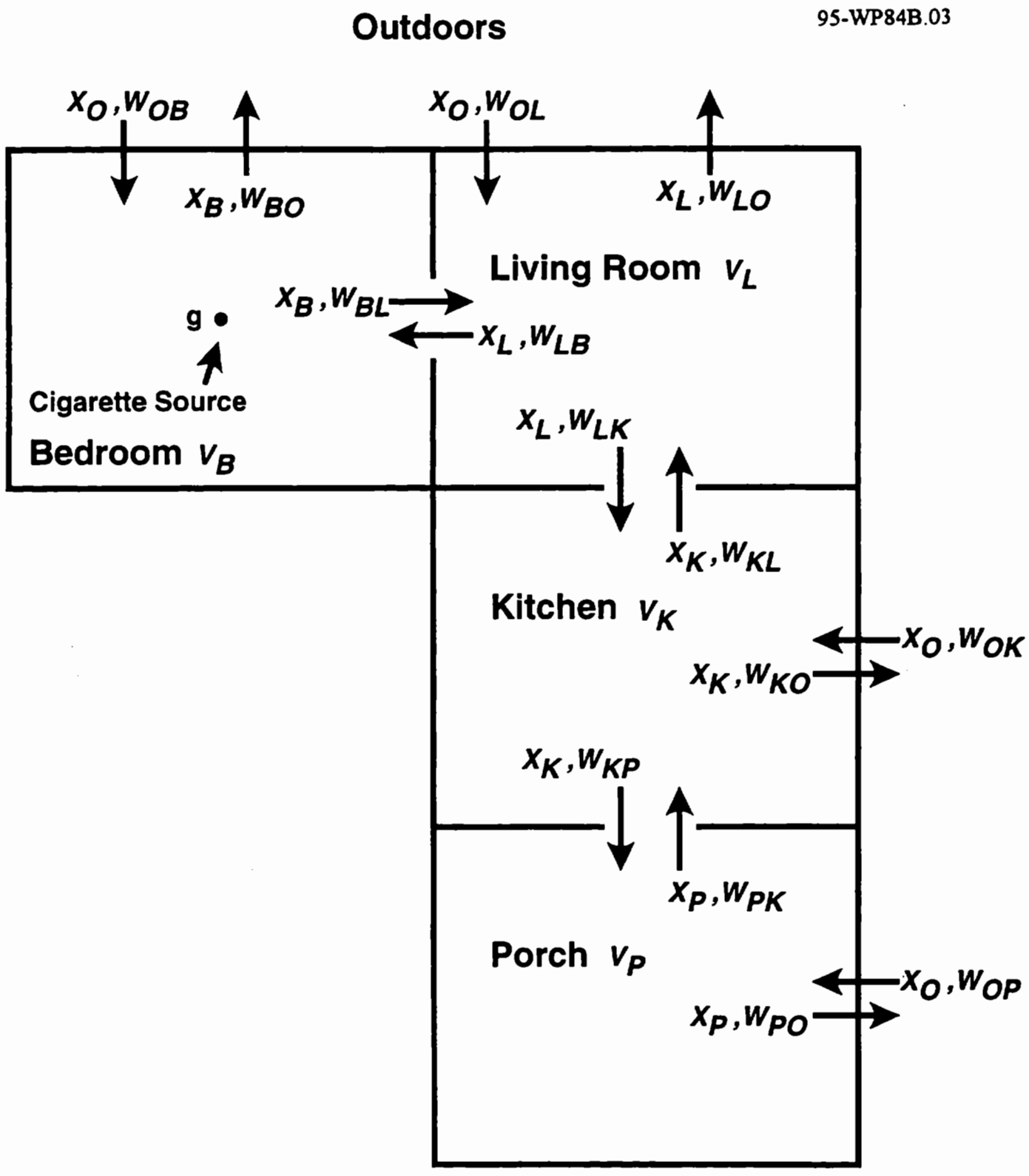

Figure 1. Schematic showing air flow paths and pollutant concentrations in a 4-room house for which the time series model was developed.

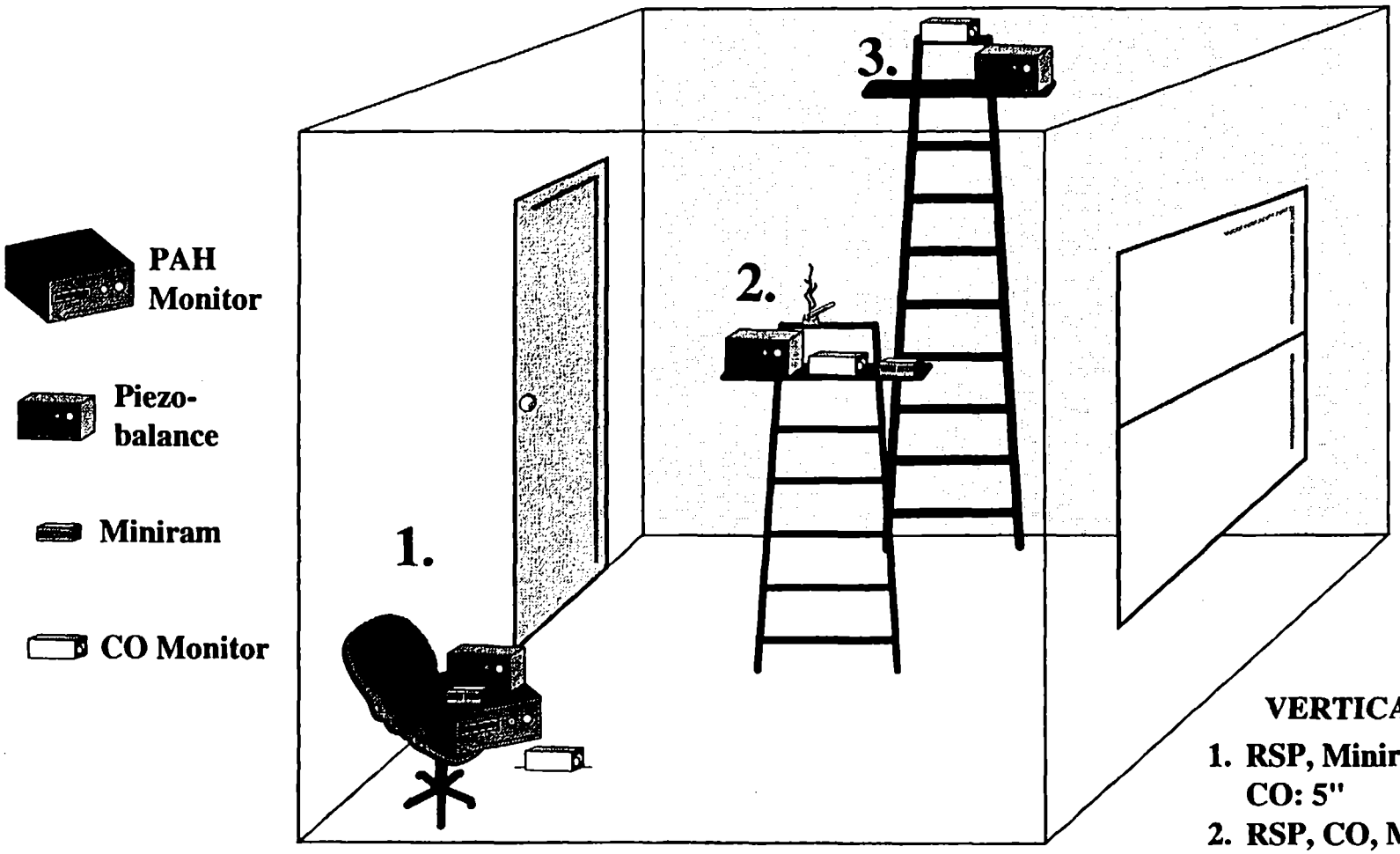

Figure 2. Monitoring Locations in Bedroom of Partridge Avenue House.

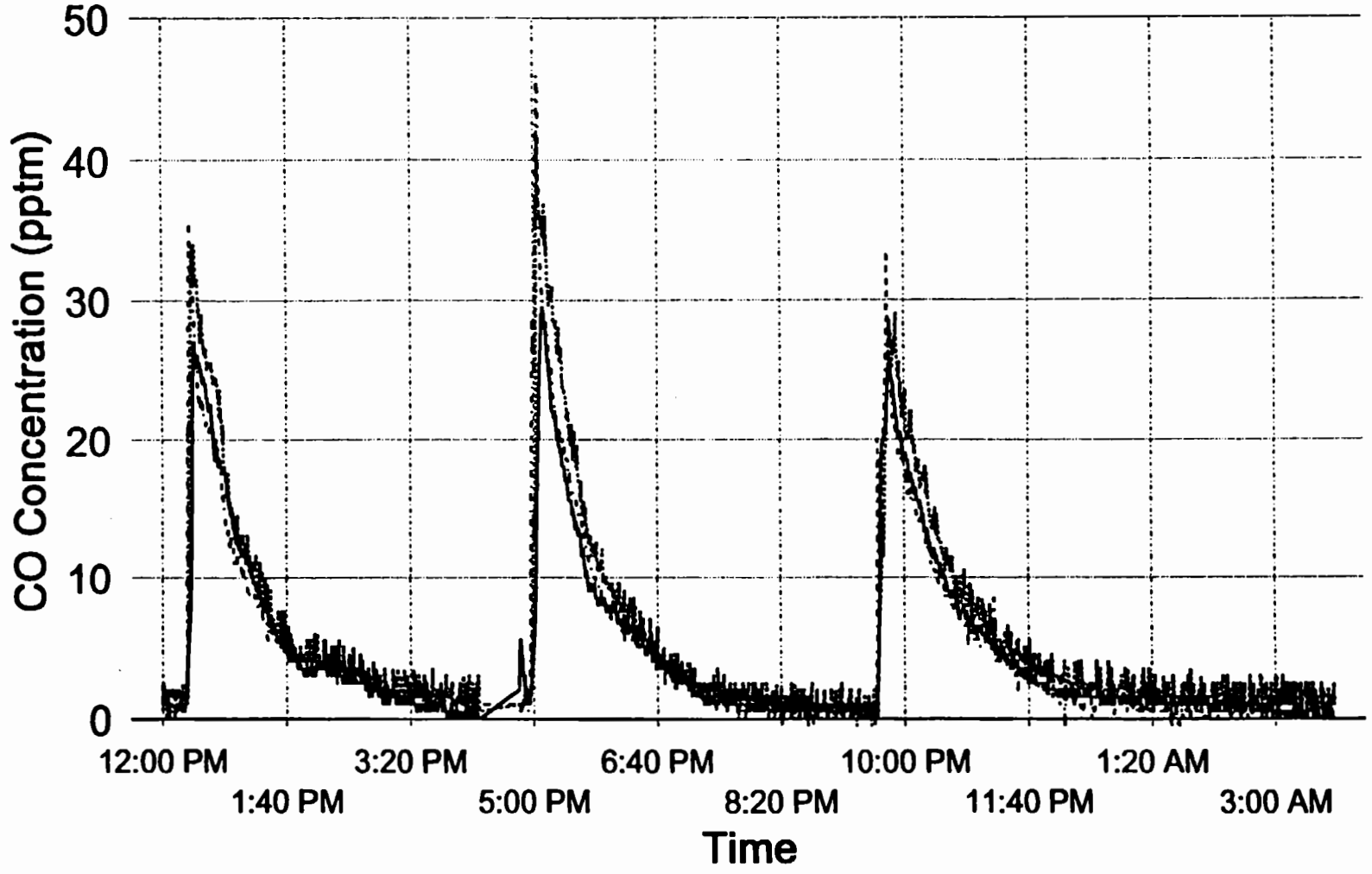

Figure 3. CO Concentration measured in a 25.7 m^3 bedroom over a 16-hour period during which 3 Marlboro regular filter tip cigarettes were smoked.

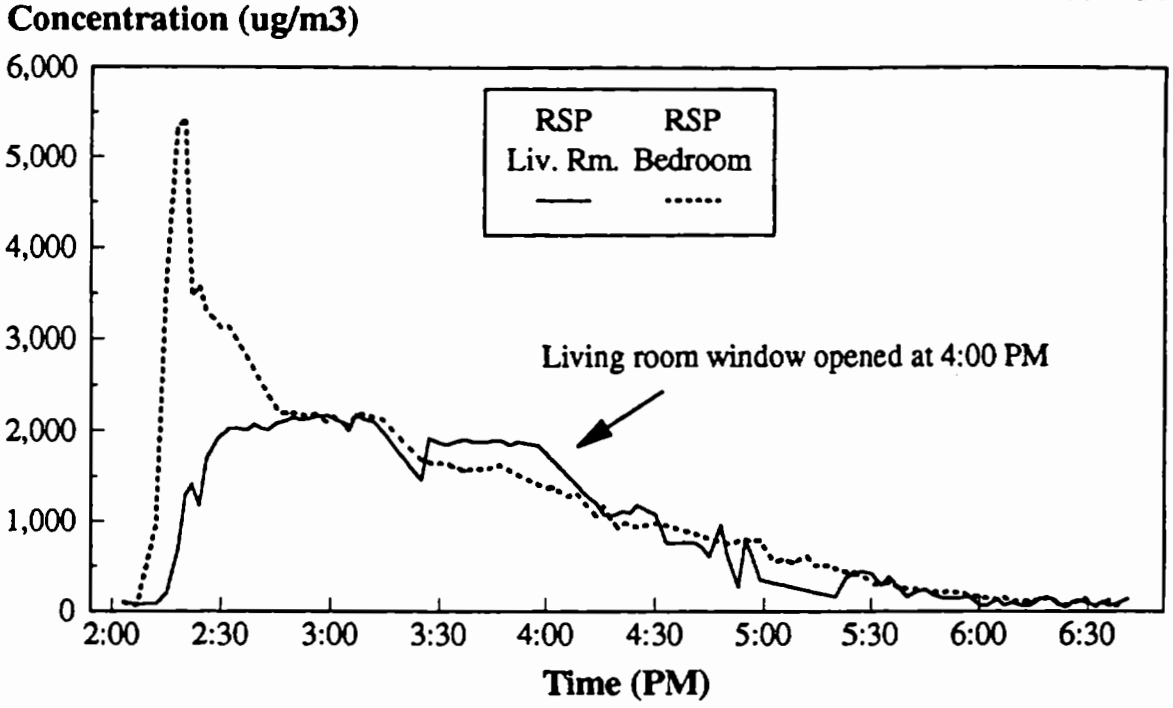

Figure 4. RSP concentrations measured in the bedroom and living room with the door open after three Kentucky No. 2R1 reference cigarettes were smoked.

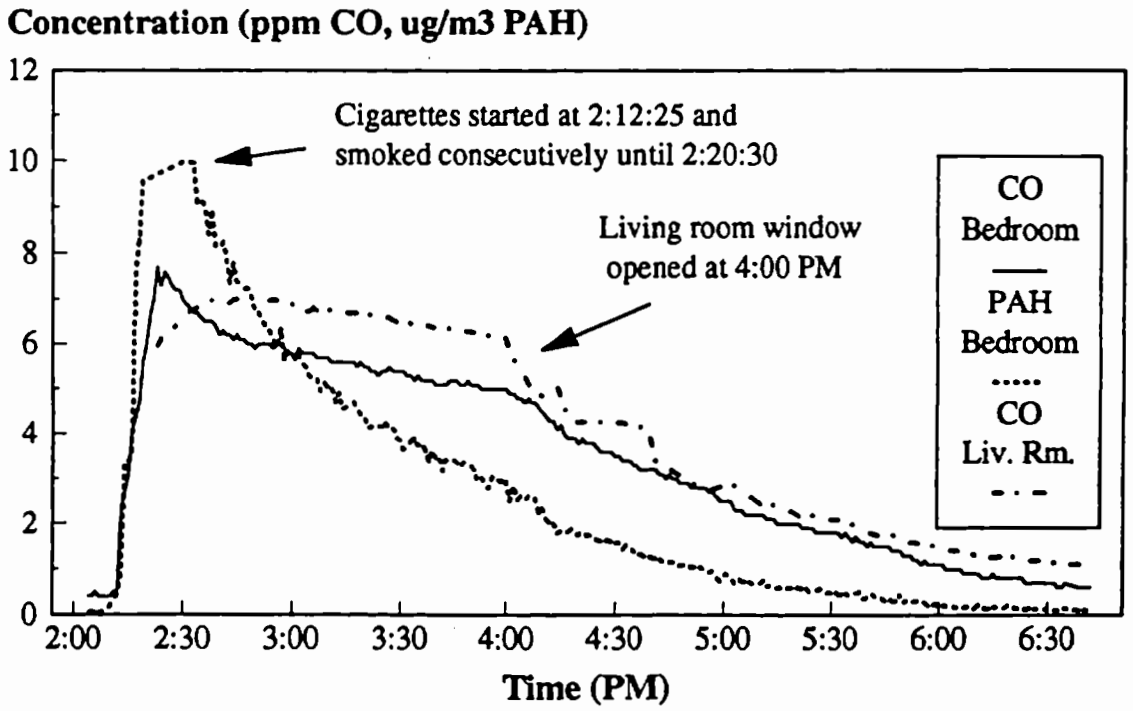

Figure 5. CO and PAH concentrations measured in the bedroom and the living room with the door open after three Kentucky No. 2R1 reference cigarettes were smoked.

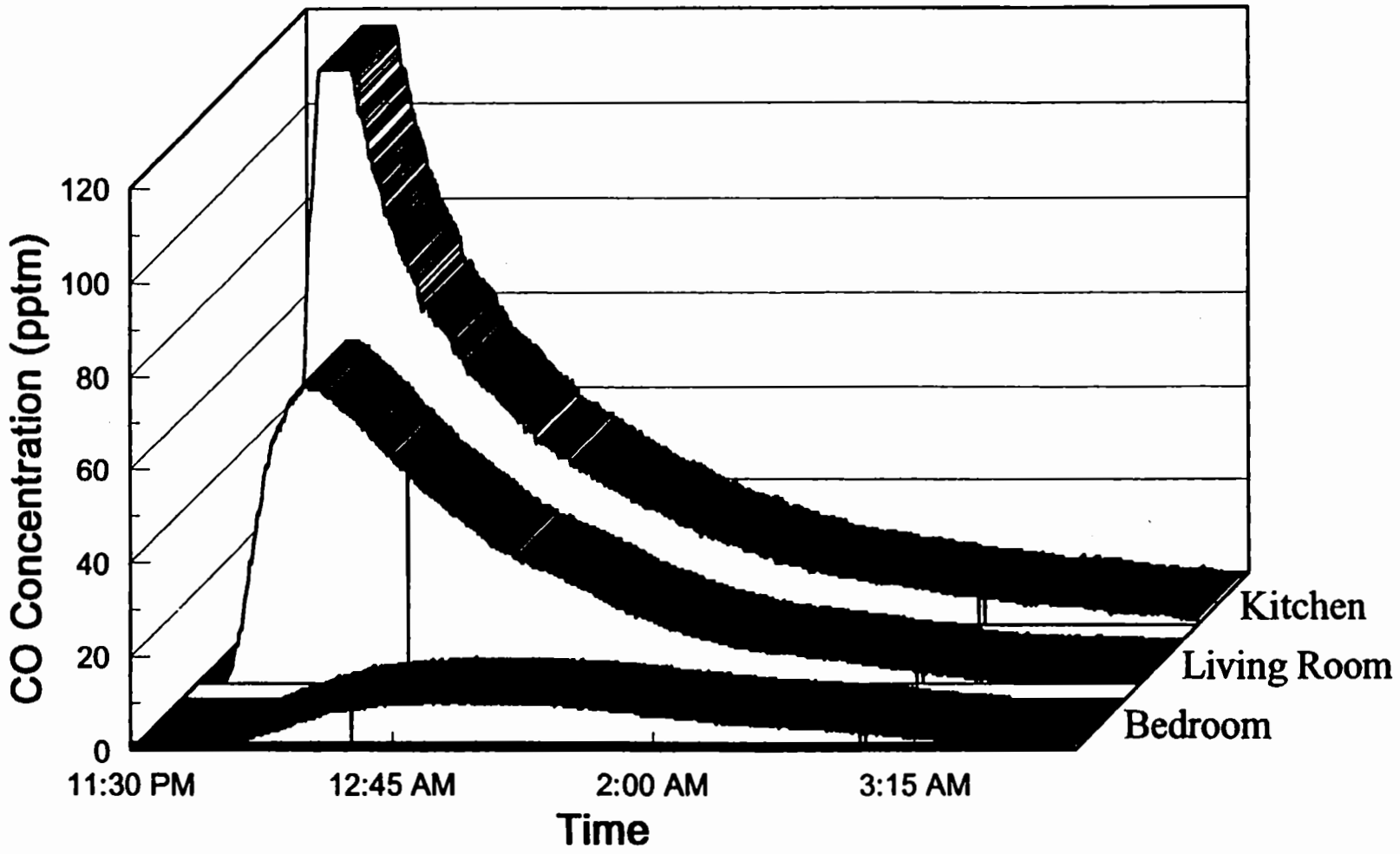

Figure 6. The CO time series in three rooms of the house after a cigar was smoked in the kitchen. The kitchen door was open 3" and the bedroom window and door were closed. The background concentration has been subtracted from each CO monitor.

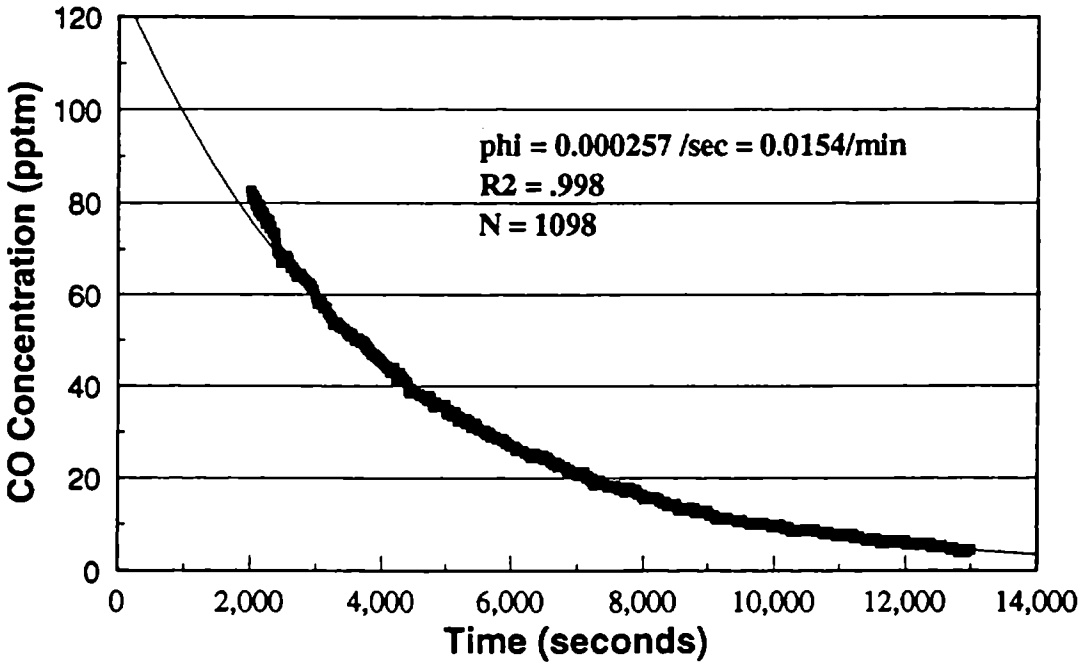

Figure 7. The CO concentration measured in the kitchen after a cigar was smoked along with the exponential fit to the data. The kitchen door was open 3"

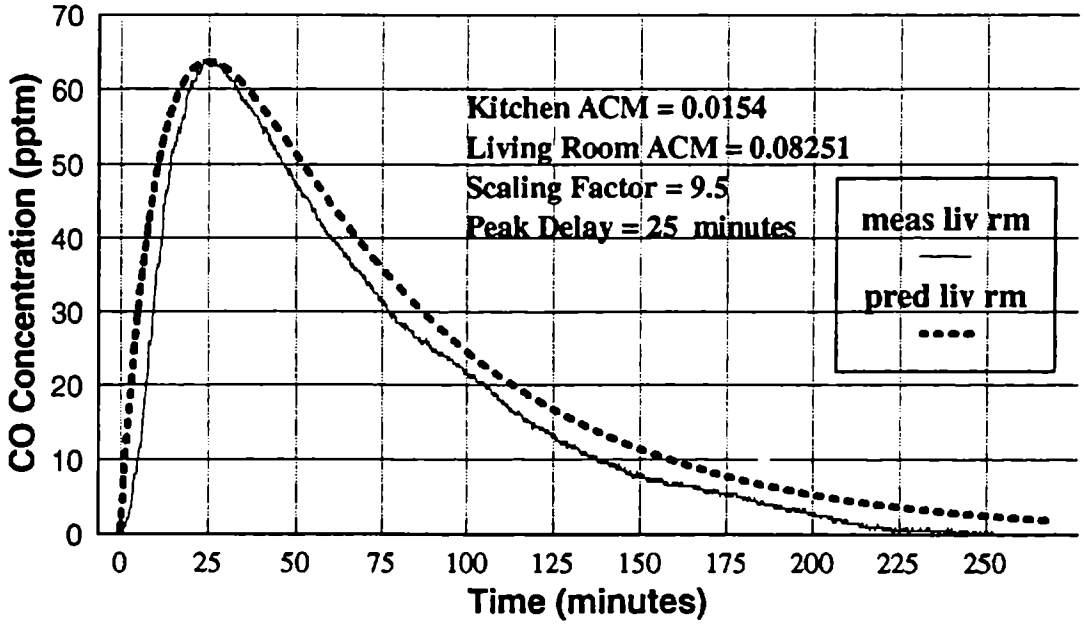

Figure 8. Comparison of measured and predicted levels of CO in the living room after a cigar was smoked in the kitchen. The door between the kitchen and the living room was open 3".

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15. SUPPLEMENTARY NOTES

16. ABSTRACT

This paper presents the theoretical and practical development of a multi-compartment indoor air quality model designed for predicting pollutant concentrations from environmental tobacco smoke (ETS) in the home. The model is developed using transfer functions for each compartment, thereby obtaining analytical solutions that can be expressed mathematically and do not require a computer. The input parameters to the model are the cigarette source emission rate, smoking activity patterns, room volumes, compartmental air exchange rates, and intercompartmental flow rates. Field experiments are conducted in an unoccupied home using a cigar and cigarettes as sources to evaluate the performance of the model, and real-time measurements are made in the home of carbon monoxide (CO), respirable suspended particles (RSP), and polycyclic aromatic hydrocarbons (PAH). The time series predicted from the equations by the model agree well with the concentration time series measured in the rooms of the home. The transfer function approach can be applied to any home simply by inspecting the floor plan and then writing the transfer functions by following simple rules. The experimental data show that the door and window positions in each room exert considerable influence on the pollutant concentrations observed in the home.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field Group
Exposure Modeling Mathematical Modeling Indoor Air Quality Modeling Environmental Tobacco Smoke (ETS) Indoor Air Quality Carbon Monoxide		

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