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Macromodel for Assessing Residential Concentrations of Combustion-Generated Pollutants: Model Development and Selected Sensitivity Analyses

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MACROMODEL FOR ASSESSING RESIDENTIAL CONCENTRATIONS OF COMBUSTION-GENERATED POLLUTANTS: MODEL DEVELOPMENT AND SELECTED SENSITIVITY ANALYSES

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Abstract

An indoor air quality simulation model (also called a "macromodel") was developed to assess indoor concentration distributions of combustion pollutants across homogeneous groups of houses. The model inputs include the market penetration of indoor pollution sources, (e.g., percentage of houses using kerosene heaters), pollution source characteristics (e.g., pollutant emission rates, source usage rates), building characteristics (e.g., house volume, air exchange rate), and meteorological parameters (e.g., outside temperature). The model uses time-averaged parameters and assumes a single well-mixed zone for each house. A series of sensitivity analyses was conducted on the model. The results consistently showed the importance of source emission rate and usage rate information. In addition, the indoor reactivity rate was important for simulating NO_2 concentrations, and the appliance venting factor was important for estimating indoor pollutant concentrations in houses with forced-air furnaces. Other causative parameters are ranked in importance. Future field studies in this area should collect information on those macromodel input parameters shown to significantly affect indoor air pollutant concentrations.

Introduction

Research on indoor air pollution has expanded significantly in recent years. One outgrowth of this expansion has been the need for models that can characterize indoor air pollution concentrations and exposures of homogeneous populations or housing stocks. Human exposures to air pollutants are often dominated by indoor air pollutant exposures for two reasons. First, indoor concentrations of many pollutants are higher, often much higher, than outdoors.[1-5] Second, people spend approximately 90% of their time indoors.[1,6-8]

An indoor air pollution simulation model (also called a "macromodel") has been developed for characterizing combustion pollutant concentration distributions in homogeneous housing stocks and will sometimes be referred to as the "combustion macromodel."[9] The term "macromodel" is used to describe the *application* of this modeling approach, not the model itself. Macromodels describe concentration distributions in homogeneous housing stocks, whereas micromodels describe indoor concentration profiles (time and/or space profiles) within a single house or structure. Both modeling approaches depend upon the same, or variations of the same, physical models. The combustion macromodel is based on the physical principles that describe indoor air pollution and includes source usage models and building characteristics that affect indoor air pollution levels. Key equations of the model will be described in this paper.

Selected sensitivity analyses were conducted to determine the input parameters with the greatest influence on the outcome (i.e., indoor pollutant concentrations). In these analyses, explicit attempts were made to identify the parameters that caused certain households to have indoor pollutant concentrations significantly higher than the average concentration for the house-type modeled. A generalized technique (nonparametric) employing the Kolmogorov-Smirnov test was used for the sensitivity analyses.[10-15]

Modeling

All indoor air quality models are based on the principle of mass balance. Time-dependent versions of the well-mixed, single-room, mass-balance indoor air quality (IAQ) model have been widely published,[9,16-19] and one version follows.

$$C(t) = \frac{(PaC_o + S/V)}{a + k} \left[1 - e^{-(a+k)t}\right] + C(0)e^{-(a+k)t} \quad , \qquad (1)$$

where

- C = indoor pollutant concentration ($\mu g/m^3$ or ppm);
- t = time (h);
- P = pollutant penetration factor, i.e., fraction of outdoor pollutants that penetrate the building shell (unitless, 1 = 100% penetration);
- a = air exchange rate (h^{-1});
- C_o = outdoor pollutant concentrations ($\mu g/m^3$ or ppm);
- S = indoor pollutant source strength ($\mu g/h$ or cm^3/h);
- V = volume (m^3); and
- k = indoor pollutant reactivity rate (h^{-1}).

The steady-state or time-averaged version of the well-mixed, single-room IAQ model is

$$C(t) = \frac{(PaC_o + S/V)}{a + k} \quad . \tag{2}$$

Equation (2) was the kernel of the IAQ modeling work used by Traynor et al.[9]

Additional modeling of the indoor air pollution source strength can be accomplished. The indoor pollutant source strength, S, can be described by the following equation:

$$S = QEF_v \quad , \tag{3}$$

where

- Q = source usage rate, same as house space heating requirements for space heaters (kJ/h or cigarettes/h);
- E = source pollutant emission rate (μg/kJ, cm^3/kJ, or μg/cigarette); and
- F_v = appliance venting factor (unitless, ranges from 0 for completely vented to 1 for completely unvented).

For space heating appliances, the source usage rate can be modeled further[9,20]:

$$Q = \frac{b(UA\Delta T + aVq\Delta T - Q_f)}{\epsilon} \quad , \tag{4}$$

where

- b = life-style factor (unitless);
- ϵ = appliance efficiency (unitless);
- U = overall building thermal conductance or "U-value" (kJ/hm^2 °C);
- A = total house surface area (m^2);
- ΔT = indoor/outdoor temperature difference (°C);
- V = house volume (m^3);
- q = heat content of air (1.2 kJ/m^3 °C); and
- Q_f = house "free" heat (kJ/h).

The overall house U-value is calculated from the individual U-values and surface areas of the ceiling, walls, doors, windows, and floors. The house "free" heat was calculated from estimates of internal sources of heat (e.g., appliances, occupants), and solar gain.[9]

Finally, the air exchange rate can be further characterized as follows[21]:

$$a = \frac{(ELA^2 f_s^2 \Delta T + ELA^2 f_w^2 v^2)^{0.5}}{V} \tag{5}$$

and

$$ELA = SLA \times A_f \times 10^{-4} \quad , \tag{6}$$

where

ELA = effective leakage area (m^2);
f_s = reference stack parameter for infiltration model ($m/h\ °C^{0.5}$);
f_w = reference wind parameter for infiltration model (m^2/km^2);
v = wind speed (km/h);
SLA = specific leakage area (cm^2/m^2); and
A_f = floor area (m^2)

Indoor pollutant concentration distributions are simulated using the Monte Carlo simulation technique.[9] Each simulation uses a housing stock of 3500 houses. Distributions of all input parameters were constructed from data in the literature.[9] For each house modeled, each input parameter assigned to that house was chosen, using the Monte Carlo simulation technique, from the probability distribution of that particular parameter. Once the input parameters for a house were chosen, an indoor pollutant concentration was calculated using the above equations. This process was repeated for all 3500 houses and an indoor pollutant concentration distribution was constructed for the housing stock modeled. All model inputs and outputs are averaged over one week. The simulations made in this report are for houses with a single combustion source with a prescribed outdoor air temperature and wind speed.

Approach

A general nonparametric sensitivity analysis technique employing the Kolmogorov-Smirnov test[10-15] was chosen as the most applicable method for the combustion macromodel. The advantages of this method are (1) the technique is consistent with intuition regarding sensitivity analyses, (2) the technique does not depend on linear relationships or normal distributions, and (3), most importantly, the results are easily interpreted. A simplified description of the technique is presented here, and the reader is referred to other documents for further information.[10-15]

The basic approach to the combustion macromodel sensitivity analysis is to determine the differences in input parameter distributions between the houses with high indoor air pollution levels and the remainder of the houses (i.e., those with moderate or low indoor air pollution levels). Houses with their indoor concentrations in the top 20% of the concentration distribution, within a homogeneous housing stock with the same indoor source, were arbitrarily designated as having a "high" concentrations. The full macromodel was run for houses with specific sources and the input parameters for each of the 3500 houses modeled were saved. The houses were then separated according to their indoor pollutant concentration (i.e., the model input parameter vectors were separated for the houses in the top 20% -- a group of 700 houses -- and the bottom 80% -- a group of 2800 houses). The particular input parameters (e.g., house volume, outdoor CO concentration) for each group of houses were combined. The cumulative distributions of the separated input parameter distributions were then plotted along with the parent distribution (inputs for all 3500 homes). If, for a particular input parameter, the cumulative distribution of the top 20% and the bottom 80% were similar to the parent distribution, then that particular input parameter does not have a significant effect on whether a particular house has a "high" indoor air pollution concentration. If, however, the input parameter distributions of the top 20% and the bottom 80% greatly diverge from the parent distribution, then that particular input parameter has a significant (or, at least, relatively greater) affect on the indoor air pollution level.

The degree of input parameter separation can be quantified. If we call the cumulative input parameter distribution of the top 20% and the bottom 80% $S_t(x)$ and $S_b(x)$ respectively, then the Kolmogorov-Smirnov "D" can be defined as the maximum deviation between $S_t(x)$ and $S_b(x)$ for all values of x. Mathematically, the deviation measure, D, can be defined as the following:

$$D = \max_{-\infty<x<\infty} |S_t(x) - S_b(x)| \quad 0 \le S \le 1 \quad . \tag{7}$$

To reiterate, if the distribution of an input parameter that characterizes the houses with the highest 20% of the indoor concentrations is similar to the input parameter distribution of the bottom 80%, then that parameter is not significant in determining which houses have high indoor pollutant levels. Conversely, if the input parameter distribution of the houses in the top 20% differs greatly from the distribution of the houses in the bottom 80%, then that parameter has a much greater affect on the indoor concentrations of the modeled housing stock. The Kolmogorov-Smirnov statistic, "D," will be used to rank the the various input parameters in terms of importance.

A representative housing stock with a specific indoor combustion source was modeled. The effects of unvented and partially vented space heaters and selected non-space-heating sources were analyzed.

Results and Discussion

A total of five representative sensitivity analyses were conducted, three on non-space-heating sources, and two on space-heating sources. The sensitivity analyses were chosen to ensure that all relevant parameters were analyzed at least once. Two parameters were not addressed: the market penetration of sources, and the outdoor temperature. The market penetration of sources was not addressed because the presence or absence of a source has obvious implications regarding indoor air pollution from that source, and no further elucidation is needed. Outdoor temperature was not addressed because (1) it has only an indirect effect on indoor air pollution from non-space-heating sources through the air exchange rate, which is addressed by the specific leakage area of the house, and (2) it clearly drives the source usage rate of space-heating sources. For space-heating sources, the housing stocks are modeled with a given one-week-average temperature for a given region; therefore, the temperature itself does not determine which houses have high concentrations, it only affects space heating use. Table I lists most of the independent parameters used in the sensitivity analyses. The housing stock used in the combustion macromodel for the Rochester, NY, region was used for all sensitivity analyses.[9] Where appropriate, an indoor/outdoor temperature difference of 23.5 °C and a wind speed of 20 km/h (5.6 m/s) were used for the analyses.[9]

Table II summarizes the sensitivity analysis results for carbon monoxide (CO) from gas stoves. Figure 1 shows the three input cumulative distributions generated by the macromodel (all houses, the 20% of houses with the highest indoor concentrations, and the 80% of houses with the lowest indoor concentrations) for the outdoor CO concentration, a parameter that was not a significant factor in influencing which houses were in the top 20% of the concentration distribution. Note that all three cumulative distributions are quite similar and did not "separate" when the houses were divided into the top 20% and bottom 80% when using the indoor concentration as the guiding parameter. Figure 2 shows an example of an independent parameter, the gas range CO emission rate, that "separated" when the parent distribution was disaggregated into the top 20% and bottom 80%. As a consequence, the "D" value listed in Table II for the gas stove/CO analysis is very low for the outdoor CO concentration and is very high for the gas range (or range top) CO emission rate. In fact, the two most important parameters in determining which houses have high indoor CO levels from gas stoves are the range CO emission rate (E_{range})

and the oven CO emission rate (E_{oven}). The importance of E_{range} and E_{oven} is also reflected in the very large differences between the geometric means of these parameters for the houses in the top 20% and the bottom 80%. The third most important factor is the specific leakage area of the house, followed by the oven usage rate, the house volume, and the range usage rate. The least important factor was the outdoor CO concentration.

When the gas stove sensitivity analysis was conducted with the indoor nitrogen dioxide (NO_2) as the dependent parameter, the order of significant parameters changed compared with the CO results (see Table III). The indoor pollutant reactivity rate of NO_2 was the most important factor in determining which houses had the highest indoor NO_2 concentrations. The important factors in the next group are all related to the source and consist of the oven and range NO_2 emission rates and the oven and range usage rates. As with CO, the outdoor NO_2 concentration had very little impact on which houses had high indoor NO_2 concentrations from gas stoves.

Table IV shows the sensitivity analysis results for respirable suspended particles (RSP) from smoking. The most important determinant for indoor RSP from smoking is the indoor smoking rate followed by the specific leakage area of the house. The smoking emission rate, which has a very narrow distribution with a geometric standard deviation of 1.2, was the third most important factor, with a 12.2% difference between the means of the high and low concentration groups. As with the previous analyses, the outdoor concentration was not an important factor in determining which houses had high indoor RSP concentrations.

The sensitivity analysis results for houses with space-heating sources are summarized in Tables V and VI. For the convective kerosene heater analysis, the CO emission rate was by far the dominant factor in determining which houses have high indoor CO levels (see Table V). In fact, it was so dominant that the relative ranking of the remaining parameters may be meaningless, although the two other "source-related" parameters, the house U-value and the specific leakage area (SLA), were second and third in importance. Outdoor air concentration and house volume were the least important.

The results for houses with gas forced-air furnace (FAF), analyzed for CO, show that the outdoor CO concentration and the venting factor are the two dominant parameters in determining which houses have the highest concentrations (see Table VI). This makes sense, because only 6.8% of the housing stock have non-zero vent factors and most houses with non-zero vent factors would be expected to fall into the highest 20%. The remainder of the houses would be in the top 20% because of high outdoor concentrations, since outdoor air is the only other source of indoor CO for this analysis. For CO from gas FAFs, the appliance venting factor is the single most important factor in determining the very highest indoor concentrations (e.g., the 5% of houses with highest concentrations, as opposed to the 20% used in this analysis), yet very little is known about this very critical parameter.

Conclusions

In general, the sensitivity analysis results demonstrated the importance of indoor pollutant source emission rates and usage rates in determining which houses have high indoor air pollution levels and, therefore, which population groups are at greatest risk. In addition, the reactivity rate of NO_2 was identified as a very important factor in determining indoor NO_2 levels. The most critical factor for houses with forced-air furnaces leading to very high CO concentrations was the appliance venting factor, yet very little is known about this parameter.

Many of the important causal parameters identified in this report have been ignored

in past IAQ field studies, and this trend must be reversed. Field studies must pay attention to source parameters, appliance venting factors, and at least for NO_2, reactivity rates. Although the sensitivity analysis results show many clear trends, the results are dependent on the input parameters used in the model, and the fine or subtle implications of the sensitivity analyses may not be significant.

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Table I. Macromodel Input Parameters Used in Sensitivity Analyses.[a]

Parameter	Geometric Mean	Geometric Standard Deviation	Empirical Distribution Range
Volume (m^3)			325-775
Specific Leakage Area (cm^2/m^2)	2.84	1.44	
Oven CO Emission Rate (μg/kJ)	38.6	4.1	
Oven NO_2 Emission Rate (μg/kJ)	7.4	1.80	
Range CO Emission Rate (μg/kJ)	81.3	3.1	
Range NO_2 Emission Rate (μg/kJ)	11.8	1.40	
Convective Kerosene Heater CO Emission Rate (μg/kJ)	42.1	3.4	
Forced-Air Furnace CO Emission Rate (μg/kJ)	11.4	6.4	
Smoking RSP Emission Rate (μg/cig)	15,900	1.20	
Oven Usage Rate[b] (kJ/h)	556	1.50	
Range Usage Rate[b] (kJ/h)	566	1.50	
Smoking Rate[b] (cig/h)	0.8	1.50	
NO_2 Reactivity Rate (h^{-1})	0.77	1.69	
RSP Reactivity Rate (h^{-1})	0.08	1.26	
Outdoor CO Concentration (ppm)	0.70	1.20	
Outdoor NO_2 Concentration (ppm)	0.006	1.95	
Outdoor RSP Concentration ($\mu g/m^3$)	19.0	1.50	
Forced-Air Furnace Venting Factor for 6.8% of the Furnaces[c] (unitless)			0.05 to 0.95
House U-values	d	d	

a Data from a previously published report using the Rochester Gas and Electric region, where appropriate.[9]

b Usage rates for convective kerosene heaters and forced-air furnaces were modeled using an indoor/outdoor temperature difference of 23.5° C and a wind speed of 20 km/h.[9]

c Only 6.8% of the forced-air furnaces had non-zero venting factors.

d House U-values calculated from component U-values.[9]

Table II. Sensitivity Analysis for CO from Gas Stoves.

Parameter	Top 20% Geometric Mean	Bottom 80% Geometric Mean	Difference in Geometric Means (%)	D	SR[a]
V (m^3)	499	481	3.7	0.169	5
SLA (cm^2/m^2)	2.37	2.95	-19.7	0.258	3
E_{oven} (μg/kJ)	100	29.3	241	0.381	2
E_{range} (μg/kJ)	204	64.9	214	0.467	1
Q_{oven} (kJ/h)	608	557	9.2	0.093	6
Q_{range} (kJ/h)	658	547	20.3	0.196	4
C_o (ppm)	0.69	0.68	1.5	0.047	7

[a] Significance Ranking

Table III. Sensitivity Analysis for NO_2 from Gas Stoves.

Parameter	Top 20% Geometric Mean	Bottom 80% Geometric Mean	Difference in Geometric Means (%)	D	SR[a]
V (m^3)	459	491	-6.5	0.141	6
SLA (cm^2/m^2)	2.68	2.86	-6.3	0.095	8
E_{oven} (μg/kJ)	9.9	6.9	43.5	0.263	3
E_{range} (μg/kJ)	13.8	11.4	21.1	0.244	4
Q_{oven} (kJ/h)	658	548	20.1	0.175	5
Q_{range} (kJ/h)	700	536	30.6	0.271	2
k (h^{-1})	0.48	0.85	-43.5	0.497	1
C_o (ppm)	0.007	0.006	16.7	0.116	7

[a] Significance Ranking

Table IV. Sensitivity Analysis for RSP from Smoking.

Parameters	Top 20% Geometric Mean	Bottom 80% Geometric Mean	Difference in Geometric Means (%)	D	SR[a]
V (m^3)	477	488	-2.3	0.109	5
SLA (cm^2/m^2)	2.28	3.05	-25.2	0.345	2
$E_{smoking}$ ($\mu g/cig$)	17,500	15,600	12.2	0.259	3
$Q_{smoking}$ (cig/h)	1.23	0.72	70.8	0.572	1
k (h^{-1})	0.076	0.082	-7.3	0.137	4
C_o ($\mu g/m^3$)	19.6	18.8	4.3	0.066	6

[a] Significance Ranking

Table V. Sensitivity Analysis for CO from Convective Kerosene Heaters.

Parameter	Top 20% Geometric Mean	Bottom 80% Geometric Mean	Difference in Geometric Means (%)	D	SR[a]
V (m^3)	494	482	2.5	0.100	4
SLA (cm^2/m^2)	2.54	2.91	-12.7	0.170	2
U (kJ/hm^2 °C)	0.70	0.66	6.1	0.147	3
E_{kero} (μg/kJ)	213	27.5	676	0.820	1
C_o (ppm)	0.69	0.68	1.5	0.044	5

[a] Significance Ranking

Table VI. Sensitivity Analysis for CO from Gas Forced-Air Furnaces.

Parameter	Top 20% Geometric Mean	Bottom 80% Geometric Mean	Difference in Geometric Means (%)	D	SR/[a]
V (m^3)	484	484	0.0	0.025	5
SLA (cm^2/m^2)	2.81	2.83	-0.7	0.021	6
U (kJ/hm^2 °C)	0.68	0.66	3.0	0.066	3
E_{faf} (μg/kJ)	13.0	11.7	11.1	0.046	4
F_v	0.094[b]	0.005[b]	1,780[b]	0.737	2
C_o (ppm)	0.85	0.65	30.8	0.797	1

[a] Significance Ranking

[b] Arithmetic means and differences are used because 93.2% of gas forced-air furnaces had vent factors of zero.

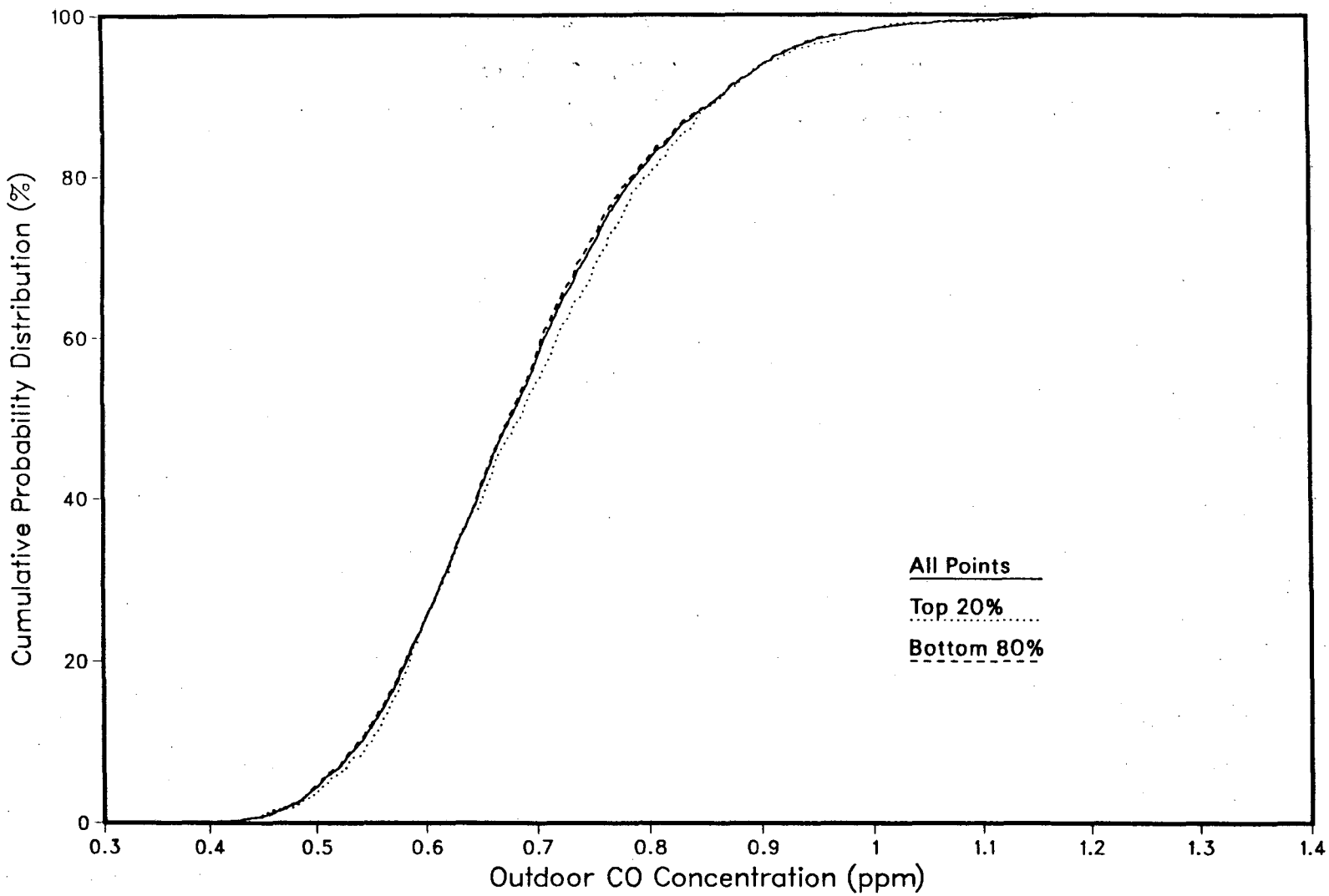

Figure 1. Cumulative outdoor CO concentration distributions for all houses, the 20% of houses with the highest indoor CO concentrations (top 20%), and the 80% of houses with the lowest indoor CO concentrations (bottom 80%).

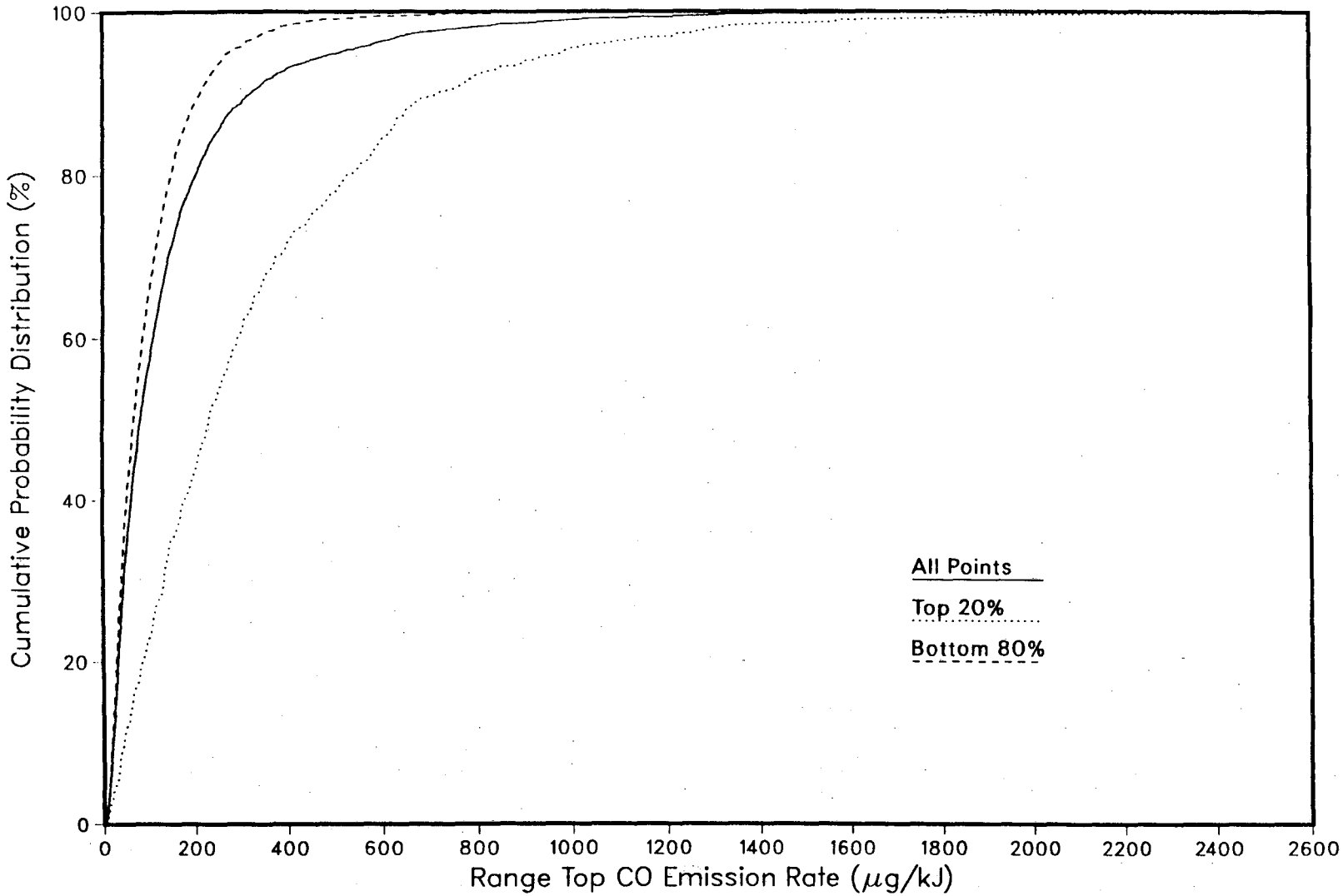

Figure 2. Cumulative range top CO emission rate distributions for all houses, the 20% of houses with the highest indoor CO concentrations (top 20%), and the 80% of houses with the lowest CO indoor concentrations (bottom 80%).

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