Section 7.0

MODEL VERIFICATION AND EVALUATION

A model validation plan was developed for the project (see Appendix D) that included a series of verification steps for Level 1-2 and both verification and evaluation steps for Level 3. Temporary trace files providing intermediate outputs from the Level 1-2 and Level 3 components of the model were programmed as an aid to the verification efforts and were removed from the software after testing was completed. The procedures described below are largely in accordance with the validation plan. Results of evaluation steps (comparisons of model outputs with measurements where such measurements are available) are also presented.

7.1 EXPOSURE/DOSE CALCULATIONS

Strictly speaking, an evaluation cannot be performed for this part of the model. To do so would require concentration inputs for all environments, for a pollutant for which 24-hour personal exposure also has been monitored. There are not, as yet, any pollutants for which this full range of data is available. Indeed, in most cases concentration data are limited to residential environments.

A number of verification efforts were carried out for various components of the exposure/dose model. These efforts were intended to verify the following:

- Proper computation of time spent in different environments at different activity levels, as derived from the original activity data files provided by ARB staff
- Proper choice of matched activity profiles for selected criteria relating to population subgroups
- Proper use of time and concentration inputs in computing exposure
- Proper use of time spent in different environments at various activity levels in computing dose
- Proper summation of exposures and doses across locations

- Proper sampling from each description of the concentration distribution (normal, lognormal, etc.), resulting in statistics and distributional shapes that faithfully depicted the inputs
- Appropriate selection from multiple descriptions of concentration distributions, that is, in accordance with specified weights for each description.

Each of these checks was satisfied by the software, based on independent calculations performed with a calculator or using spreadsheet software. Examples of some of these efforts and their results are provided below.

Proper choice of matched activity profiles was verified by selecting population-subgroup criteria for which the count of matched profiles reported by the model could be compared with counts published by ARB (Wiley et al. 1991). For example, selecting only adults (age 18 or over) should result in 1,579 matches, as reported by the model. Similarly, there should be 1,200 children (under age 12), as also reported by the model. Agreement was found for subsets of adults defined by region (e.g., South Coast), sex, education, age subgroup, county, and month of year and day of week when activities were recorded. As a final check, combinations of criteria were selected (e.g., females in South Coast region), and the results were compared with results of tabulations using SPSS/PC software with the adult activity data base as input. Agreement was found in all cases.

Proper sampling from various types of concentration distributions was verified by comparison of the mean and standard deviation of sampled values with original input specifications and plotting the sampled distributions to verify that the shape of the input distribution was faithfully depicted. For example, proper sampling from normal, lognormal and triangular distributions was verified based on residential concentration inputs for 117 adults whose activity status was "keep house." A normal distribution for residential concentrations was first input, with a mean of 75 $\mu g/m^3$ and a standard deviation of 25. The values sampled by the model averaged 77.5 ± 23.4 $\mu g/m^3$ with a normal shape as shown in the histogram in Figure 7-1. For a lognormal distribution input with a mean of 75 $\mu g/m^3$ and a standard deviation of 50, the sampled values averaged 77.4 ± 45.0 $\mu g/m^3$ and the histogram showed the lognormal shape in Figure 7-2. For a triangular distribution input with a minimum of 0, mode of 75, and maximum of 200 $\mu g/m^3$, the modal interval in

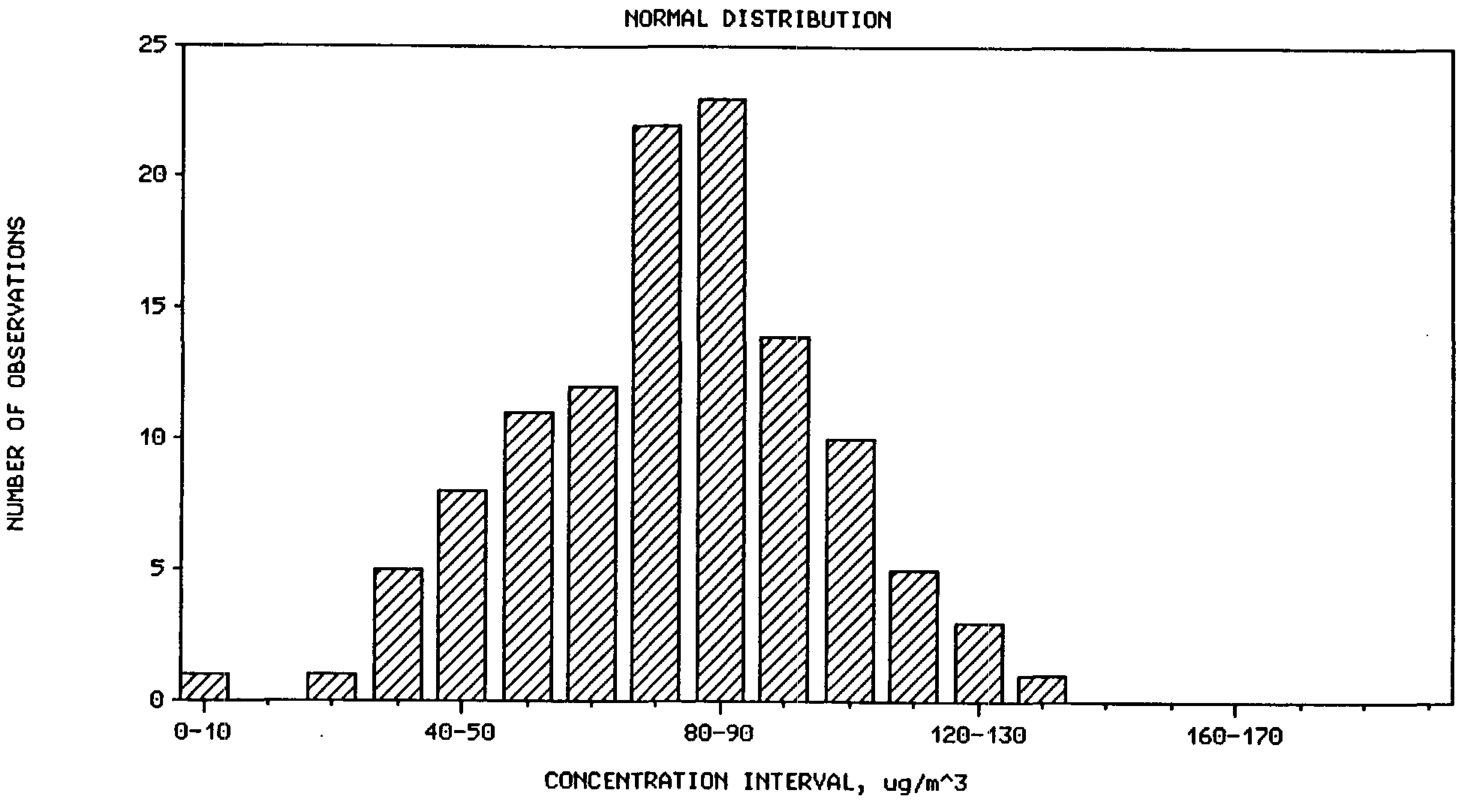

Figure 7-1. Histogram of Values Sampled from a Normal (75, 25) Distribution

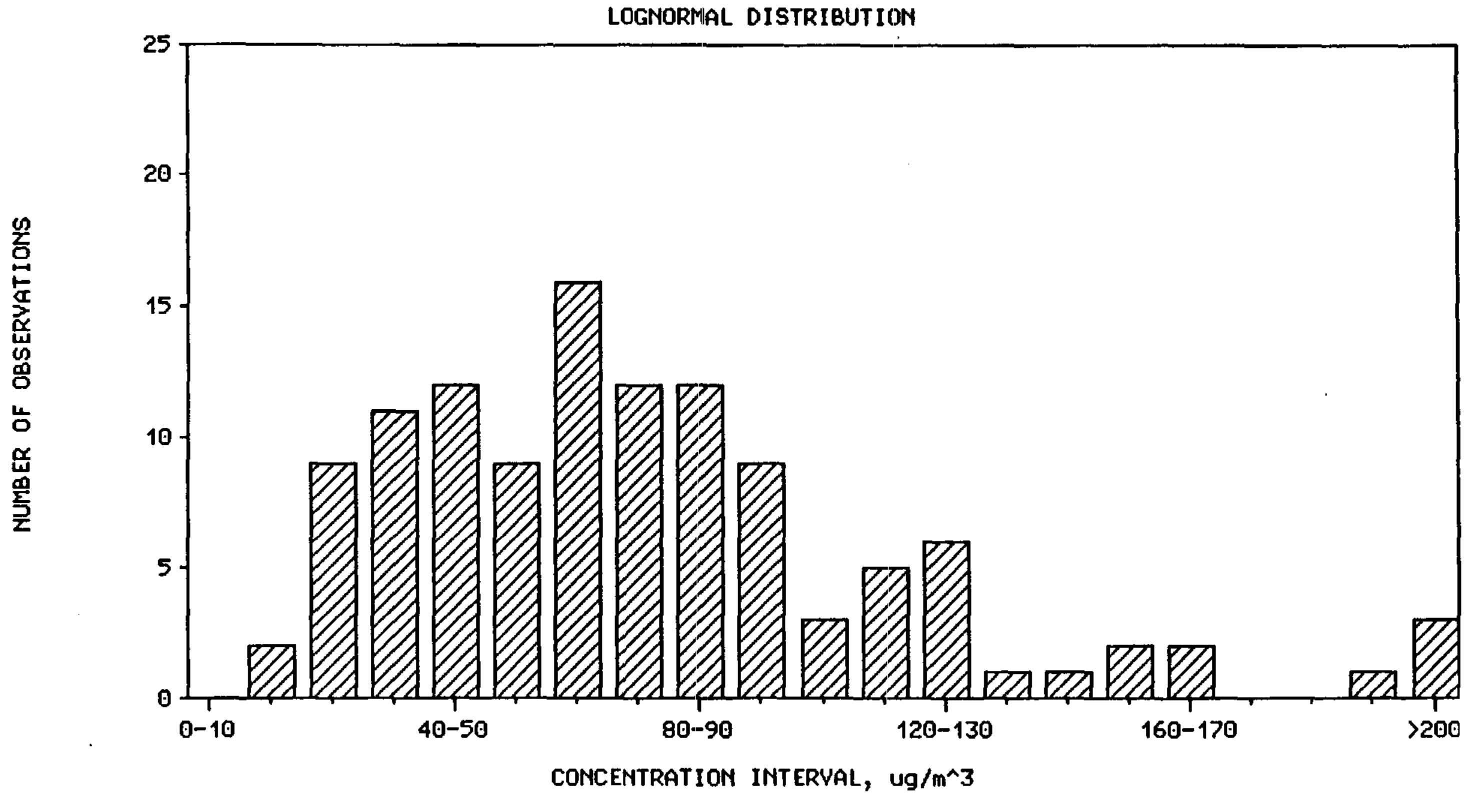

Figure 7-2. Histogram of Values Sampled from a Lognormal (75, 50) Distribution

the histogram (Figure 7-3) was the 70-80 $\mu g/m^3$ interval, the shape approached triangular, and the largest sampled value did not exceed 200 $\mu g/m^3$.

An additional assessment, along the lines of model evaluation, was performed using inputs from the Harvard NO_2 study in Los Angeles. As part of this study (Colome et al. 1992), a subset of participants wore one personal sampler while at home, a second personal sampler while away from home, and a third personal sampler throughout the 24-hour period. The study was conducted in eight different cycles; one of these (cycle 4) was arbitrarily selected for the validation effort. The average concentration for the sampler worn at home was 57.4 ± 34.6 $\mu g/m^3$ (average ± standard deviation) and the average concentration for the sampler worn away from home was 106.1 ± 57.0 $\mu g/m^3$.

To match the conditions of the NO_2 study as closely as possible, activity profiles were selected for individuals in the South Coast area between the ages of 8 and 75 years whose activities were recorded during the winter. A total of 138 matching profiles was found; on the average, these individuals spent 17.8 hours per day at home. Assuming a lognormal distribution, the mean and standard deviation for "at home" monitoring were used for the residential location, and the mean and standard deviation for "away from home" monitoring were assigned for all other locations. Using the same mean and standard deviation for each of the other locations may bias the standard deviation for 24-hour total exposure downward, because certain environments (e.g., travel in vehicle) are likely to exhibit greater variability due to relatively short time spent, in many cases, coupled with inherent variability from place to place (especially for the commuting environment).

The simulation was run ten times to assess the stability of various parameters of the distribution estimated by the model. Average values for each parameter from the model are compared with measurement values from the Harvard study in Table 7-1. The mean modeled "personal exposure" (total exposure across all environments, divided by 24 hours) of 73.0 $\mu g/m^3$ was very close to the measured value of 71.7 $\mu g/m^3$. The modeled standard deviation of 29.9 $\mu g/m^3$ was 11.5 percent lower than the measured value of 33.8 $\mu g/m^3$; as noted above, this downward bias was expected because of the restricted information from which concentration inputs for nonresidential environments were constructed. The

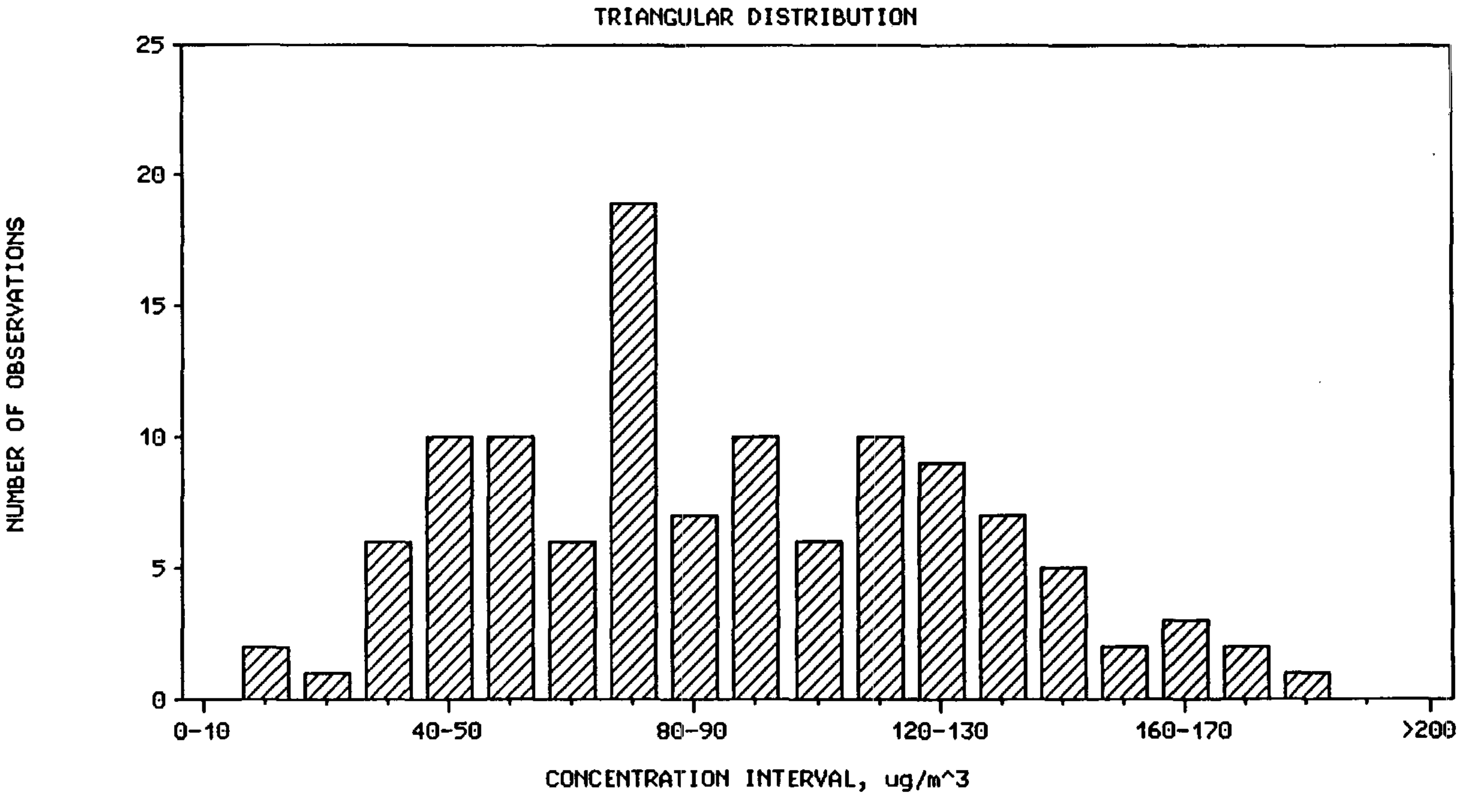

Figure 7-3. Histogram of Values Sampled from a Triangular (0, 75, 200) Distribution

various percentiles of the distributions indicated that the model largely followed the measurements near the center of the distribution but did not capture the minimal and maximal extremes.

Table 7-1. Comparison of Personal Monitoring Measurements and Model Outputs for Nitrogen Dioxide (in $\mu g/m^3$)

Statistics	Harvard Study Measurements	Model Outputs[a]
Average	71.7	73.0
Standard Deviation	33.8	29.9
Minimum	10.5	19.0
10th Percentile	31.6	41.0
25th Percentile	47.4	51.8
50th Percentile	68.5	68.0
75th Percentile	92.2	88.0
90th Percentile	115.9	109.8
Maximum	305.5	203.1

[a] Averaged across 10 model runs with different random number seeds; results of individual runs are shown in Table 7-11.

For the ten separate runs of the model, only the random number seed was changed in going from one run to the next; all concentration inputs were kept constant from run to run. As shown in Table 7-2, most parameters estimates for the modeled distribution were relatively stable, with a standard deviation that was ten percent of the mean or less. The only exceptions were the minimum and maximum, with a coefficient of variation (ratio of the standard deviation to the mean) on the order of 25 percent.

Table 7-2. Summary Statistics on 24-hour-average NO_2 (in $\mu g/m^3$) for Individual Model Runs

Run Number (Random Seed)	Arith. Mean	Std. Deviation	Minimum	Percentiles of the Distribution					Maxi-mum
				10th	25th	50th	75th	90th	
1 (4279)	71.1	26.4	19.3	41.7	55.0	65.2	84.7	103.0	216.0
2 (6351)	71.8	25.2	23.4	41.8	53.0	69.9	85.0	104.2	156.8
3 (9549)	77.5	30.7	20.3	42.2	53.0	71.9	103.4	118.0	192.6
4 (3736)	77.2	36.0	9.5	43.4	56.5	70.9	89.6	114.4	293.8
5 (9476)	71.4	28.4	13.3	40.1	50.5	69.4	90.7	101.2	249.6
6 (1363)	70.9	26.7	19.6	38.5	48.8	67.1	86.6	106.5	143.5
7 (128)	73.9	26.3	23.0	47.6	54.5	68.3	87.4	108.6	156.7
8 (452)	75.2	28.3	23.3	41.9	57.7	70.3	90.9	108.8	166.9
9 (8706)	76.0	33.4	23.8	41.7	55.6	68.0	89.5	117.7	241.8
10 (3016)	75.4	33.1	14.1	40.7	52.7	67.5	90.3	118.7	213.4
Average, all Runs	74.0	29.5	19.0	42.0	53.7	68.9	89.8	110.1	203.1
Std. Deviation	2.6	3.8	5.0	2.4	2.7	2.0	5.3	6.6	48.8
Coefficient of Variation	0.03	0.13	0.26	0.06	0.05	0.03	0.06	0.06	0.24

7.2 CONCENTRATION CALCULATIONS

For evaluation of this component of the model, pollutants were selected for which (1) the various types of model parameters, especially indoor sources, could be reliably quantified from existing information and (2) field monitoring studies have been conducted in California residences to provide a basis for comparison with modeling outputs. The following three pollutants satisfied these criteria:

- Chloroform
- Benzo[a]pyrene
- Nitrogen dioxide.

The subsections that follow describe the assembly of model input parameters for each pollutant and comparisons between measured and modeled residential concentrations.

7.2.1 Chloroform

Residences in the Los Angeles metropolitan area were monitored for various VOCs, including chloroform, as part of the EPA total exposure assessment methodology (TEAM) study that was conducted in February and July of 1987. Chloroform concentrations in drinking water were determined for a subset of the participating households. The concentrations averaged 6.8 ± 3.9 μg/L (mean ± standard deviation) in February and 11.0 ± 3.4 μg/L in July. Although there are some consumer products that can release some quantity of chloroform, water use represents the dominant indoor source. The five primary types of water use are toilet flushes, water draws from faucets, bathing or showering, and use of dishwashers and clothes washers. The inputs required for these sources, other than the chloroform concentration in the water, are the quantities and rates of water use and the volatilization coefficient (i.e., fraction of chloroform volatilized from water); these inputs are summarized for each type of water use in Table 7-3.

Table 7-3. Summary of Existing Information on Rates of Water Use and Volatilization Coefficients

Rate of Use and Volatilization	Type of Indoor Water Use				
	Toilet	Faucet	Bath/Shower	Dishwasher	Clothes Washer
Gallons per Household[a] per Day	84	34	73	15	56
Gallons per Usage Event[a]	3.5[b]	2.1	25[c]	15	45
Volatilization Coefficient[d]	0.95	0.5	0.55	0.9	0.9

[a] Metropolitan Water District of Southern California, "Urban Water Use Characteristics in the Metropolitan Water District of Southern California," draft document dated August 1991.

[b] Values given as 1.6 gallons for 1992 California plumbing code, 3.5 gallons for 1979 code, and 5-7 gallons for pre-1979 code; the intermediate value of 3.5 gallons was chosen.

[c] Values given as 20 gallons for bath, and 25 (1979 code) or 40 (pre-1979 code) gallons for shower; the intermediate value of 25 gallons was chosen.

[d] C.R. Wilkes, M.J. Small, C.I. Davidson, J.B. Andelman, and M.D. Pandian. 1993. "A Human Activity--Indoor Air Quality Model for Predicting Inhalation Exposures to VOCs," presented at Indoor Air '93, Helsinki.

The various types of water use listed above and in Table 7-3 represent frequently occurring indoor sources that are independent of house volume in some cases but correlated in others (i.e., to the extent that larger families occupy larger houses). To achieve better control over inputs for rates of use, the water uses were entered in the model as a frequent source without a loading factor. Inputs are required for usage events per day, duration of the event (in minutes), rate of water use (liters per minute), and chloroform emission rate (μg per liter). Multiplication of the duration, water use rate, and emission rate (performed by the model's calculation routine for emissions) yields the quantity of chloroform (in μg) emitted during each event. Model inputs for these parameters are summarized in Table 7-4. Events per day, rates of water use, and emission rates were input as lognormal distributions with the mean values given in the table and standard deviations as described in footnotes to the table. The event durations were input as constants for each type of water use, by specifying normal distributions with the mean values given in the table and standard deviations set to zero. The model for frequent sources also requires inputs for the distribution of events by time of day. The distributions given in Table 7-5 were arbitrarily chosen to spread the events across the day while giving higher percentage weights to selected morning and evening hours.

The remaining inputs required for the model relate to the distributions for outdoor concentrations, penetration factors, indoor sinks, and air exchange rates. The input values used for these model parameters are summarized in Table 7-6. Season-specific (February and July) values were provided for outdoor concentrations and air exchange rates. For both of these parameters, as well as the indoor volumes, the parameter estimates were based on measurements that were taken as part of the TEAM study. Little information was available to guide the choice of inputs for penetration factors and indoor sinks; as a conservative approach, it was assumed that chloroform concentrations outdoors can penetrate to indoors without any intermediate losses (constant value of 1 used as input) and that there are no losses to indoor sinks (constant value of 0 used as input).

Table 7-4. Inputs for Five Types of Indoor Water Use Modeled as Frequent Sources

Model Input Parameters	Type of Indoor Water Use				
	Toilet	Faucet	Bath/Shower	Dishwasher	Clothes Washer
Usage Events per Day	24[a]	16[a]	3[a]	1[b]	1.25[c]
Duration of Event (min)	1	1	15	45	30
Rate of Water Use (L/min)[d]	13.25	7.95	6.31	1.26	5.68
Chloroform Emission Rate (μg/L)[e]					
Winter (Feb. 1987)	6.5	3.4	3.7	6.1	6.1
Summer (July 1987)	10.5	5.5	6.1	9.9	9.9

[a] Input as a lognormal distribution with a mean equal to the indicated value and a standard deviation equal to 50% of the mean.

[b] Input as a frequency distribution as follows:
0 events - 25%
1 event - 50%
2 events - 25%

[c] Input as a frequency distribution as follows:
0 events - 25%
1 event - 45%
2 events - 15%
3 events - 10%
4 events - 5%

[d] Input as a lognormal distribution with a mean equal to the indicated value and a standard deviation equal to 25% of the mean.

[e] Input as a lognormal distribution with a mean ± standard deviation equal to winter values (6.8 ± 3.9) or summer values (11.0 ± 3.4) multiplied by the volatilization coefficients given in Table 7-1.

Table 7-5. Time-of-Day Distribution (%) for Five Types of Indoor Water Use

Hour of Day	Type of Indoor Water Use				
	Toilet	Faucet	Bath/Shower	Dishwasher	Clothes Washer
00-01	1	1	0	0	0
01-02	1	1	0	0	0
02-03	1	1	0	0	0
03-04	1	1	0	0	0
04-05	1	1	0	0	0
05-06	1	1	0	0	0
06-07	5	5	10	0	0
07-08	8	8	10	0	0
08-09	8	8	5	0	0
09-10	5	5	5	5	5
10-11	5	5	5	5	5
11-12	5	5	5	5	5
12-13	5	5	5	5	10
13-14	5	5	5	10	10
14-15	5	5	5	5	5
15-16	5	5	5	5	5
16-17	5	5	5	5	5
17-18	5	5	5	5	10
18-19	8	8	5	15	10
19-20	8	8	5	15	10
20-21	5	5	10	10	10
21-22	5	5	10	10	5
22-23	1	1	0	0	5
23-24	1	1	0	0	0

Table 7-6. Model Inputs for Outdoor Concentrations, Penetration Factors, Indoor Sinks, Volumes, and Air Exchange Rates

Input Parameter	Type of Distribution	Mean	Standard Deviation
Outdoor Concentrations, μg/m³			
February	Lognormal	0.49	0.80
July	Lognormal	0.79	1.36
Penetration Factors	Normal	1	0
Indoor Sinks, 1/h	Normal	0	0
Volumes, m³	Lognormal	274.9	110.6
Air Exchange Rates, 1/h			
February	Lognormal	0.94	0.82
July	Lognormal	2.83	2.54

One run with 100 trials was made for each season, with a random number seed of 649 for February and 8658 for July. The results of these initial evaluation runs are summarized in Table 7-7 as comparisons between measurements and model outputs for selected statistics describing their respective distributions. Although there is general agreement, as indicated by the model average being within 1 μg/m³ of the measured average and differing by no more than 50 percent, there is some evidence of systematic departures. In particular, the standard deviation for model outputs is consistently lower, relative to the mean (see the coefficient of variation in Table 7-7), than for the field measurements. One reason for this type of departure is that the five types of water use are input to the model as five separate sources. With this approach, the model will randomly select an emission rate for each type of source within a given house, resulting in variable source-specific emission rates for the house. In reality, however, the emission rates in a given house will tend to be highly correlated across the various types of water uses.

Table 7-7. Comparison of Field Measurements and Initial Modeling Outputs for Chloroform (in $\mu g/m^3$)

	February		July	
Statistics	TEAM Study Measurements	Model Outputs	TEAM Study Measurements	Model Outputs
Average	1.41	2.16	1.20	1.55
Standard Deviation	1.52	1.90	1.65	1.35
Coefficient of Variation	1.08	0.88	1.38	0.87
Minimum	0.07	0.18	0.07	0.12
10th Percentile	0.11	0.43	0.07	0.52
25th Percentile	0.34	0.99	0.34	0.75
50th Percentile	0.97	1.71	0.65	1.15
75th Percentile	1.79	2.63	1.28	1.93
90th Percentile	3.64	4.42	2.47	2.74
Maximum	7.23	10.54	7.79	10.24

To overcome this potential deficiency, all types of water use were combined to represent a single indoor source. The average household water use for the Los Angeles area, 262 gallons or 992 liters, was treated as an average of 10 uses per day at a rate of 99.2 liters per use. As shown in Table 7-8, the uses per day and water use per event were input as lognormal distributions with the above averages and arbitrarily assigned standard deviations, to provide variability across houses for these parameters. For consistency with model calculations of the indoor source term, the event duration was set to a constant value of 1 minute (an equivalent result could have been obtained, for example, by using a constant duration of 10 minutes and an average use rate of 9.92 liters per minute). The chloroform emission rates for February and July were obtained by weighting the emission rates specific to each type of water use (Table 7-4) by their respective daily usage rates (gallons per household per day, Table 7-3). All other model input parameters (outdoor concentrations, etc.) were kept as before (Table 7-6). The distribution given in Table 7-9 for usage events by time of day was assumed.

Table 7-8. Model Inputs for Combined Chloroform Sources

Input Parameter	Type of Distribution	Mean	Standard Deviation
Usage Events per Day	Lognormal	10	5
Duration of Event (min)	Normal	1	0
Rate of Water Use (L/min)	Lognormal	99.2	24.8
Chloroform Emission Rate (μg/L)			
February	Lognormal	5.2	3.0
July	Lognormal	8.5	2.6

Table 7-9. Time-of-Day Distribution (%) for Combined Chloroform Sources

Time of Day	Percent	Time of Day	Percent
00-01	1	12-13	6
01-02	1	13-14	4
02-03	1	14-15	4
03-04	1	15-16	4
04-05	1	16-17	6
05-06	2	17-18	8
06-07	4	18-19	8
07-08	6	19-20	8
08-09	8	20-21	6
09-10	6	21-22	4
10-11	4	22-23	2
11-12	4	23-24	1

The modeling results based on the refined inputs, using combined sources, are compared with measurement results from the TEAM study in Table 7-10. The model was run three times for each time period, changing only the random number seed, to explore the variability in model outputs. For these runs, the model outputs were closer to the measurement results in terms of the coefficient of variation (ratio of the standard deviation to the mean). The mean model output generally was about 50 percent higher than the mean measurement result, and model-based estimates for various percentiles of the distribution generally were higher than measurement-based estimates throughout the distribution. This systematic difference could be largely due to the conservative model inputs of 100 percent penetration of outdoor concentrations and no losses to indoor sinks, but may also be due in part to over- estimates of inputs such as frequency/rate of water use.

7.2.2 Benzo[a]pyrene

Residences in Riverside, California, were monitored for various PAHs, including benzo[a]pyrene (BaP), as part of the PTEAM study conducted in the fall of 1990. Both indoor and outdoor concentrations were measured. Based on a mass-balance modeling approach, the researchers (Sheldon et al. 1992b) estimated penetration factors for the subset of homes with no apparent indoor sources and estimated average emission rates in homes with apparent sources, assuming that the average penetration factor estimated from "no source" homes prevailed in the "source" homes. Both of the estimates were based on the assumption of a zero sink rate (i.e., no pollutant decay indoors).

The average source strength (arithmetic mean) estimated from the PTEAM study was 390 ng/h, with a range from near zero to 8800 ng/h. Such a skewed distribution is best represented as lognormal. The standard deviation about the average source strength was not provided by the researchers, but was estimated using limited statistics that they reported. More specifically, the source strength was assumed to be 5 ng/h for the first through the 25th percentiles of the distribution, 10 ng/h for the 26th through the 50th percentiles, and 20 ng/h for the 51st through 75th percentiles. For the 76th and higher percentiles, the preceding value was multiplied by a constant value of 1.27, yielding 25.4 ng/h for the 76th percentile, 32.3 ng/h for the 77th percentile, and so on, with a value of

Table 7-10. Comparison of Field Measurements and Refined Model Outputs (Combined Sources) for Chloroform (in $\mu g/m^3$)

Statistics	TEAM Study Measurements	Model Outputs[a] Run 1	Run 2	Run 3
February				
Average	1.41	1.52	1.96	2.12
Std. Deviation	1.52	1.29	1.55	2.71
Coefficient of Variation	1.08	0.85	0.79	1.28
Minimum	0.07	0.20	0.07	0.21
10th Percentile	0.11	0.40	0.40	0.44
25th Percentile	0.34	0.57	0.73	0.78
50th Percentile	0.97	0.99	1.50	1.33
75th Percentile	1.79	1.97	2.76	2.31
90th Percentile	3.64	3.41	3.98	3.97
Maximum	7.23	6.71	7.55	23.00
July				
Average	1.20	1.81	1.68	1.66
Std. Deviation	1.65	2.09	1.46	1.48
Coefficient of Variation	1.38	1.15	0.87	0.89
Minimum	0.07	0.20	0.23	0.08
10th Percentile	0.07	0.42	0.40	0.43
25th Percentile	0.34	0.65	0.62	0.75
50th Percentile	0.65	1.20	1.23	1.15
75th Percentile	1.28	2.39	2.28	1.96
90th Percentile	2.47	3.52	3.45	2.92
Maximum	7.79	16.43	7.91	8.71

[a] The model was run three times, changing only the random number seed, to explore the variability in statistics across runs; the seeds were 649, 5718 and 2967 for February and 8658, 257 and 5754 for July.

6199 ng/h ultimately assigned to the 99th percentile. The reported maximum of 8800 ng/l was also used. The average source strength across the 100 values so constructed was near 390 ng/h, with a standard deviation of 1,285; this value is close to that (1,467) obtained using the range divided by six (i.e., 8,800/6) as a rough indicator of the magnitude of the standard deviation.

Model input parameters are summarized in Table 7-11. Because an average source strength was used, based on researchers' estimates from a steady-state model, the indoor BaP source was modeled as a long-term (always present) source that is independent of the house volume. Based on information provided by the PTEAM researchers, it was assumed that BaP sources were present in 28 percent of the homes. The source strength was input as a lognormal distribution with a mean and standard deviation as indicated above. The outdoor concentration was also modeled as a lognormal distribution with a mean and standard deviation as reported from the PTEAM study. The penetration factor and decay rate (indoor sink) were each set to constant values (0.6 and 0, respectively), consistent with values estimated or assumed by the PTEAM researchers. Parameter estimates for indoor volume distributions from three studies in Southern California were input with equal weights, and the distribution for the air exchange rate was based on estimates reported from the PTEAM study.

Ten separate runs of the model were made, using the inputs described in Table 7-11 and changing only the random number seed in going from one run to the next. Average values across the 10 runs for various statistics describing the modeled distribution are compared with measurement-based statistics in Table 7-12. Model-based estimates for the mean and percentiles through the 75th are very consistent with those based on measurements, but there are differences at the 90th percentile and for the standard deviation. As shown in Table 7-13, parameter estimates for the standard deviation, 90th percentile and maximum values are relatively unstable (indicated by a relatively large standard deviation across model runs in comparison to the mean) because the distribution for the emission rate has a broad tail, as indicated in Table 7-11 by a standard deviation that is more than three times the mean.

Table 7-11. Summary of Model Inputs for Benzo[a]pyrene

Input Parameter	Distribution/Value
Percent of Residences with Indoor Sources	28
Number of Indoor Sources	Normal (1,0)[a]
Emission Rate, ng/h	Lognormal (390, 1285)
Outdoor Concentration, ng/m^3	Lognormal (0.30, 0.36)
Penetration Factor	Normal (0.6, 0)
Indoor Sink, 1/h	Normal (0,0)
Indoor Volume, m^3	
TEAM Study[b]	Lognormal (274.9, 110.6)
SoCal Study	Lognormal (309.5, 159.8)
ADM Study	Lognormal (354, 101)
Air Exchange Rate, 1/h	Lognormal (1.25, 1.02)

[a] Values in parentheses are the mean and standard deviation of the distribution

[b] Inputs for volume from three different studies in Southern California were equally weighted

Table 7-12. Comparison of Field Measurements and Model Outputs for Benzo[a]pyrene (in ng/m^3)

Statistics	PTEAM Study Measurements	Model Outputs[a]
Average	0.70	0.68
Standard Deviation	4.00	2.17
Minimum	NR[b]	0.02
10th Percentile	NQ[c]	0.04
25th Percentile	0.08	0.08
50th Percentile	0.19	0.15
75th Percentile	0.36	0.36
90th Percentile	0.65	1.15
Maximum	NR	17.6

[a] Averages across 10 model runs with different random number seeds; results of individual runs are shown in Table 7-13.

[b] Not reported.

[c] Not quantifiable (below the measurement method's quantifiable limit).

Table 7-13. Summary Statistics for Individual Model Runs for Benzo[a]pyrene (in ng/m^3)

Run Number (Random Seed)	Arith. Mean	Std. Deviation	Minimum	Percentiles of the Distribution					Maximum
				10th	25th	50th	75th	90th	
1 (8740)	0.70	1.86	0.01	0.05	0.07	0.16	0.35	1.21	13.8
2 (6611)	0.42	1.04	0.02	0.05	0.08	0.14	0.29	0.65	7.2
3 (903)	0.64	2.94	0.02	0.04	0.07	0.14	0.32	0.81	28.5
4 (9296)	0.44	0.86	0.02	0.04	0.09	0.19	0.41	0.82	5.3
5 (4515)	1.31	5.58	0.01	0.03	0.07	0.12	0.38	1.07	42.4
6 (544)	0.72	3.02	0.02	0.05	0.07	0.14	0.34	0.70	27.9
7 (1852)	0.66	1.58	0.01	0.05	0.08	0.17	0.45	1.55	11.7
8 (3820)	0.63	1.43	0.01	0.05	0.08	0.15	0.33	1.86	11.3
9 (532)	0.60	1.47	0.01	0.04	0.07	0.15	0.28	1.72	10.9
10 (6459)	0.63	1.91	0.02	0.04	0.08	0.14	0.46	1.08	17.2
Average, all Runs	0.68	2.17	0.02	0.04	0.08	0.15	0.36	1.15	17.6
Std. Deviation	0.24	1.39	0.01	0.01	0.01	0.02	0.06	0.43	11.7
Coefficient of Variation	0.35	0.64	0.50	0.25	0.13	0.13	0.17	0.37	0.66

7.2.3 Nitrogen Dioxide

Residences in the Los Angeles metropolitan area were monitored for NO_2 as part of a field study conducted by the Harvard University School of Public Health between May 1987 and May 1988. Both indoor and outdoor NO_2 concentrations were measured over a 48-hour period, and measurements were taken at various times throughout the year.

The primary source of NO_2 indoors is use of a gas range for cooking breakfast, lunch or dinner. Model inputs relating to this source, derived from the Harvard study and published/unpublished data from the gas industry, are summarized in Table 7-14. The three primary uses of the range -- cooking breakfast, lunch and dinner -- were initially modeled as separate sources. The Harvard researchers reported that 73.3 percent of the study homes had gas ranges. Average fuel consumption by the range for cooking, based on unpublished data from the gas industry, is 2.56 ± 2.93 ft^3 (average ± standard deviation) for breakfast, 4.33 ± 5.10 ft^3 for lunch, and 6.19 ± 5.34 ft^3 for dinner. Assuming a heating value of 1,030 Btu/ft^3, these values translate to an average of 2636.8 Btu for breakfast, 4459.9 Btu for lunch, and 6375.7 Btu for dinner. Using an average fuel input rate of 150 Btu/minute (9,000 Btu per hour), roughly equivalent to that of one range top burner at full input or a cycling oven, the fuel inputs translate to an average duration of 17.6 minutes for breakfast, 29.7 minutes for lunch, and 42.5 minutes for dinner, as shown in the table. The distribution of the emission rate for the gas range was based on published data from the gas industry (Billick 1988). The estimates for percent of days on which each meal is cooked were based on a survey (Koontz et al. 1992) indicating that the range is used an average of 2.4 days per week for cooking breakfast, 2.1 days for lunch, and 4.9 days for dinner. The times of day for cooking each meal were arbitrarily chosen to provide some separation in time between individual cooking events within households.

Table 7-14. Summary of Model Inputs for Cooking Meals

Input Parameter	Breakfast	Lunch	Dinner
Percent of Residences with Indoor Source	73.3[a]	73.3[a]	73.3
Quantity Used (Btu/min)	Lognormal (150, 50)	Lognormal (150, 50)	Lognormal (150, 50)
Episodes per Day (0,1)	66%, 34%	70%, 30%	30%, 70%
Hour of Day	07-08	12-13	18-19
Duration (min)	Lognormal (17.6, 20.1)	Lognormal (29.7, 35.0)	Lognormal (42.5, 36.7)
Emission Rate (μg/Btu)	Normal (9.15, 2.3)	Normal (9.15, 2.3)	Normal (9.15, 2.3)

[a] Modeled as 100 percent of cases, linked to dinner cooking (73.3 percent of cases).

The other major indoor source of NO_2 is the pilot light(s) present on some gas ranges. This source was modeled as a long-term source whose magnitude is independent of the house volume. The amount of fuel consumed by range pilot lights, based on unpublished data from the gas industry, ranges from 3 ft^3 per day (3,090 Btu/day or 128.8 Btu/hour) to 15 ft^3 per day (643.8 Btu/hour), with intermediate values of 6, 8 and 10 ft^3 per day for the 25th, 50th and 75th percentiles, respectively. The Harvard researchers reported that 68.1 percent of the ranges in their study homes had pilot lights. This source was input with a link to dinner cooking so that pilot lights would only appear as a source within a subset of the 73.3 percent of households with gas ranges. The emission-rate distribution for pilot lights was assumed to be the same as that for range cooking (see Table 7-14).

Values used for the remaining model inputs are summarized in Table 7-15. The distribution of outdoor NO_2 concentrations was that measured by the Harvard researchers outside their study homes. A penetration factor of one was assumed for all homes. One source (Billick 1988) reported an average NO_2 decay rate of 0.5/hour and another (Spicer et al. 1989) reported an average rate of 0.8/hour. Thus, the model was run twice to accommodate these two different estimates. The Harvard researchers did not report the volumes or air exchange rates for their study homes. Model inputs for volume were based on two other studies (equally weighted) in the Los Angeles area, and six estimates of the distribution of air exchange rates at different times of the year for Los Angeles were equally weighted as inputs for this modeling parameter.

Table 7-15. Model Inputs for Outdoor Concentrations, Penetration Factors, Indoor Sinks, Volumes, and Air Exchange Rates

Input Parameter	Type of Distribution	Mean	Standard Deviation
Outdoor Concentrations, $\mu g/m^3$	Lognormal	72.0	39.3
Penetration Factors	Normal	1	0
Indoor Sinks, 1/h	Lognormal	0.5 (0.8)	0.3
Volumes, m^3			
TEAM Study	Lognormal	274.9	110.6
SoCal Study	Lognormal	309.5	159.8
Air Exchange Rates, 1/h			
TEAM Study (Feb.)	Lognormal	0.94	0.82
TEAM Study (July)	Lognormal	2.83	2.54
SoCal Study (Mar.)	Lognormal	0.78	0.63
SoCal Study (July)	Lognormal	1.51	1.47
SoCal Study (Jan.)	Lognormal	0.58	0.47
Cal IAQ Study	Lognormal	0.77	0.57

As shown in Table 7-16, the outputs of the model run assuming an average decay rate of 0.8/hour best matched the measurement results, in terms of the average indoor NO_2 concentration across houses. As with chloroform, the standard deviation from modeling underestimated that based on measurements. Treating the three meals separately in the model resulted in assignment of a variable emission rate to the range in each household. For a revised model run, the cooking events for the three meals were combined into a single source (Table 7-17) with up to three episodes per day. The percentage distribution in the table for episodes per day provides an average of 1.35 episodes per day, consistent with published data indicating an average of 9.4 episodes per week. The distribution for hour of day in the table was intended to proportionally represent the times when breakfast, lunch or dinner would be cooked. The distribution for cooking duration was synthesized, through a Monte Carlo simulation using Level 1-2 of the model, from the respective distributions for each meal. The assumed distribution for the emission rate was kept the same as before.

Table 7-16. Comparison[a] of Field Measurements and Initial Modeling Outputs for Nitrogen Dioxide (in $\mu g/m^3$)

Statistics	Measurements from Harvard Study	Model with Average Decay Rate of 0.5/h	Model with Average Decay Rate of 0.8/h
Average	·51.2	62.9	50.2
Standard Deviation	30.4	31.3	24.8
Minimum	6.6	16.6	12.5
10th Percentile	18.7	27.0	21.4
25th Percentile	31.4	38.7	29.7
50th Percentile	46.3	55.1	46.1
75th Percentile	65.8	81.6	64.4
90th Percentile	84.3	101.5	75.9
Maximum	289.4	167.9	131.6

[a] The field-measurement results are based on a 48-hour averaging period, whereas the modeling results are based on a 24-hour averaging period; a smaller standard deviation would be expected for a longer averaging period, other things being equal.

Table 7-17. Summary of Model Inputs for Combined Cooking Events

Input Parameter	Distribution/Value(s)
Percent of Residences with Indoor Source	73.3%
Quantity Used (Btu/min)	Lognormal (150, 50)
Episodes per Day	
0	15%
1	50%
2	20%
3	15%
Hour of Day	
07-08	26%
12-13	22%
18-19	52%
Duration (min)	Lognormal (33.3, 33.3)
Initial Emission Rate (μg/Btu)	Normal (9.15, 2.3)
Decline in Rate (inverse hours)	Normal (0, 0)

The comparison of initial model outputs with measurements (Table 7-16) also indicated that the model underestimated the tail (90th percentile and above) of the measured indoor NO_2 distribution. The values near the tail are believed to represent isolated cases where the range was used as a source of supplemental heat. For the Harvard study, 11.1 percent of participating homes indicated that the range was sometimes used as a source of heat. Because such usage occurs only during the winter and NO_2 modeling was intended to represent the entire year, this percentage was reduced by a factor of four (to 2.8 percent). Range use for heating was modeled as a frequent source with one episode per day on 34 percent of days (zero episodes otherwise), consistent with published estimates (Koontz et al. 1992) of range use for heating on an average of 2.4 days per week during the winter. A fuel input rate of 300 Btu/minute (18,000 Btu/hour) was assumed together with an average duration of 144 ± 72 minutes (lognormal distribution), consistent with published estimates of 2.4 hours per day as the average duration of range use for heating. The time of use (start hour) was assumed to be late evening (hours 8-9 and 9-10) or early morning (hours 5-6 and 6-7). The emission rate was assumed to be the same as that for range cooking and range pilot lights.

Ten separate runs of the refined model were made, using a different random number seed for each run. Average values across the 10 runs for various statistics describing the modeled distribution are compared with measurement-based statistics in Table 7-18. Model-based estimates for the mean, standard deviation and percentiles through the 90th are very consistent with those based on measurements. On the average, the model output underestimated the maximum of the measured distribution, but one of the individual model runs (Table 7-19) had a maximum (247 $\mu g/m^3$) approaching the measured maximum (289 $\mu g/m^3$) . Most of the modeled parameters of the distribution were relatively stable, with a coefficient of variation (CV, ratio of the standard deviation across the 10 runs to the average) of less than 10 percent. The exceptions were the standard deviation, with a CV of 17 percent, the minimum, with a CV of 20 percent, and the maximum, with a CV of 24 percent.

Table 7-18. Comparison of Field Measurements and Refined Modeling Outputs for Nitrogen Dioxide (in $\mu g/m^3$)

Statistics	Harvard Study Measurements	Model Outputs[a]
Average	51.2	50.5
Standard Deviation	30.4	28.5
Minimum	6.6	10.3
10th Percentile	18.7	21.3
25th Percentile	31.4	30.1
50th Percentile	46.3	44.5
75th Percentile	65.8	63.4
90th Percentile	84.3	83.5
Maximum	289.4	163.2

[a] Averages across 10 model runs with different random number seeds; results of individual runs are shown in Table 7-19.

Table 7-19. Summary Statistics for Individual Model Runs for Nitrogen Dioxide (in $\mu g/m^3$)

Run Number (Random Seed)	Arith. Mean	Std. Deviation	Minimum	Percentiles of the Distribution					Maxi-mum
				10th	25th	50th	75th	90th	
1 (1096)	48.6	28.4	13.4	22.7	28.7	40.4	60.7	79.1	154.1
2 (4105)	51.6	25.6	12.5	22.6	28.8	49.0	68.2	83.6	126.0
3 (6593)	51.2	30.3	7.4	20.5	29.9	47.4	60.8	82.8	189.9
4 (4931)	48.6	31.0	9.9	18.6	27.5	40.6	62.1	87.9	183.8
5 (7654)	50.3	27.0	10.6	24.2	30.2	43.7	62.0	86.7	141.8
6 (9752)	58.3	34.9	10.3	21.5	33.1	50.1	76.1	99.4	181.3
7 (2858)	45.2	23.1	8.0	21.3	30.3	41.2	54.4	71.2	160.1
8 (1822)	54.6	37.2	9.1	23.1	31.5	45.2	65.1	86.0	247.5
9 (2531)	45.4	24.5	8.9	17.6	27.7	39.7	57.1	76.4	137.4
10 (610)	50.8	23.0	13.0	20.8	33.3	47.9	67.3	82.2	110.4
Average, all Runs	50.5	28.5	10.3	21.3	30.1	44.5	63.4	83.5	163.2
Std. Deviation	3.9	4.9	2.1	2.0	2.0	3.9	6.1	7.5	39.4
Coefficient of Variation	0.08	0.17	0.20	0.09	0.07	0.09	0.10	0.09	0.24

7.3 DISCUSSION OF EVALUATION RESULTS

Verification steps for the Level 1-2 module indicated that inputs (activity profiles, concentration distributions) are properly accessed and used by the model, and that exposures and doses are correctly computed and accumulated across environments. Evaluation of Level 1-2 estimates, based on data from an NO_2 study in Los Angeles that included both personal and stationary monitoring, indicated (1) that the average total (personal) exposure estimated from the simulation agreed closely with that based on the field study, and (2) that the standard deviation of the modeled exposure distribution was about 11 percent lower than that for the field study. This downward bias in the standard deviation was expected because of the limited information available for constructing concentration inputs for environments other than the residence.

Estimates from the Level 3 module for the residential environment were evaluated for three pollutants--chloroform, benzo[a]pyrene (BaP) and nitrogen dioxide (NO_2). For both chloroform and NO_2 the modeled standard deviation, relative to the mean, initially was lower than that for field measurements. This is believed to be due to an initial separate description of each type of indoor source (water uses for chloroform and cooking meals for NO_2). When the sources were described in this manner, the model sampled a different emission rate for each source within each trial, whereas the emission rates are likely to be very similar. When these sources were combined, to enable a common emission rate within each residence, the modeled ratio of the standard deviation to the mean better reflected the ratio based on measurements. These outcomes suggest that similar types of indoor sources should be combined whenever possible.

For BaP, a single long-term source was modeled that had a lognormal distribution with a broad tail. Model-based estimates for the mean and percentiles through the 75th were very consistent with those based on measurements, but there were differences toward the upper tail of the distribution. Because the percentiles near either tail of the distribution tend to be less stable statistically than measures of central tendency such as the mean, the model should be run with a sufficient number of trials (e.g., 500) to increase the stability of such parameter estimates.

Although the principles on which both components of the model are based are scientifically and mathematically sound, the accuracy of the outputs is limited by that of the inputs. Data on concentration distributions, needed for Level 1-2 of the model, are not yet available for many of the environments. For Level 3 of the model, there is a notable lack of information at present for many of the indoor sources as well as pollutant-specific penetration factors and decay rates.

All estimates provided by the model are subject to some degree of uncertainty, but the model offers a means to estimate this uncertainty. Once the user has specified all inputs, the model can be run several times with all inputs the same except the random number seed. Variability for each output parameter (e.g., average exposure, 95th percentile of the exposure distribution) across repeated model runs can then be characterized through a measure such as the coefficient of variation.

Section 8.0

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Appendix A

SOFTWARE REQUIREMENTS DOCUMENT

Software Requirements Document

California Air Resources Board

Indoor Exposure Model

Revision 3.00 May 15, 1992

REQUIREMENT 1

The model shall perform its calculations for a time interval of 24 hours (one day).

TYPE: Processing

ORIGIN: Implicit (not explicitly stated in RFP)

COMMENTS: The model needs some defined time interval over which to perform the calculations.

REQUIREMENT 2

The model shall calculate exposures and doses, for averaging/integrating times of 1, 8, 12, or 24 hours, depending on the specific contaminant for which calculations are requested by the user.

TYPE: Processing, input

ORIGIN: RFP page 3

COMMENTS: The "exposure" is defined as the time-weighted average pollutant concentration encountered by an individual in the course of his/her daily activities. The "dose" (amount inhaled) is the time integral of the product of the exposed person's breathing rate and the concentration encountered. These averaging or integration times are not specified in the RFP, which refers only to "several."

Although, in concept, the user can select from the three choices given above, the integrating time in most cases will be dictated by the time base of available concentration data. The program will indicate a default averaging/integrating time equal to the time base of the concentration data, when available.

Depending on the pollutant, either an integrating time or an averaging time, or both, may apply. For air toxics (e.g., VOCs), whose primary health effects are long term (e.g., cancer), the notion of a 24-hour integrating time is more appropriate. For criteria pollutants much as CO and NO_2 that may have short-term effects, the notion of an averaging time (i.e., average hourly or daily concentration encountered) may be more applicable. For CO, an 8-hour averaging period (i.e., running 8-hour averages) will also be provided as an option. For each model run, the user will have the option to calculate exposure, dose, or both of these quantities.

REQUIREMENT 3

The random number seed for each run shall be read from the system clock; there shall also be an option to override the clock value and force the seed to a user-specified value.

TYPE: Processing, input

ORIGIN: Not in RFP

COMMENTS: The pseudorandom-number seeding of a Monte Carlo simulation is of vital importance, and needs to be controllable by the user. The seed will be displayed, and also stored in the main output file (this file is optional; see Requirement 4), and there will be an option to force the seed to a particular value, so that a run can be exactly reproduced. The option to force the seed can also be used in mitigation studies, if the program is designed to accommodate this variance-reduction strategy (TBD). Reading the seed from the clock, as a default, eliminates the need for the user to invent a new seed for each run; displaying/storing and inputting it will allow a run to be replicated, as needed.

REQUIREMENT 4

The model shall find estimates of the differential (density) and cumulative probability distribution functions, for a user-input sample size, for concentration, exposure, and inhaled dose.

TYPE: Processing, input, output

ORIGIN: Pages 3, 7, 8 in RFP

COMMENTS: The RFP is silent on the required form(s) of model output; see Requirement 13. The PDF and CDF information will be presented in the form of on-screen and printer (option) percentile tabulations, and on-screen plots. An option to write the distribution information, and the random-number seed, to a disk file will be provided. Summary statistics (mean, median, standard deviation) also will be provided. The percentile tabulations will be provided in 5% increments.

The sample size is not addressed as a user input in the RFP (page 8: "sufficient number of iterations"); in Monte Carlo analysis the sample size is driven by considerations of the precision of the final (output) estimator. The model will present one or more "default" sample sizes to choose from, in addition to accepting a user-input value. One of the default values will be the sample size of the population being studied in that run (i.e., the number of available activity profiles).

REQUIREMENT 5

The model exposure calculations shall be performed for either a general population or a user-specified subgroup of that population.

TYPE: Processing, input

ORIGIN: RFP page 1

COMMENTS: The "general population" is understood to be that of the state of California. The user will input, through a menu, the specification of the subgroup. If the sample size which results from this specification is too small for modeling purposes, a warning message will be displayed to the user, and with the model output.

Potential criteria for defining subgroups (per correspondence from P. Jenkins dated June 27, 1991) include geographic region, urban/suburban/rural location, county, season, weekday/weekend, age, gender, income level, education status, and employment status.

REQUIREMENT 6

The model calculations shall be performed for an expandable list of pollutants.

TYPE: Processing, input

ORIGIN: RFP page 3

COMMENTS: The pollutants in Table 3-1 of the GEOMET proposal will be included. The model will be structured in such a manner that additional pollutants can be added. The user will input the desired pollutant from a menu at the start of a run.

REQUIREMENT 7

The model exposure calculations shall be performed using either existing measured concentration data, or model-calculated concentration values. The measured data shall be expandable.

TYPE: Processing, input

ORIGIN: RFP page 8

COMMENTS: The choice between existing concentration data (which will be sampled) and model-calculated concentration values will be a user input. The measured-concentration data will be expandable. The calculated-concentration values will be found using a single-compartment "mass-balance" model, the parameters of which will be sampled from existing data, or from various PDF's, at the user's choice.

The source terms for the mass-balance model will include combustion sources, consumer products, material sources, and water (RFP page 8). The calculations will include consideration of the source emission rate, load factor, and duration factor.

The air exchange rates, pollutant removal rates, and outdoor concentrations will be sampled; sampling will be done via "re-sampling" existing data sets directly or based on parameters describing the distribution of such data sets.

Data and/or parameters for any of these factors will be interfaced to the model in a manner that will permit modification or expansion, as needed. Some information may need to be calculated "off-line" in stand-alone program(s); if such programs are necessary, they will be included in the model "package."

It is possible to merge two or more data sets for a given pollutant to produce a new, combined data set. The model will provide for combining of data sets (e.g., for pollutant concentrations) by allowing the user to specify more than one data set. The data sets will be "combined" through user-defined weights indicating the relative proportions of cases to be sampled from the data sets to be combined.

REQUIREMENT 8

The exposure calculations shall use expandable activity-pattern data.

TYPE: Processing

ORIGIN: RFP pages 2, 3, 7

COMMENTS: To start, the activity-pattern data will be taken from the "California activity study data base" (RFP page 7). These activity patterns will be resampled. Further activity data can be added, provided they are put in the format required by the model. The activity-pattern data interact with the population subsets chosen under Requirement 5. The use of weights to reflect different selection probabilities for survey participants will be accommodated in developing model outputs. Options to use selected (as opposed to combined) activity data bases will be provided.

REQUIREMENT 9

The exposure calculations shall be performed for eight types of indoor microenvironments and for the outdoor environment.

TYPE: Processing, input

ORIGIN: RFP page 4

COMMENTS: The model will perform its calculations for all microenvironments requested by the user for which data are available in the model or for which the user provides data through the model. Data initially will be provided in the model for the residence only; supplemental data for other microenvironments will be provided as such data become available in the course of the model development effort. The model will be structured so that the user can readily add new information as it become available for any of the nine types of microenvironments. The nine microenvironments are residences, offices, plants, schools, public access buildings, restaurants/lounges, travel in enclosed vehicles, other indoors, and outdoors.

REQUIREMENT 10

The model shall be designed to permit the addition of multiple pathways.

TYPE:	Processing, input
ORIGIN:	RFP page 4
COMMENTS:	To start, the pathway will be inhalation only; later (i.e., subsequent projects), other pathway calculations can be added. This will require modification of the model (pathway-specific calculation code), in addition to the interfacing of any required data. The interfacing of the additional pathways will be done in the "accumulator" portion of the model, where exposures are summed.

REQUIREMENT 11

The exposures for a given pollutant shall be accumulated across microenvironments and pathways.

TYPE:	Processing
ORIGIN:	RFP page 4
COMMENTS:	As pathways are added, the exposure accumulation also can be updated to include the contribution from the new pathway.

REQUIREMENT 12

The model outputs shall be organized in a manner that will permit the performance of mitigation studies.

TYPE:	Processing, output
ORIGIN:	RFP page 4
COMMENTS:	The model itself will NOT perform any mitigation-study calculations. However, thought must be given to techniques for conducting such studies, so that the program can be designed accordingly. The model shall have an option to produce an output file, for mitigation studies, which contains the daily/hourly

exposures, per person, per microenvironment, with appropriate identifying header information, per run.

REQUIREMENT 13

The model shall have an option to produce an output file, for mitigation studies, which contains the daily exposures or doses, per person, per microenvironment, with appropriate identifying header information, per run.

TYPE:	Output
ORIGIN:	Implicit (not explicitly stated in RFP)
COMMENTS:	This output will be needed to perform some types of analysis for mitigation (comparison) studies; it is an adjunct to the information presented under Requirement 4. To save storage space, this output will only be produced on user request (input option to save detailed output file).

REQUIREMENT 14

The model shall execute on an IBM-AT type computer, shall be coded in Microsoft QuickBasic, and shall be "user-friendly."

TYPE:	General
ORIGIN:	RFP page 5, 6
COMMENTS:	The model will be developed in such a way that it will not require highly specialized input data. The user interface will be through a menu system, and defaults will be provided so that the program can run without the user needing to input large quantities of data. The model will permit the storage of the run parameters, so that runs can readily be reproduced, or modified slightly from a baseline case (e.g., mitigation studies), without the need to input a lot of information. In some cases (e.g., new pollutant added to the model after its initial development), the user may need to provide significant new information, but the model will provide a structured user interface for doing this.

Appendix B

ACTIVITY CODES

VALUE	LABEL
1	main job
2	unemployment
3	travel during work
4	at work not used
5	second job
6	eating at work
7	before-after work
8	breaks
9	travel-work
10	food preparation
11	meal cleanup
12	cleaning house
13	outdoor cleaning
14	clothes care
15	car repair
16	other repairs
17	plant care
18	pet care
19	other hh
20	baby care
21	child care
22	helping-teaching
23	talking-reading
24	indoor playing
25	outdoor playing
26	medical care
27	other child care
28	pick up-drop off at dry cleaners
29	travel child care
30	grocery shopping
31	durable shopping
32	personal services
33	medical services
34	govt.-financial services
35	car repair services
36	other repair services
37	other services
38	errand
39	travel goods and services
40	washing, hygiene
41	medical care
42	help and care
43	meals at home

VALUE	LABEL
44	meals out
45	night sleep
46	naps
47	dressing
48	no activity given
49	travel personal care
50	student classes
51	other classes
52	unused
53	unused
54	homework
55	library
56	other education
57	unused
58	unused
59	travel education
60	professional union
61	special interest
62	political civic
63	volunteer-helping
64	religious groups
65	religious practice
66	fraternal
67	child youth family
68	other organizational
69	travel organizational
70	sports events
71	entertainment events
72	movies
73	theatre
74	museums
75	visiting
76	parties
77	bars-lounges
78	other social
79	travel social events
80	active sports
81	outdoor
82	walking hiking bicycling
83	hobbies
84	domestic crafts
85	art literature
86	music drama dance

VALUE	LABEL
87	games
88	computer use
89	travel recreation
90	radio
91	TV
92	records-tapes
93	read books
94	read magazines
95	read newspapers
96	conversations
97	writing
98	think relax smoking
99	travel communications
124	cleaning and laundry together
149	clothes care: at laundromat
165	darkroom photographic work
166	repairing the boat
167	painting a room or house
169	building a fire
474	washing and dressing
801	golf
802	bowling
803	yoga - health spa
914	TV-eat
939	TV-read
954	TV-knitting

Appendix C

BIBLIOGRAPHY RESULTING FROM LITERATURE REVIEW

BIBLIOGRAPHY FOR CALIFORNIA AIR RESOURCES BOARD PROJECT

"Development of a Model for Assessing Indoor Air Exposure to Air Pollutants"

The bibliography is divided into the categories defined briefly here. The bibliographic entries are grouped in these categories, identified with corresponding subheads.

California Data: These papers actually contain pollutant-of-interest emission or concentration data for interior locations in California. Hard copies of the papers included here have been reviewed, and are available.

USA (Non-California) Data: Papers included here contain interior emission or concentration data for pollutants of interest. Not all of the papers have been physically reviewed; in some cases abstracts or titles were the only data available. The data are for locations in the United States, outside of California.

Other Indoor Air Pollution: These papers report relevant studies or analyses, but do not contain interior pollutant emission or concentration data. Of particular interest in the literature search for this group were papers dealing with computer modelling, and related efforts.

Motor Vehicles: Where relevant papers turned up incidental to the main thrust of the literature review effort they were included here, primarily on the expectation that future work modelling carbon monoxide indoors would have to consider automotive sources.

Surveys/Overviews: Relevant papers and monographs reporting broad reviews of the indoor air pollution problem are presented in this group; they include other literature reviews.

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Appendix D

MODEL VALIDATION PLAN

MODEL VALIDATION PLAN

"Development of a Model for Assessing Indoor Exposure
to Air Pollutants"
(ARB Contract No. A933-157)
January 8, 1993

INTRODUCTION

ASTM designation D5157-91 (Standard Guide for Statistical Evaluation of Indoor Air Quality Models) defines model evaluation as "a series of steps through which a model developer or user assesses the performance of a model for selected situations" and model validation as "as series of evaluations undertaken by an agency or organization to provide a basis for endorsing a specific model (or models) for a specific application (or application)." A related concept is model verification, which involves computational and logical checks to verify proper flow and accuracy of calculations performed by the model.

Two segments of the model referenced above required validation:

- Modeling of exposures/doses for one or more microenvironments (Level 1/2)
- Modeling of concentrations for a microenvironment (Level 3).

To the extent that data sets resulting from measurements are available to provide a basis for comparison with modeling outputs, the model validation effort will be slanted more toward evaluation than verification. This distinction will be made clearer in the discussion that follows for each segment of the model.

VERIFICATION OF MODELED EXPOSURES/DOSES (LEVEL 1/2)

Level 1/2 of the model involves sampling from concentration distributions for one or more microenvironment and combining each sampled concentration with the amount of time spent by an individual in that microenvironment (as determined by a sampled activity profile) to develop a time-weighted average concentration to which an individual is exposed over a (user-specified) period of 1, 8, 12 or 24 hours. The sampled activity profile indicates not only the amount of time spent in each microenvironment but also the activity level (heavy, moderate, light or resting) for which a breathing rate is assigned by the model user. For each microenvironment, the concentration to which the individual is exposed ($\mu g/m^3$) is multiplied by the time duration in the microenvironment (h) and the activity-dependent breathing rate (m^3/h) to calculate an inhaled dose (μg). The total inhaled dose is the sum of the calculated doses across all microenvironments for which the user has provided inputs.

There are some measurement data sets (e.g., 12-hour personal exposures measured in the 1984 and 1987 TEAM studies) that could provide a basis for comparison with Level 1/2 outputs (exposures, but not doses) if concentration inputs were available from all nine microenvironments in the model, which collectively account for 100 percent of an individual's time. The difficulty, however, is that reliable estimates of concentration distributions do not, as yet, exist for most microenvironments; they are, in fact, largely restricted to residences. This fact requires that validation for the Level 1/2 model segment will need to be slanted toward model verification.

Model verification for Level 1/2 will involve the following steps:

1. Verifying that various ways of describing concentration distributions, as input by the user, are faithfully reproduced by the sampling schemes in the model's calculation module.
2. Verifying that individuals' time allocations and activity levels are correctly accessed by the calculation module.
3. Verifying that time-weighted average exposures and accumulated inhaled doses are computed correctly by the calculation module.

Ways of describing concentration data sets include supplying parameters of a distribution (normal, lognormal, triangular or uniform), percentiles of a distribution or an actual data set to be sampled. Faithful reproduction of the concentration inputs will be determined through comparisons of summary statistics for the input versus sampled distributions, percentiles of the two distributions, and histograms depicting the shapes of each distribution. Statistical tests can be utilized to assess the similarity of certain statistics (e.g., mean, standard deviation) or to assess the general agreement between distributions (e.g., nonparametric tests for goodness of fit).

Verifying individuals' time allocations and activity levels will be performed based on a model run with a relatively small number of trials (e.g., ten). We will verify (1) that the correct activity profiles were sampled, using the random numbers generated by the model as a frame of reference and (2) that the quantities of time and associated activity levels for each microenvironment were properly accessed by the model. This information, together with the sampled concentration values for each microenvironment, will be entered in a spreadsheet to compute time-weighted average concentrations and accumulated inhaled doses for direct comparison with the results output from the model. This exercise will be performed for two cases--one where concentration inputs are provided for only one microenvironment (e.g., residence) and one where concentration inputs are provided for all microenvironments.

VALIDATION OF MODELED CONCENTRATIONS (LEVEL 3)

In this case it should be possible to locate some data sets with measurement results, so that the validation exercise can include aspects of model evaluation as well as verification. As in the previous case, model verification will address (1) whether input distributions (for volumes, air exchange rates, emission rates, etc.) are correctly reproduced by the model and (2) whether resultant indoor concentrations are correctly calculated using these inputs. Such verification checks will be provided for two different pollutants (e.g., CO, benzene) using a number of trials on the order of ten. Unlike Level 1/2, these intermediate outputs (sampled volumes, etc.) are not part of the model output, so that the Level 3 code will need to be temporarily revised to output these values.

The aspect of model evaluation will involve comparison of the distribution of modeled concentrations with the distribution based on measurement results from a field study. The distributions will be compared in terms of summary statistics (e.g., mean, standard deviation, 50th percentile, 90th percentile) as well as general agreement (goodness-of-fit tests). In making these contrasts, there are several important facts to keep in mind:

- Measured and modeled results may disagree because the measurements are subject to some degree of error and uncertainty.

- Measured and modeled results may disagree because of our ignorance with respect to the distributions of some model parameters.

With the second fact in mind, we will strive to find data sets for which some of the pertinent mass-balance parameters (volumes, air exchange rates, outdoor concentrations, presence/absence of various types of indoor sources) were characterized for the structures involved in the measurements. This would be possible, for example, for the 1984/1987 TEAM studies in Los Angeles or for the recent ARB study of PAHs and CO in northern California. Both of these studies involved measurements in residences.

Model evaluation is planned to be conducted for one combustion pollutant (preferably CO) and one VOC (preferably benzene). These pollutants are preferred because (1) CO concentrations have been measured as a time series of hourly average concentrations, whereas benzene concentrations have been measured as 12-hour or 24-hour average values, and (2) the two pollutants have some differences in types of indoor sources, yet the indoor sources have been fairly well characterized for each pollutant. If CO data are not available from the ARB study, then a possible alternative is to use NO_2 data for the SoCal study (recognizing that this study provided measurements for a sampling duration longer than 24 hours, such that we would expect the distribution of measured values to have a smaller variance than for a 24-hour measurement interval, other things being equal).

The measured and modeled results may not correspond very well. This outcome would not necessarily mean that the model is poorly conceived or poorly implemented. More likely, such an outcome would point to our ignorance about the distribution of some critical input parameter (e.g., emission rates). If the measured and modeled results do diverge, then we will investigate whether some relatively simple adjustment (e.g., changing the shape of an input distribution, adjusting the mean and/or variance of an input distribution, or adding a new indoor source) can bring the results into relatively chose agreement. If not, then we may need to "rethink" the model formulation.