DRAFT MEMORANDUM

SUBJECT: **Analysis Of Uncertainty In Ozone Population Exposure Modeling**

FROM: John Langstaff

TO: Ozone NAAQS Review Docket (OAR-2005-0172)

DATE: July 24, 2006

The attached technical memorandum describes a methodology for an analysis of the uncertainties associated with the population exposure modeling conducted in support of the review of the ozone NAAQS, and plans for completion of this analysis. We are soliciting input from the Clean Air Scientific Advisory Committee (CASAC) and the public on the methodology laid out in this memorandum. We plan to address comments received on the methodology described here in completing this analysis, and to include the results of this analysis in a final memorandum that will inform the discussion of our exposure analysis in our final Ozone Staff Paper.

Analysis Of Uncertainty In Ozone Population Exposure Modeling

Draft Technical Memorandum

July 24, 2006

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Glossary of Acronyms

Acronym	Meaning of Acronym	page first used
AER	air exchange rate	28
APEX	Air Pollution Exposure Model (EPA, 2006c,d)	1
BM	body mass	41
BME	Bayesian maximum entropy	15
BSA	body surface area	57
CART	classification and regression trees (Breiman et al., 1984)	38
CD	Ozone Air Quality Criteria Document (EPA, 2006b)	1
CDS	Child Development Supplement (CDS, 2005)	40
CHAD	Consolidated Human Activity Database (EPA,2002)	37
CMAQ	Community Multiscale Air Quality Model (www.epa.gov/asmdnerl/cmaq/)	19
CSA	combined statistical area (OMB, 2005)	9
CV	coefficient of variation	11
ECF	energy conversion factor	41
EPOC	excess post-exercise oxygen consumption	56
EVR	effective ventilation rate	41
FEM	Federal equivalent method	11
FRM	Federal reference method	11
GM	geometric mean	5
GSD	geometric standard deviation	5
HVAC	heating, ventilation, and air conditioning	34
MET	metabolic equivalent (see Ainsworth, 2003)	41
NAAQS	national ambient air quality standard	1
NO	nitric oxide	18
NO_x	nitrogen oxides	9
PAI	physical activity index	41
PEM	personal exposure monitor	5
PM	particulate matter	1
PSID	Panel Study of Income Dynamics (CDS, 2005)	40
RMR	resting metabolic rate	41
RMSE	root mean square error	13
TSD	technical support document	1
UV	ultraviolet	11
Ve	expiration ventilation rate	57
VO_2	oxygen consumption rate	57
VOC	volatile organic compounds	9

INTRODUCTION

When models are applied in decision-making processes an evaluation of the uncertainty of the model predictions is of the utmost importance. The decision maker needs to know whether or not the level of uncertainty in modeled results are acceptable in the context of the decisions to be made. Without some knowledge of the uncertainty, the model essentially lacks useful predictive power. In practice it is difficult, if not impossible, to gain a complete understanding of all of the sources of model uncertainty and take them into account. However, it is incumbent on modelers to assess and report model uncertainty to the extent that it is feasible.

At the time the 1996 ozone CD was published, available information indicated that only 40 percent of the variability in personal exposures was explained by exposure models (CD, Appendix AX3, page 196). Since that time there have been considerable improvements in population exposure models and data for these models. However, a comprehensive evaluation of population exposure models for ambient air pollutants has never been performed, and significant uncertainties in the predictions of these models remain.

The importance of specific limitations of exposure models is application- and pollutant-specific. For example, the distribution of air exchange rates is one of the more important model input data for PM exposure modeling. For some air toxics, uncertainties in the emissions and air concentrations of the pollutant will be the overriding limitation. For pollutants where time spent outdoors is an important parameter (for example, ozone), activity diary construction may be a significant source of uncertainty.

This analysis of model uncertainty is performed as part of the exposure analysis conducted in support of the ozone NAAQS review, described in Chapter 4 of the Ozone Staff Paper (EPA, 2006a) and the Exposure Analysis Technical Support Document (EPA, 2006b). The exposure model, APEX, is documented in a user's guide and technical document (EPA, 2006c,d). We will refer to these four documents in the remainder of this report as the Staff Paper, the Exposure Analysis TSD, the APEX User's Guide, and the APEX TSD.

This report presents interim results and identifies the work still to be completed. A final version will be available with the release of the final ozone Staff Paper in October, 2006.

In the remainder of this section, we cover some of the basic concepts of model variability and uncertainty. The next section gives an overview of our approach for quantitatively characterizing the uncertainty of the exposure modeling performed as part of the ozone NAAQS review, followed by sections on estimation of the uncertainty of the inputs to the exposure model APEX and treatment of the uncertainty of the formulation of the APEX model. The results of the uncertainty analysis will be presented in the final section.

Concepts

Uncertainties arise from errors in the values of data and parameters input to the model and the necessarily simplified representation by the model of complex physical and human behavioral processes. The model inputs are assumed to be representative of the area being modeled, and many of them are (e.g., population demographics, air quality and meteorological data). However, some of the inputs are derived from data collected at locations and/or time periods that differ from those being modeled, and these can contribute to the uncertainty of the model results. It is difficult to judge the significance of these different sources of uncertainty without conducting a thorough assessment of the uncertainties and also of the variability of the model inputs and results. The distinctions between uncertainty and variability and between sensitivity and uncertainty analyses are fundamental to this discussion. These are defined as follows.

Uncertainty refers to the lack of knowledge of the actual values of physical variables (parameter uncertainty) and of physical systems (model uncertainty). For example, parameter uncertainty can result when non-representative sampling (to measure the distribution of parameter values) gives sampling errors. Model uncertainty results from simplification of complex physical systems. Uncertainty can be reduced through improved measurements and improved model formulation.

Variability represents the diversity or heterogeneity in a population or property, and is an inherent property of a physical property or population characteristic. This is sometimes referred to as *natural variability*. Examples are the variation in the heights of people and the variation of temperature over time. Variability cannot be reduced by using more measurements or measurements with increased precision (taking more precise measurements of people's heights does not reduce the natural variation in heights). *Inter-individual (between-individual) variability* refers to the differences in a property between individuals in a population. The variation of a property for one individual over time is *intra-individual (within-individual) variability*.

Sensitivity Analysis assesses the effect of changes in individual model input parameters on model predictions. This is often done by varying one parameter at a time and recording the associated changes in model response. One primary objective of a sensitivity analysis is to rank the input parameters on the basis of their influence on, or contribution to, the variability in the model output.

Uncertainty Analysis involves the propagation of uncertainties and natural variability in a model's inputs to calculate the uncertainty and variability in the model outputs. It can also involve an analysis of the uncertainties resulting from model formulation. The contributions of the uncertainty and variability of specific model inputs to the uncertainty and variability of the model predictions can in some cases be explicitly quantified.

Data Uncertainty and Model Uncertainty

In general, limitations and uncertainties result from variability not modeled or modeled incorrectly, erroneous or uncertain inputs, errors in coding, simplifications of physical, chemical, and biological processes to form the conceptual model, and flaws in the conceptual model. Sources of uncertainty in exposure modeling can be classified into two primary areas: errors in the model input data and parameters, and errors in the formulation of the model itself (structural uncertainty).

Parameter or Input Data Uncertainty. When parameters or input data are estimated from measurements or samples from within a larger population, uncertainties can arise from:

- small sample sizes
- imprecise measurements (systematic and random errors)
- non-representative samples, extrapolation errors
- temporal period and/or spatial extent too limited to detect trends
- flawed study design (systematic errors in the data collection process)
- flawed statistical estimation method
- the use of surrogate measures

Model Formulation or Structural Uncertainty. Model uncertainty can result from:

- simplifying assumptions
- incorrect assumptions
- incomplete knowledge of the physico-chemical processes
- not accounting for important variables
- temporal and spatial aggregation errors
- mis-specification of the problem
- applying a model in a situation for which it was not designed

A simple example which illustrates the difference between model input uncertainty and structural uncertainty is modeling the distribution of heights in a population by a normal distribution, parameterized by the mean and variance. Estimates of the mean and variance are the "model input data." The uncertainty which results from the difference between the shape of the true distribution and the normal distribution leads to structural uncertainty. The parameters of the distribution are estimated by measuring a sample of the population, and thus are subject to sampling errors, which result in the model inputs uncertainty. Increasing the sample size will reduce these errors and the associated uncertainty of the modeled distribution. However, if the form of the distribution is incorrect, increasing the sample size will help only up to a point, and then model uncertainty will dominate. The only way to reduce the uncertainty further would be to improve the model by finding a distribution whose shape more accurately reflects the true distribution of heights.

Note that an input value can be very uncertain and yet have little contribution to the uncertainty of the model results. This depends on the degree of leverage or influence the particular model input has. Thus the most uncertain inputs do not necessarily contribute the most to the uncertainty of the model results. In some cases, the amount of influence that a

parameter has can depend on values of other parameters. For example, the proportion of houses with air conditioning may be an influential model input when temperatures are high, and not when temperatures are low.

The primary difficulty in performing an uncertainty analysis is the quantitative characterization of the uncertainties of the model inputs and model formulation. We often have information about the variability of model inputs, and sometimes the variability and uncertainty combined, but it is usually difficult to estimate the uncertainty separately from the variability. We seldom know the quantitative uncertainty resulting from model formulation, except in cases where a model evaluation has been performed.

The Uncertainty of Uncertainty Analysis

If all of the important sources of uncertainty are not taken into account, an analysis of uncertainty will give a misleading picture. Unfortunately, the major sources of uncertainty tend to be the most difficult to characterize, since if we have data for good quantitative characterization of uncertainty, these data can often then be used to reduce the uncertainty. Thus, estimates of uncertainty are themselves uncertain. Model evaluation, where model predictions are compared with measured values, is useful in this context.

APPROACH FOR ASSESSMENT OF EXPOSURE MODELING UNCERTAINTY

The goal of this uncertainty analysis is to quantify the uncertainty in the APEX model output that results from uncertainty in the model inputs and uncertainty due to the model itself.

There are two general methods we are using to assess the uncertainty due to uncertain model inputs. The primary method involves first quantifying the uncertainties of each of the model inputs, and then propagating those uncertainties through the model to estimate the resulting uncertainty of the model results. We do this using the Monte Carlo method, which has the advantage of being very flexible (Morgan and Henrion, 1990; Vose, 1996). The second method involves sensitivity analyses. Certain model inputs are very complex and difficult to treat with a Monte Carlo approach, and we conduct sensitivity analyses to quantify their effect on uncertainty.

APEX is a Monte Carlo simulation model which explicitly incorporates the inherent variability of the modeled population and physical processes leading to exposures. Most of the inputs to APEX are distributions. For example, instead of using a single decay rate for the decay of ozone indoors, a distribution of hourly decay rates is input to APEX, specified by its form (lognormal) and parameters (a geometric mean (GM) of 2.5 and geometric standard deviation (GSD) of 1.5), as shown in Figure 3. The development of the distributions representing variability which are input to APEX is described in the Exposure Analysis TSD (EPA, 2006a).

The Monte Carlo approach entails performing many model runs with model inputs randomly sampled from distributions reflecting the uncertainty of the model inputs. For ozone decay rates, we are assuming that the form of the distribution is approximately correct, but realize that the GM and GSD are not known precisely. We estimate that the errors of the GM are normally distributed with mean 0 and standard deviation 0.18 (Figure 1), and the errors of the GSD are normal with mean 0 and standard deviation 0.05 (Figure 2). Then we run APEX numerous times, and for each run we randomly select values from these error distributions, add them to the GM (2.5) and GSD (1.5) of the decay rates, and use these for model inputs. Figure 4 illustrates six decay rate distributions that result from adding these uncertainty terms (randomly selected from the distributions depicted in Figure 1 and Figure 2) to the GM and GSD of the base distribution.

Our approach to the assessment of the uncertainty resulting from model formulation and structure primarily involves a careful review of the scientific basis of the algorithms that make up APEX. We have also conducted a limited evaluation of APEX by comparing its predictions to 6-day average personal exposure measurements of ozone (see the Exposure Analysis TSD). A diagnostic evaluation with personal exposure monitors (PEMs), indoor, and outdoor measurements of ozone with shorter averaging times (1 hour or less) would be very informative, if the data were available.

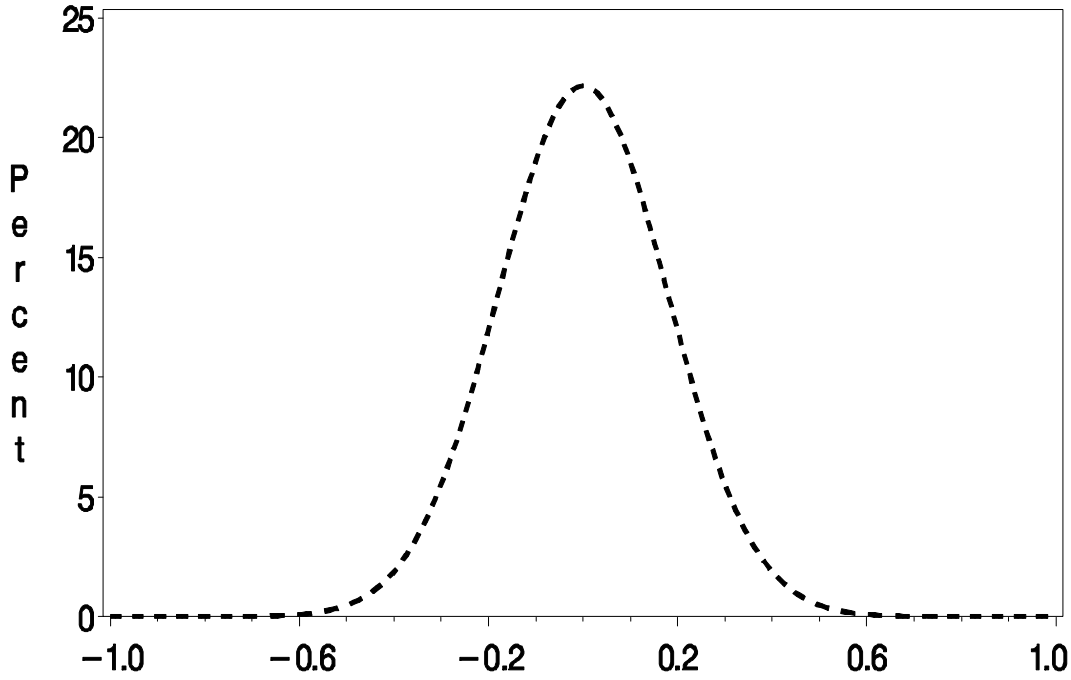


Figure 1. The distribution of the uncertainty of the GM (normal, mean=0, stdev=0.18)

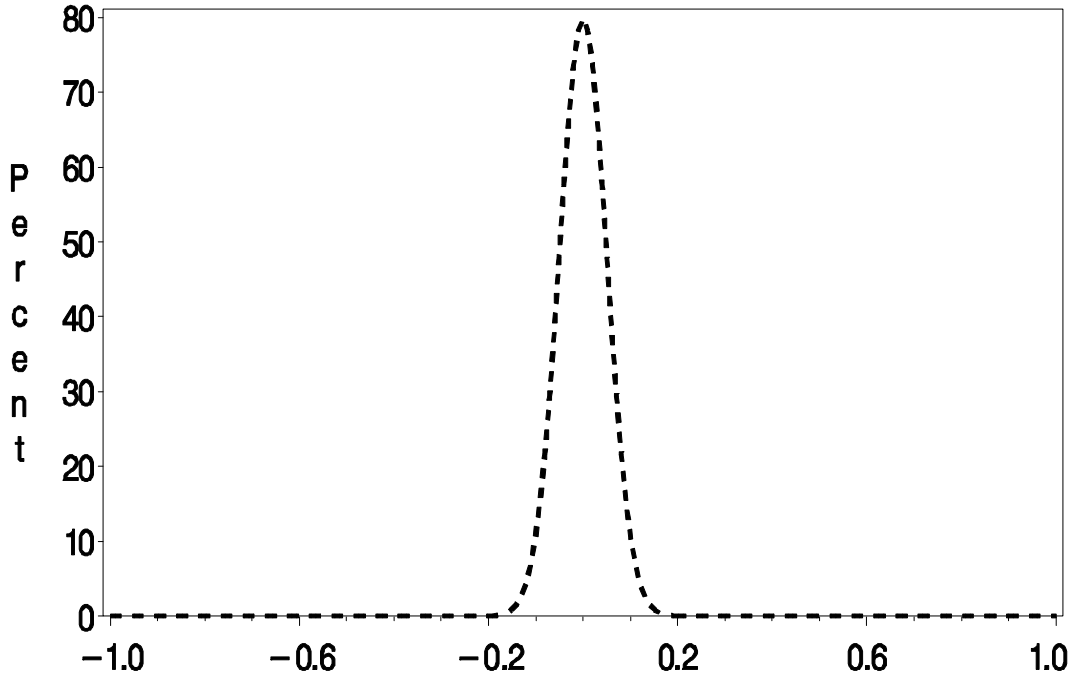


Figure 2. The distribution of the uncertainty of the GSD (normal, mean=0, stdev=0.05)

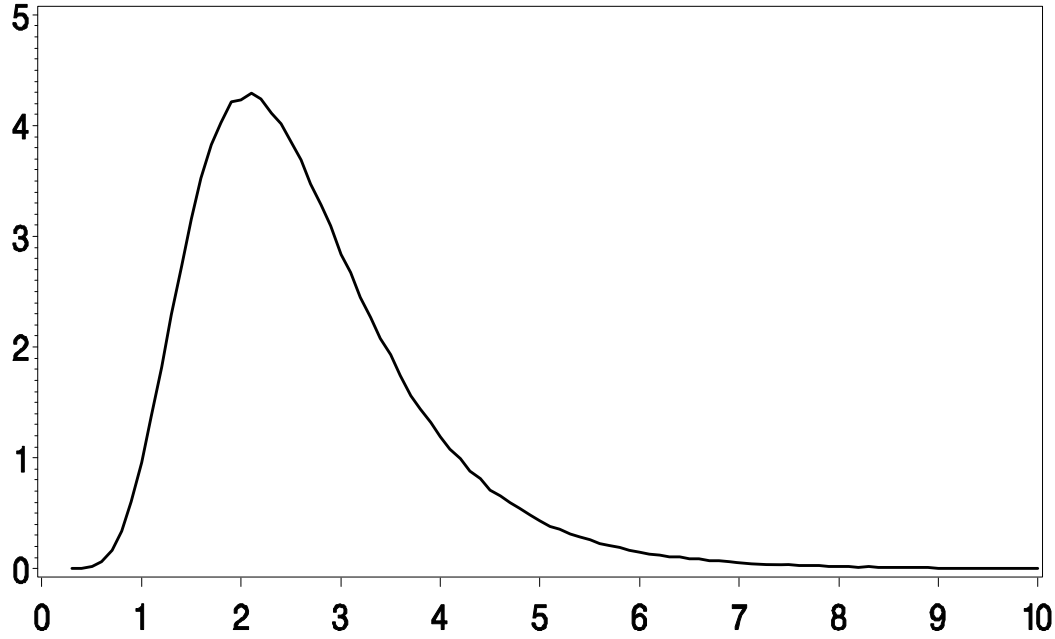


Figure 3. The base decay rates variability distribution (lognormal, GM=2.5, GSD=1.5)

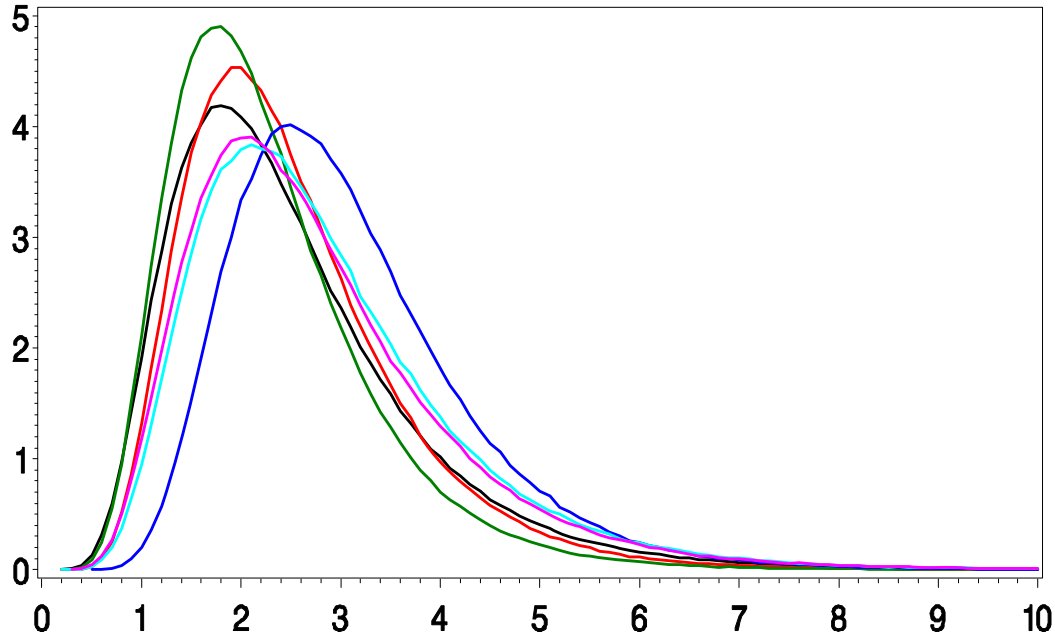


Figure 4. Six realizations of the combined variability and uncertainty distribution

The primary obstacle to performing an acceptable uncertainty analysis for this type of modeling is the quantitative characterization of the uncertainties of the model inputs. We often have information about the variability of model inputs, and sometimes the variability and uncertainty combined, but it is usually difficult to estimate the uncertainty separately from the variability. Developing appropriate distributions representing variability and uncertainty in various model inputs (e.g., air exchange rates, ozone decay rates, physiological parameters) is a key part of this modeling effort.

A Note About the Lognormal Distribution

Most of the inputs to APEX which have population variability are best fit with a lognormal distribution, and in some cases only the parameters of lognormal fits to data are reported in the literature. Typically there are not much data or information available for estimating the uncertainty of the distributions representing variability which are input to APEX, and a decision must be made about the distributional form of the uncertainty. Given an estimate of the uncertainty of an unbiased estimate of the GM, the question arises whether the uncertainty interval for the GM should be symmetric about the GM (e.g., $[GM-\Delta, GM+\Delta]$) or symmetric in the data space (symmetric about the GM multiplicatively, e.g., $[GM/\Delta, GM\cdot\Delta]$), and whether or not the GSD should be concurrently varied. Changing the GM (or the GSD) changes both the mean and the standard deviation of a distribution, so care must be exercised when varying one or the other of these to ensure that the GM,GSD pair is valid. Therefore, if the estimate of the mean of a lognormal distribution is unbiased, then the GM and GSD must be varied concurrently in the Monte Carlo simulations in such a way that the average of the means of the Monte Carlo distributions is approximately equal to the original estimate of the mean.

QUANTIFYING THE UNCERTAINTY OF APEX MODEL INPUTS

In this section we describe how the distributions of uncertainty were developed for this assessment of uncertainty of our application of APEX to model population exposures to ozone pollution in 12 U.S cities.

Ambient Air Quality Concentrations

Hourly ambient concentrations are input to APEX, accounting for temporal variability. If concentrations from only one monitor are used, then spatial variability is not accounted for and cannot be properly modeled. If multiple monitors are used, then spatial variability is accounted for, but some uncertainty remains for concentrations at locations distant from monitors. The uncertainties associated with these concentrations in relation to spatial representativeness can be significant. For this modeling analysis, there is fairly good spatial coverage of the areas modeled. Table 1 lists the numbers of monitoring sites in the study areas for the two years modeled. Using Boston as an example, the placement of monitors for the Boston greater metropolitan area is shown in Figure 5 (the monitoring sites are indicated by squares and the combined statistical

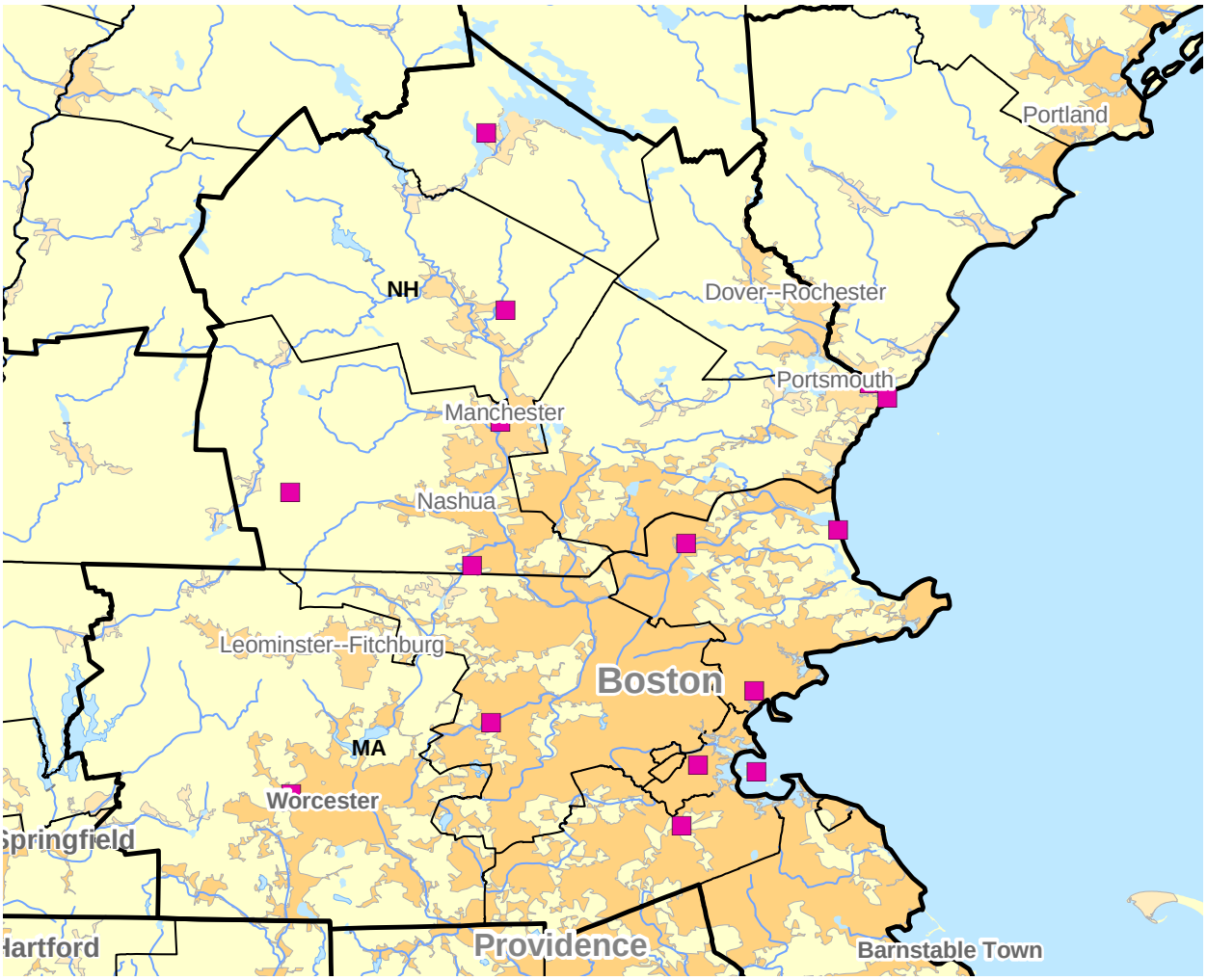


Figure 5. Boston CSA with ozone monitoring sites

area (CSA) by the heavy black lines). However, spatial variations in ozone concentrations can be considerable, resulting in uncertainty if these are not accounted for by the model (CD, Section 3.3).

If a single ozone season is modeled, another source of uncertainty results from the year-to-year variability of ozone concentrations, meteorology and NO_x and VOC emissions. We have modeled the 2002 and 2004 ozone seasons, which have different ozone concentrations due to a combination of different weather patterns and emissions of ozone precursors. In this way we account for the sensitivity of the exposure modeling results to year-to-year variability of air quality and meteorology.

Table 1. The number of ozone monitors in each of the study areas

Study Area (CSA)	Number of monitors	
	2002	2004
Atlanta-Sandy Springs-Gainesville, GA-AL	13	12
Boston-Worcester-Manchester, MA-NH	17	15
Chicago-Naperville-Michigan City, IL-IN-WI	32	27
Cleveland-Akron-Elyria, OH	11	11
Detroit-Warren-Flint, MI	10	10
Houston-Baytown-Huntsville, TX	21	21
Los Angeles-Long Beach-Riverside, CA	45	44
New York-Newark-Bridgeport, NY-NJ-CT-PA	30	29
Philadelphia-Camden-Vineland, PA-NJ-DE-MD	18	16
Sacramento--Arden-Arcade--Truckee, CA-NV	21	22
St. Louis-St. Charles-Farmington, MO-IL	18	17
Washington-Baltimore-N. Virginia, DC-MD-VA-WV	28	26

In addition to modeling exposures for 2002 and 2004, we are modeling exposures for scenarios of attainment of the current ozone standard and a number of potential alternative standards. For areas which do not meet these standards for these modeled years, attainment of these hypothetical scenarios would occur in the future. Modeling exposures for future years under different emission control strategies has, in addition to the uncertainties involved with modeling historical scenarios, the uncertainties of the complex process of projecting to future years air quality, population demographics, activity patterns, and other parameters which change over time. We employ a quadratic rollback technique to calculate ozone concentrations for these scenarios. This technique and the rationale for using it are described in the draft Staff Paper.

The primary uncertainties in the air quality data input to the model, discussed in the remainder of this section, result from:

- Instrument measurement error
- Estimation of missing data (temporal interpolation)
- Estimation of neighborhood-scale concentrations at locations which are not close to monitoring sites (spatial interpolation)
- Estimation of micro-scale concentrations (e.g., near-roadway)
- Adjustment of concentrations to reflect alternative standards (rollback)

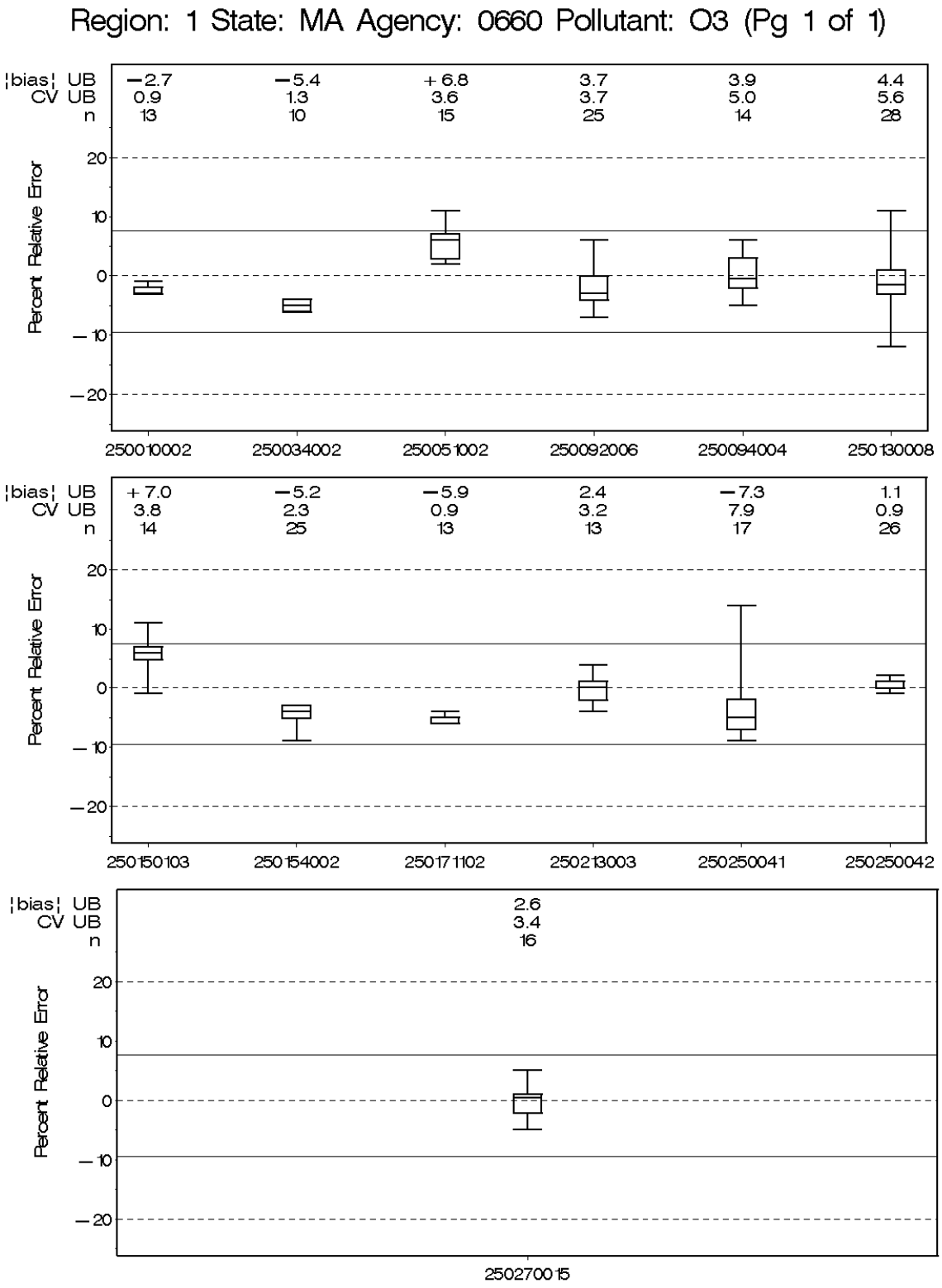
Uncertainty Due To Measurement Error

The Federal reference method (FRM) for ozone is based on chemiluminescence. However, chemiluminescence has not been widely used in instrumentation since the mid-1980s. Most instruments in use today employ ultra-violet (UV) absorption, a Federal equivalent method (FEM) (CD, Section 2.6). The equivalency test requires instruments to be within 5 ppb of known ozone concentrations (1-hour average) (40 CFR Ch. 1, section 53.2). Interference with other pollutants and humidity can lead to errors in measurements. This does not seem to be well quantified (CD, pages 2-25 to 2-26), but can range from a few ppb to up to 20-40 ppb in highly polluted areas (CD, page 2-23).

For this uncertainty analysis we will estimate the errors of the hourly average measurements from the site-specific single point precision and bias estimates from the *2003 Criteria Pollutant Quality Indicator Summary Report* (Battelle, 2004) and the *2004 Single Point Precision and Bias Graphics for Criteria Pollutants* (EPA, 2005a,b). Figure 6, taken from the Battelle report, illustrates these errors for some of the Massachusetts monitors. The "Bias" is the 95% confidence upper limit on the mean of the absolute values of relative percent differences for the monitoring season, and the "CV" is the 90% confidence upper limit of the coefficient of variation (CV) of relative percent difference values for the monitoring season. A positive bias means that the monitor readings are too high. Table 2 lists the 2003 and available 2004 values for monitors in the Boston CSA. Note that the 2003 and 2004 values do not correlate well, which indicates that the bias may be random for a given monitor. We estimate the measurement error uncertainty as normally distributed, with mean and CV taken to be the overall average of the precision and bias values. For example, the numbers in Table 2 give an average bias of 0.22% and an average CV of 4.4%.

Table 2. 2003 and 2004 Single Point Precision and Bias for Boston Monitors

	2003		2004	
AQS ID	**Bias (%)**	**CV (%)**	**Bias (%)**	**CV (%)**
250090005-1	-2.71	0.90	+2.66	2.55
250092006-1	+3.73	3.74	-5.70	5.71
250094004-1	+3.89	4.96	+2.49	2.28
250095005-1			+0.72	0.81
250171102-1	-5.86	0.91	-5.73	6.23
250213003-1	-2.41	3.21	-2.82	2.89
250250041-1	-7.35	7.87	-4.01	1.66
250250042-1	-1.07	0.94	3.54	4.51
250270015-1	-2.63	3.37	+4.09	2.40
330012004-1	+5.23	7.32		
330110020-1	+3.4	4.26		
330111010-1	3.05	4.47		
330115001-1	3.83	4.18		
330130007-1	-3.38	3.98		
330150012-1	-2.38	2.93		
330150013-1	+11.28	14.29		
330150015-1	9.28	11.90		
330173002-1	-5.36	6.79		



Data less than −25 are plotted at −25 and data greater than 25 are plotted at 25.
Solid reference lines indicate the annual agency CFR probability interval.

Figure 6. 2003 Precision and Accuracy for Massachusetts Monitors

We are treating the measurement errors at a given monitor uncorrelated. We could estimate the autocorrelation of the hourly errors through an analysis of measurements at collocated instruments.

Uncertainty in Estimation of Missing Data

Missing air quality data were estimated by the following procedure. If there were consecutive strings of missing values (data gaps) of less than 6 hours, missing values were estimated by linear interpolation between the valid values at the ends of the gap. Remaining missing values at a monitor were estimated by fitting linear regression models for each hour of the day, with each of the other monitors, and choosing the model which maximizes R^2 for each hour of the day, subject to the constraints that R^2 be greater than 0.5 and the number of regression data values is at least 50. If there were any remaining missing values at this point, for gaps of less than 9 hours, missing values were estimated by linear interpolation between the valid values at the ends of the gap. Any remaining missing values were replaced with the regionwide mean for that hour. The amount of missing data in 2002 across the 12 modeled cities is indicated in Table 3 (e.g., 75% of all of the monitors had less than 5% missing data during the 2002 ozone seasons).

Table 3. Distribution of 2002 ozone season monitor-level missing data for the 12 modeled CSAs

Percentile	10%	25%	50%	75%	90%
Percent missing	0.5%	1%	2.5%	5%	10%

The uncertainty of this method for filling in missing data was estimated by a jackknife-type approach where subsets of the data are randomly designated as "missing," then these missing values are filled in using the above procedure, and the filled in values are compared with the original values to see how well they are estimated. Since longer gap lengths generally engender more uncertainty, we calculate the frequencies of different gap lengths in the original data and set data to missing in such a way that these frequencies are reproduced. These errors turn out to be generally less than 0.004 ppm. Table 4 shows that replacement of missing data for the Boston CSA had little effect on the mean and standard deviation of the hourly ozone concentrations at each monitor. The root mean square error (RMSE) was generally less than 0.004 ppm, with insignificant bias, and the distribution of errors can be reasonably approximated by a normal distribution (Table 7 has the values used in this analysis).

Table 4. Effect of missing data replacement on the distribution of 2002 hourly ozone for monitors in the Boston CSA (ppb)

Monitor	# of hours missing	Mean of original data	Mean of filled data	Difference	St. dev. of original data	St. dev. of filled data	Difference
2500900051	290	0.0296	0.0292	0.00042	0.0188	0.0187	0.00009
2500920061	171	0.0369	0.0368	0.00013	0.0197	0.0195	0.00014
2500940041	141	0.0375	0.0374	0.00010	0.0178	0.0178	-0.00001
2501711021	483	0.0360	0.0362	-0.00016	0.0199	0.0199	-0.00004
2502130031	143	0.0427	0.0425	0.00015	0.0204	0.0203	0.00012
2502500411	157	0.0366	0.0365	0.00019	0.0187	0.0186	0.00009
2502500421	353	0.0258	0.0263	-0.00053	0.0165	0.0174	-0.00091
2502700151	1723	0.0431	0.0446	-0.00151	0.0179	0.0178	0.00014
3300120041	49	0.0373	0.0373	0.00001	0.0149	0.0149	0.00004
3301100201	47	0.0311	0.0311	-0.00001	0.0177	0.0176	0.00007
3301110101	47	0.0334	0.0334	0.00002	0.0195	0.0195	0.00007
3301150011	2634	0.0464	0.0479	-0.00145	0.0186	0.0158	0.00288
3301300071	50	0.0282	0.0283	-0.00008	0.0188	0.0188	0.00002
3301500121	39	0.0343	0.0344	-0.00003	0.0171	0.0170	0.00002
3301500131	141	0.0332	0.0333	-0.00011	0.0193	0.0192	0.00012
3301500151	162	0.0315	0.0316	-0.00010	0.0184	0.0181	0.00027
3301730021	40	0.0339	0.0339	-0.00005	0.0167	0.0167	0.00001

Uncertainty in Spatial Interpolation

We take three approaches to estimate the impacts of the errors of spatial interpolation of ozone concentrations.

Jackknife Estimates of Uncertainty

We estimate the errors of spatial interpolation using the jackknife method (Efron, 1980; Stone, 1974), in which we drop out one monitor, use the spatial interpolation method to estimate concentrations at the location of that monitor, and compare the predicted to the observed values for each hour, giving a distribution of errors for that monitor. We do this for every monitor in the study area, thereby characterizing the errors of spatial interpolation in that area by a single distribution. This method tends to overestimate the size of the errors, because all monitors are used in the actual interpolation, reducing the interpolation errors to zero at the locations where the errors are estimated.

For each site, we calculate the observed/predicted ratio for each hour, and the 25th and 75th percentiles of these ratios. For Boston, 2004, the means (over all sites) of these site-specific quartiles are 0.93 and 1.2, with a central value of 1.065, and we approximate the uncertainty of the spatial interpolation by a normal distribution of observed/predicted ratios with quartiles 0.93 and 1.2, giving a standard deviation of 0.2. Although it may appear that the interpolation generally underpredicts in this case (ratio > 1), we cannot conclude this with confidence since all sites are used in the interpolation, which acts to correct this bias. If a bias remains, we do not know whether it is positive or negative; therefore, we assume that the interpolation is unbiased.

Compare Exposure Modeling Results Using Different Spatial Interpolation Methods

A wide range of methods for spatial interpolation of ozone have been employed over the years, and no one method has emerged as clearly superior to others. We plan to perform spatial interpolation with six different methods and run APEX with the resulting concentration fields. Comparison of these exposure modeling results, taken in conjunction with jackknife assessments of how well the interpolation methods perform, will provide a quantitative assessment of the effects of spatial interpolation uncertainty on the exposure modeling results.

At this time we have results for the nearest neighbor and inverse distance squared methods (Table 5 shows this for Boston, 2004). We are planning to perform this analysis for the Voronoi neighbor averaging method, bilinear interpolation, kriging, and the Bayesian maximum entropy (BME) method (Christakos et al., 2002).

Table 5. Comparison of predicted exposures using different spatial interpolation methods

City / Interpolation Method	Jackknife RMSE, hourly O_3	Jackknife RMSE for O_3 > 0.04 ppm	Percent of population experiencing 8-hour ozone exposures above these levels		
			0.06 ppm-8hr	0.07 ppm-8hr	0.08 ppm-8hr
Boston 2004					
Nearest nhbr	0.01	0.01	30.6	8.3	1.7
1/distance^2	0.008	0.01	26.7	6.4	0.85
% difference			−13%	−23%	−50%

Decreasing Radius of Representativeness of Monitors

In general, the closer a location is to a given monitoring site, the more accurately measurements at that site will represent the concentrations at the location. APEX allows the user to specify a radius of representativeness for the air quality monitors, and only estimates exposures to population residing in a Census tracts located within this radius of a monitoring site (the center of the tract is required to be within this distance of a monitor). Conversely, the further away locations are from monitoring sites, the more uncertain the spatially interpolated concentrations tend to be at these locations. In choosing the radius of representativeness there is a tradeoff between more accurate concentrations (smaller radius) and better characterization of the population (larger radius).

We conducted a series of APEX simulations varying the radius of representativeness of air quality monitors from 10 km to unlimited (within the modeled area) for the Boston CSA and using the nearest-neighbor spatial interpolation method. The results of these simulations are depicted in Figure 7 (2004 base case), Figure 8 (2002 base case), and Figure 9 (2002 current standard). The vertical axes are the fractions of the population, and the values for the unlimited radius are plotted at 60 km in these figures. Table 6 shows the 2002 population coverage for the different radii analyzed. This analysis indicates that the nearest-neighbor method of spatial interpolation may be introducing a small positive bias into the exposure modeling results.

Table 6. Population coverage of 2002 ozone monitors in Boston CSA

Radius about monitors (km)	Population coverage within the radius
10	47%
15	65%
20	81%
25	89%
50	99%
unlimited	100%

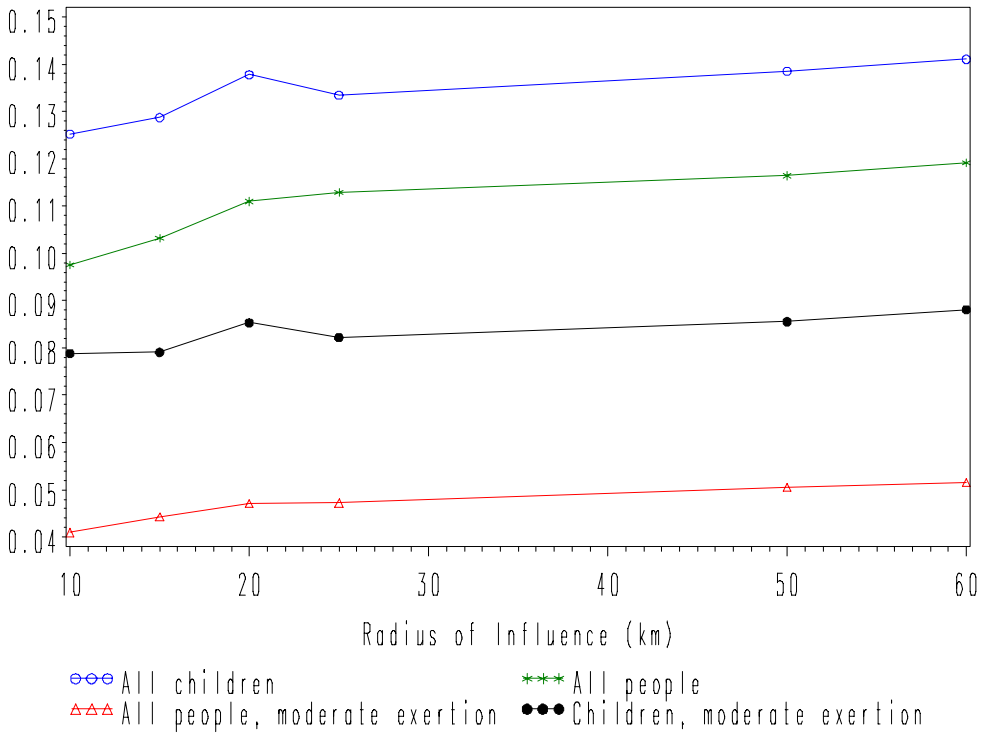


Figure 7. Sensitivity to monitor radius of influence of the fractions of four population groups with 8-hour exposures > 0.08 ppm-8hr, Boston, 2004 base case

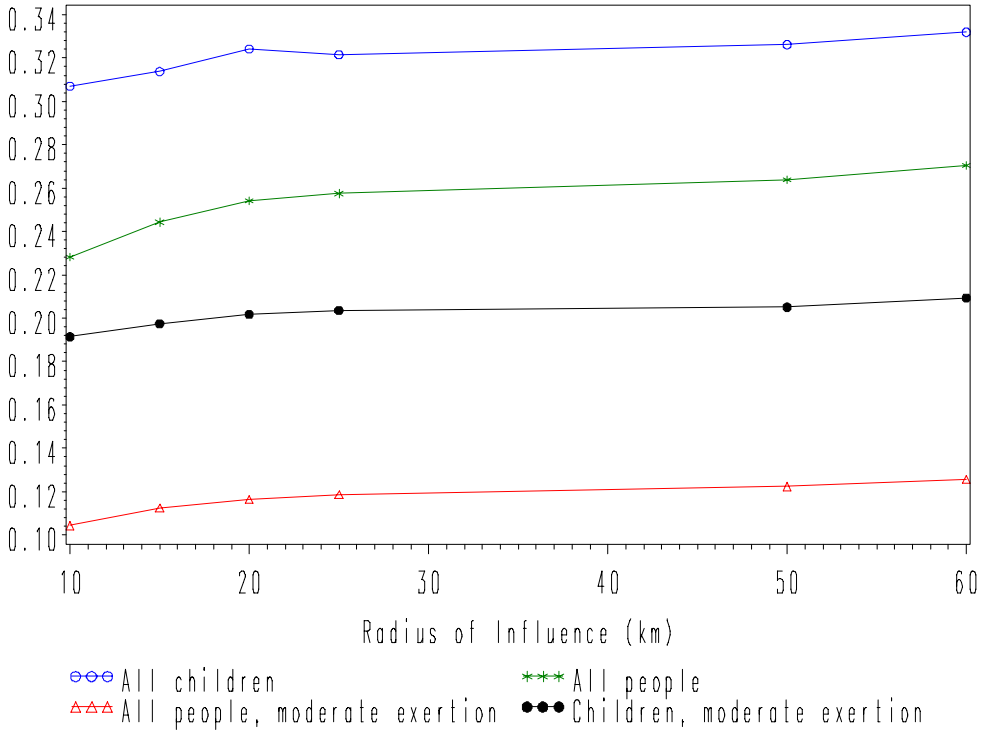


Figure 8. Sensitivity to monitor radius of influence of the fractions of four population groups with 8-hour exposures > 0.08 ppm-8hr, Boston, 2002 base case

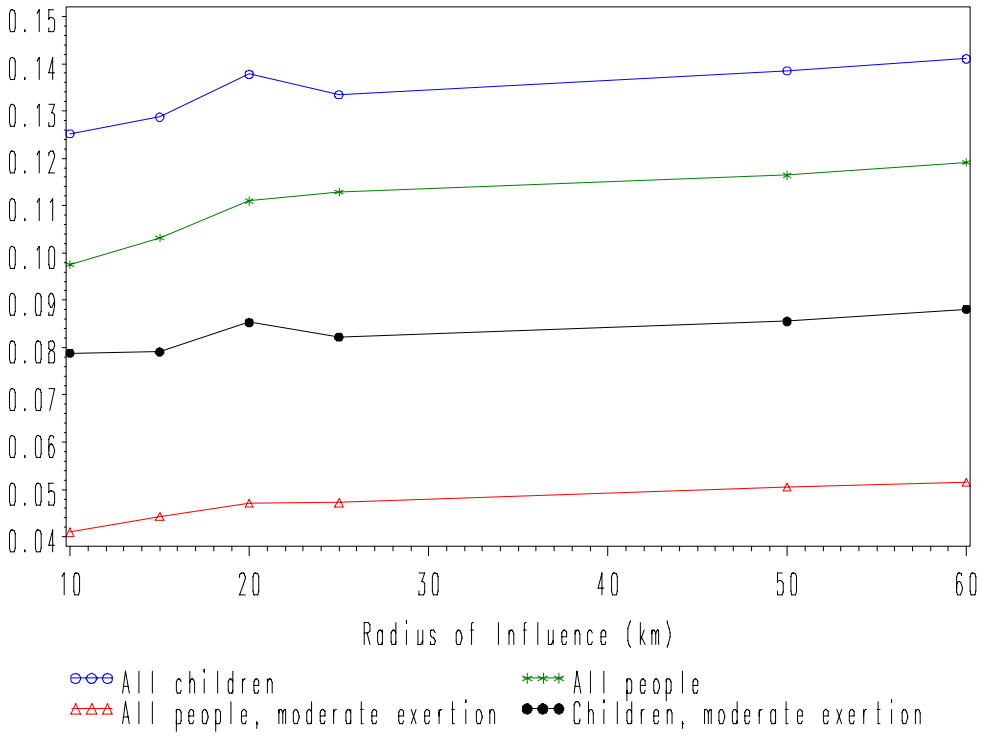


Figure 9. Sensitivity to monitor radius of influence of the fractions of four population groups with 8-hour exposures > 0.08 ppm-8hr, Boston, 2002 current standard

Summary of Uncertainty in Neighborhood-Scale Concentrations

Table 7 summarizes the uncertainties of neighborhood-scale concentrations for the Boston CSA. As discussed above, we are assuming that these uncertainties are normally distributed. It seems reasonable to assume that these three components of uncertainty are independent. The uncertainties of measurement error and missing data replacement are additive, while the spatial interpolation uncertainties are multiplicative, and so they cannot be directly combined. However, the spatial interpolation uncertainties are at least an order of magnitude greater than the other uncertainties, and we approximate the combined uncertainties by the spatial uncertainties (Table 7).

Table 7. Uncertainty distribution parameters for neighborhood-scale concentrations

Component of uncertainty	Mean (bias)	Standard deviation
Measurement error (additive)	small	0.00135 (ppm)
Missing data replacement (additive)	insignificant	0.004 (ppm)
Spatial interpolation (ratios)	none	0.2
Combined uncertainties (ratios)	none	0.2

Uncertainty of Outdoor Near-Roadway Concentrations

Concentrations of ozone near roadways are particularly difficult to estimate due to the rapid reaction of ozone with nitric oxide (NO) emitted from motor vehicles (forming NO_2 and O_2), which reduces ozone concentrations in the vicinity of the roadway.

APEX adjusts ambient ozone concentrations for NO titration near roadways through the use of proximity factors. Proximity factors which adjust concentrations according to the locations of people's activities can be input as single values or distributions to APEX. They are intended to scale the concentrations measured at fixed-site monitors to better represent the concentrations at other locations. In APEX they can serve the dual purpose of incorporating random concentration variability into the model.

We developed distributions for near-roadway proximity factors based on data from the 1994 Cincinnati Ozone Study (American Petroleum Institute, 1997, Appendix B; Johnson et al. 1995). Table 8 lists these distributions. Vehicle miles traveled in 2003 by city and road type obtained from the Federal Highway Administration were used to estimate the distribution of road types (local, urban, interstates) for each modeled city. The development of these proximity factor distributions is described in Appendix A of the Exposure Analysis TSD.

Table 8. Near-roadway proximity factor distributions

Location	Mean	Standard Deviation	Lower Bound	Upper Bound
outdoors near road and parking lots	0.755	0.203	0.422	1.0
in-vehicle, local roads	0.755	0.203	0.422	1.0
in-vehicle, urban roads	0.754	0.243	0.355	1.0
in-vehicle, interstates	0.364	0.165	0.093	1.0

We conducted a brief review of literature on near-roadway titration of ozone by NO to obtain information which could be used to estimate the uncertainty of the near-roadway proximity factor distributions. Rodes and Holland (1981) found reductions in ozone downwind of a Los Angeles freeway ranging from more than 90% at 8 meters to small reductions at 500 meters from the roadway. Lin et al. (2001) report a 30-40% reduction in ozone in a high traffic-density neighborhood. Suppan and Schadler (2004) in a modeling study using CMAQ predict ozone reductions from 3 to 20 ppb downwind of a major highway, with small changes in ozone concentrations as far as 40 km from the highway. Beckerman et al. (2006) measured ozone and other pollutants at various distances from a heavily traveled highway in Toronto and find significant variation even in 7-day average ozone concentrations, as shown in Figure 10.

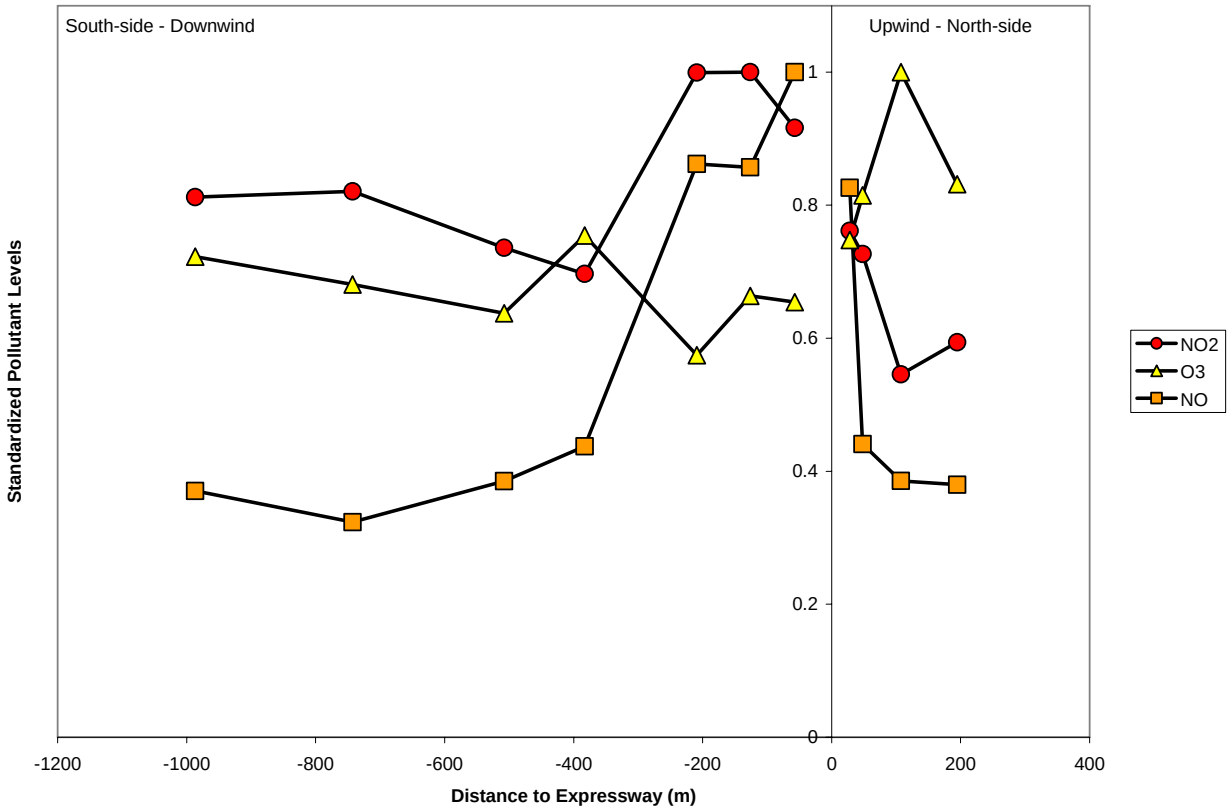


Figure 10. Pollutant concentrations around Highway 401, Toronto (Beckerman et al., 2006)

Based on this limited information we estimate the uncertainty of the means of the near-roadway proximity factor distributions to be uniformly distributed as summarized in Table 9. The standard deviations of the near-roadway proximity factor distributions have a lesser effect than the means, and we are not assigning uncertainties to them. The vehicle miles traveled by road type are much less uncertain than the titration adjustments, and therefore we are not taking into account their uncertainty.

Table 9. Uncertainty of the means of near-roadway proximity factor distributions

Location	Uncertainty of the mean of the distribution	Distribution of uncertainty (normal)		
		Uncertainty	Mean	Standard deviation
outdoors near road and parking lots	90% within [0.605, 0.905]	90% within [−0.15, 0.15]	0	0.09
in-vehicle, local roads	90% within [0.605, 0.905]	90% within [−0.15, 0.15]	0	0.09
in-vehicle, urban roads	90% within [0.604, 0.904]	90% within [−0.15, 0.15]	0	0.09
in-vehicle, interstates	90% within [0.214, 0.514]	90% within [−0.15, 0.15]	0	0.09

Uncertainty of Indoor Near-Roadway Concentrations

APEX considers a person to be near a roadway when their activity indicates this. There is no consideration of the effects of roadways on the concentrations in residences near roadways, and this is an additional source of uncertainty, since a significant portion of the population live near roadways (the 2001 American Housing Survey (U.S. Census Bureau, 2002) estimated that an eighth of the housing units in the U.S. are within 300 feet of a four or more lane highway, railroad, or airport). We plan to quantify the effects of this uncertainty by performing the exposure modeling to account for this in a simplistic way, and comparing those modeling results with the standard APEX results.

We have a data base that specifies the fraction of the population in each Census tract that live:

a) 0-75 m from a major roadway,
b) 75-200 m from a major roadway, and
c) >200 m from a major roadway.

The data are also stratified by six age groups: 0-1, 2-4, 5-15, 16-17, 18-64, 65+.

We plan to run APEX for each of these three subsets of the population, using proximity factors to decrease the ambient concentrations outside their residences in accordance with the

distance from roadways. The combined results of these three simulations will account for decreased exposures in residences near roadways. A comparison of these model results with the standard simulations will provide quantitative estimates of bias from this source of uncertainty.

Note that the phenomenon of titration by NO near roadways also has the potential to bias the exposure results in the other direction, in cases where the ozone monitors are located in areas of high traffic. Then the measurements can be biased low in comparison with other locations not affected by traffic emissions. Guidance for siting monitors gives criteria for how far to site monitors from roads to avoid interference that would make the monitor unrepresentative of the surrounding area (EPA, 1998). However, sometimes the siting of monitors near roadways is unavoidable. We are weighing the value of assessing the potential impact of traffic emissions on measurements for one or two of the modeled cities to ascertain whether or not this is an issue that needs to be considered. The location of each monitor in a city with respect to distance from roadways and traffic volume could be characterized, and adjustment factors be applied to concentrations at sites near roadways with as much specificity as the data allow (e.g., daytime vs. nighttime adjustments). APEX simulations could then be performed with the adjusted concentrations to assess the influence of this source of uncertainty.

Uncertainty of Ambient Commuting Concentrations

The ambient concentrations for a commuter are calculated in APEX as the average of the concentrations at the home and work locations, unless the worker commutes to a destination outside the study area, in which case the average ambient air concentration over all air districts in study area is used. We are considering modeling the uncertainty of this treatment by using a weighted average of the home and work tract concentrations in the Monte Carlo simulations, with weights distributed on the unit interval [0,1]. This is in addition to the general uncertainty of the ambient concentrations.

Uncertainty of the Vertical Profile of Concentrations

Ozone concentrations vary with height within the lower boundary layer, which can lead to exposure error for people living in high-rise apartment buildings (significantly higher than the ozone measurements) and in cases where an ozone monitor is significantly higher than the surrounding population. The CD (page AX3-202) states that:

> A study of the effect of elevation on O_3 concentrations found that concentrations increased with increasing elevation. The ratio of O_3 concentrations at street level (3 m) compared to the rooftop (25 m) was between 0.12 and 0.16, though the actual concentrations were highly correlated ($r = 0.63$) (Väkevä et al., 1999). Differential O_3 exposures may, therefore, exist in apartments that are on different floors. Differences in elevation between the monitoring sites in Los Angeles and street level samples may have contributed to the lower levels measured by Johnson (1997). Furthermore, since O_3 monitors are frequently located on rooftops in urban settings, the concentrations measured there may overestimate the exposure to individuals outdoors in streets and parks, locations where people exercise and maximum O_3 exposure is likely to occur.

We do not intend to address this source of uncertainty at this time, due to a lack of data on the vertical distribution of concentrations near the surface in urban areas.

Uncertainty in Concentration Rollback to Reflect Alternative Standards

One method for assessing the uncertainty of the rollback adjustments used in our modeling analyses is to apply the rollback procedure to historical air quality data and compare the observed air concentrations with the rolled-back concentrations (Rizzo, 2005). There are difficulties in translating this uncertainty into uncertainties of the APEX model inputs, and so we use a different approach.

We plan to use the quadratic rollback method to adjust ozone concentrations to reflect the current 8-hour standard for the four 3-year periods 2000-2002, 2001-2003, 2002-2004, and 2003-2005. For each of these 3-year periods, design values will be calculated, and hourly ozone concentrations rolled-back for the three years. Since each of these 3-year sets of concentrations represents just attaining the current standard, differences between them reflect uncertainty of the rollback method. Each of these four 3-year periods will be modeled using APEX for selected cities. The variability in the model results for each city will provide estimates of the uncertainty of rollback in the modeled exposures. Comparisons will be based on the distributions of modeled exposures over the 3-year periods, since it is the 3-year period which is being brought to just attaining the standard, and not each individual year.

The uncertainty of the rollback method is, to some extent, confounded with the uncertainty of a given area being in attainment, since the year-to-year variability in meteorology can have a significant effect on the design value of an area. An unusually cool and rainy summer can result in low ozone concentrations for that year, and significantly reduce the design value (which is the average of the three 4th highest concentrations for the 3-year period). A 3-year period with very different ozone levels often will have higher population exposures than a 3-year period with comparable ozone levels (where both periods have the same design value, or both being just in attainment of the standard). We can illustrate this phenomenon by comparing the distributions of air quality in an Eastern city rolled back to the current standard based on [***a***] the 2002-2004 design value and [***b***] a design value corresponding to three years of 2002 air quality. The 2002-2004 period had significant year-to-year variation in the East, and the hypothetical scenario of three years of 2002 air quality has no year-to-year variation.

Figures 11 and 12 graph the "annual design values" (the 4th highest 8-hour average concentrations at the monitor which yields the 3-year design value), respectively, for [***a***] and [***b***], for the base and "rollback to just-attaining" scenarios for New York (concentrations from Table 5A-8 in the Staff Paper). It is apparent from these figures that there would be more exposures to concentrations greater than 0.08 ppm under [***a***] than [***b***] (for the 'just-attaining" scenario), while the number of exposures to concentrations greater than 0.06 ppm may not be that different.

Figure 13 and Figure 14 contrast the distribution of hourly ozone concentrations (above 0.08 ppm) in New York for 2002 (the "high year") air quality rolled back using these two design

values these. Figure 15 combines into one chart these two figures and the corresponding distributions based on 2004 ("the low year") data. Figure 16 presents a more relevant comparison, combining the ozone concentrations for the high and low years (the most relevant comparison would combine all three years and compare population exposures instead of concentrations).

Meteorological Data

Uncertainty of Ambient Temperatures

Temperatures are the only meteorological inputs to APEX for this application. Temperatures input to APEX are specified not as distributions but as hourly and daily values measured from one or more monitors. Thus, temporal and spatial variability are accounted for. Due to the smooth nature of the temporal and spatial variability of temperatures, the uncertainty of the temperature inputs is typically small. Most of the temperature sites have no missing data; a few have 1 or 2 days missing during the year. Thus, the uncertainty from the estimation of missing temperature data is insignificant.

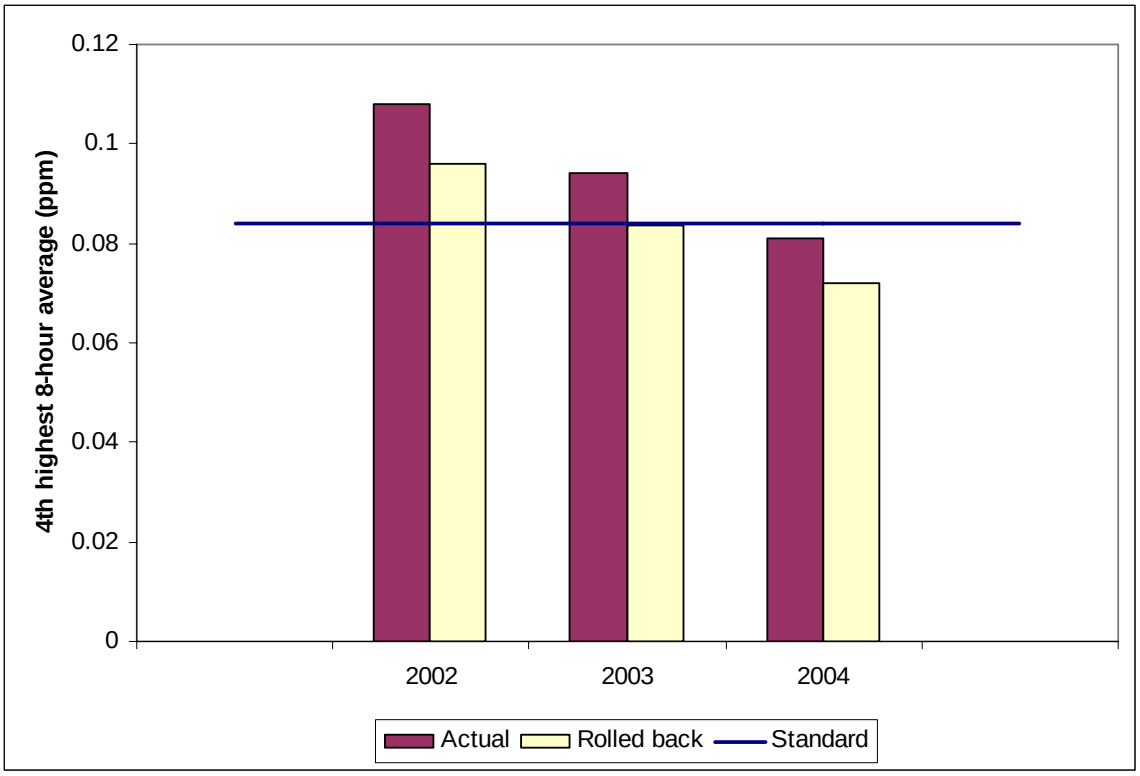


Figure 11. Rollback based on 2002 to 2004 concentrations

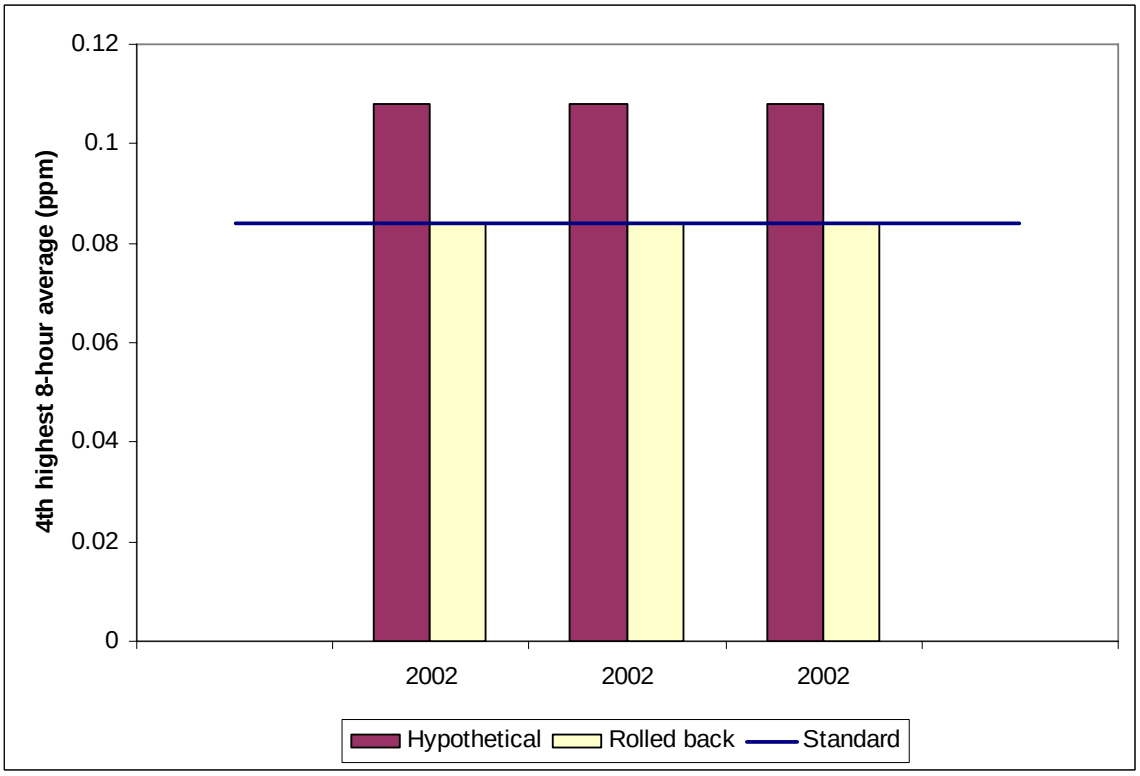


Figure 12. Rollback based on 3 years of 2002 concentrations

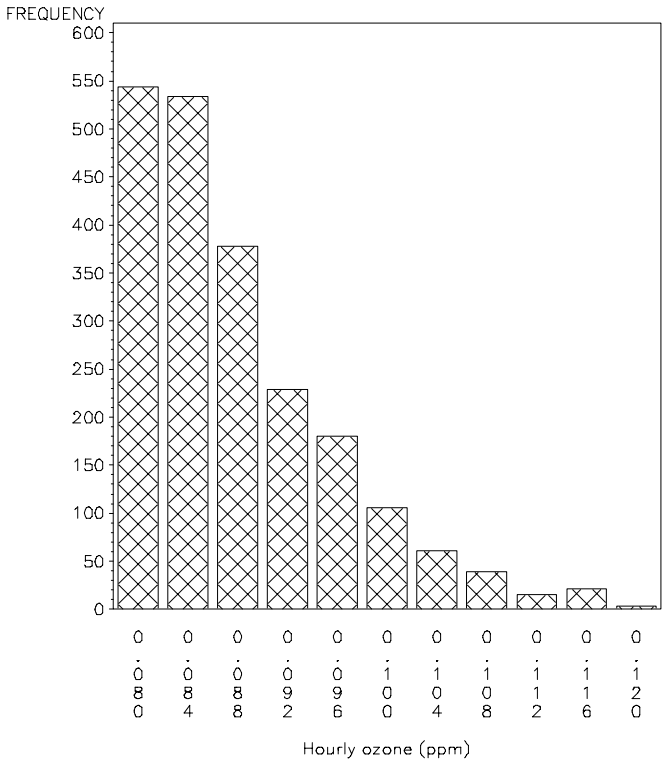


Figure 13. New York high-year (2002) ozone concentrations rolled back to the current standard, based on the 2002/2003/2004 design value

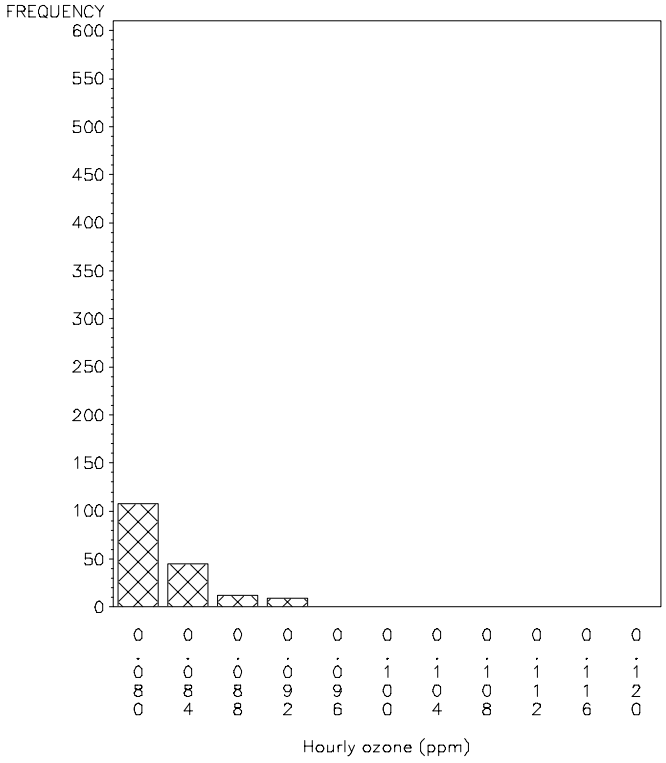


Figure 14. New York high-year (2002) ozone concentrations rolled back to the current standard, based on the 2002/2002/2002 design value

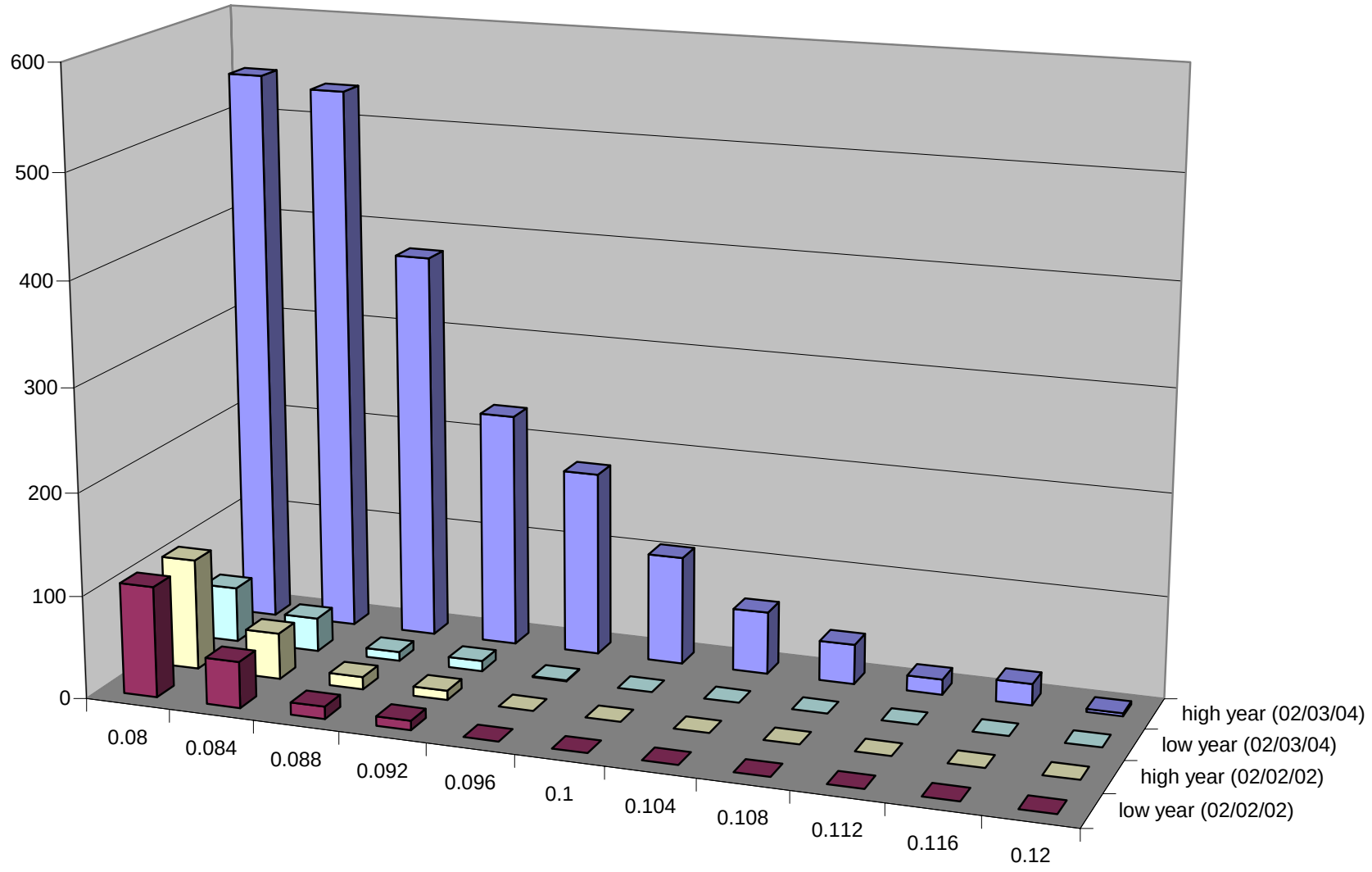


Figure 15. New York high and low year hourly ozone concentrations rolled back to the current standard, based on 2002-2004 and 3 years of 2002 design values

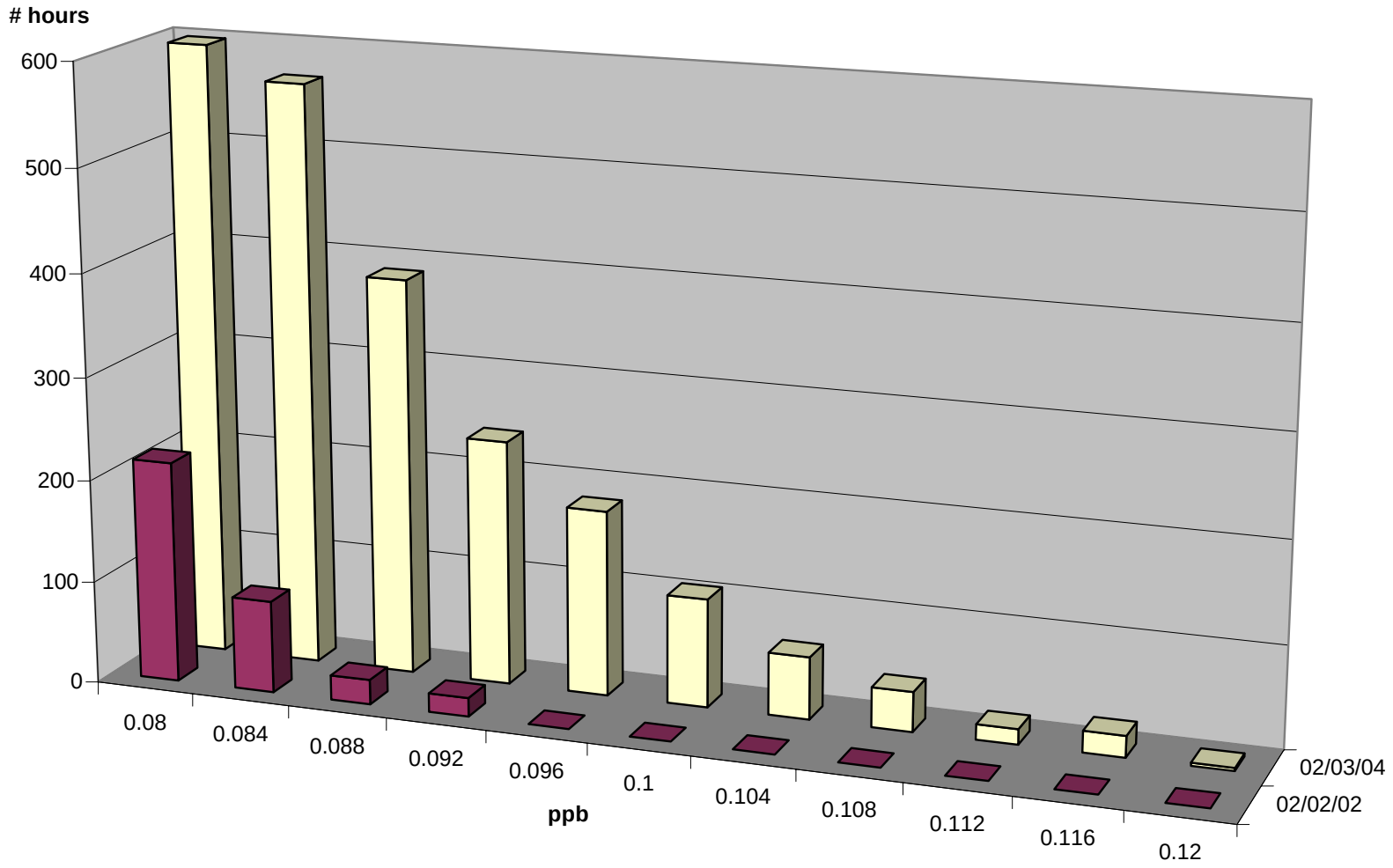


Figure 16. New York hourly ozone concentrations (high and low years combined) rolled back to the current standard, based on 2002-2004 and 3 years of 2002 design values

Modeling Concentrations in Microenvironments

The importance of estimation of concentrations in indoor microenvironments (homes, offices, schools, restaurants, vehicles, etc.) is underscored by the finding that personal exposure measurements of ozone are often not well-correlated with ambient measurements (CD, pages 3-59 to 3-61).

The microenvironmental characteristics used to model the concentrations in microenvironments tend to be highly variable, both in different microenvironments (e.g., different houses have varying characteristics) and within a single microenvironment (e.g., the characteristics of a specific house can vary over time). Since APEX is a probabilistic model, if data accurately characterizing this variability can be provided to the model, this will not result in uncertainties. However, even if we can appropriately characterize the distributions of each microenvironmental parameter, there will be significant uncertainties unless we appropriately model the relationships (correlations) between the different microenvironmental parameters, as well as the relationships between the microenvironmental parameters and other components of the exposure model (e.g., people's activities). The mass balance and factors models used to calculate ozone concentrations in the 12 microenvironments modeled (Table 10) are described in the Exposure Analysis TSD and in the APEX TSD.

Table 10. Microenvironments Modeled For Ozone Exposure

Microenvironment	Model	Parameters[1]
Indoors – Residence	Mass balance	AER and DE
Indoors – Bars and restaurants	Mass balance	AER and DE
Indoors – Schools	Mass balance	AER and DE
Indoors – Day-care centers	Mass balance	AER and DE
Indoors – Office	Mass balance	AER and DE
Indoors – Shopping	Mass balance	AER and DE
Indoors – Other	Mass balance	AER and DE
In-vehicle – Cars and Trucks	Factors	PE and PR
In-vehicle - Mass Transit	Factors	PE and PR
Outdoors – Near road	Factors	PR
Outdoors – Public garage - parking lot	Factors	PR
Outdoors – Other	Factors	PR

[1] AER: Air Exchange Rate, DE: Decay rate; PE: Penetration factor; PR: Proximity factor

Uncertainty of Air Exchange Processes

The air exchange rate (AER) is one of the most important factors in determining the ratio of outdoor to indoor concentrations of ozone. AERs are highly variable at hourly and daily time scales, both within a microenvironment over time and between microenvironments of the same type in different buildings. AERs depend strongly on the physical characteristics of a microenvironment and also on the behavior of the occupants of the microenvironment. For

example, the concentration in a house when a person enters the house will depend on the AER of the preceding hour, which could depend on whether or not there was someone else already in the house. There is also some dependence on the atmospheric conditions (temperature, humidity, and wind speed), both directly (higher wind speeds result in higher AERs in most circumstances) and indirectly (occupants can open and close windows in response to the outdoor temperature).

AER measurements (which are used to derive the APEX input distributions for a city) typically involve fitting tracer concentrations to simple mass balance models. This analysis of AER uncertainty currently does not take into account the uncertainty in this measurement/ modeling process.

Residential Air Exchange Rates

City-specific lognormal distributions of AERs for use with the APEX ozone model were developed based on an analysis of AER data from several studies (Exposure Analysis TSD, Appendix A). The parameters of these distributions depend on the outside temperature and whether or not the residence has air conditioning.

We assess the within-city uncertainty by using a bootstrap distribution to estimate the effects of sampling variation on the fitted geometric means (GMs) and standard deviations (GSDs) for each city. This analysis is described in the Exposure Analysis TSD. The bootstrap is a nonparametric method for estimating uncertainty which accounts for the correlation between the GMs and GSDs (e.g., see Figure 18), so that there are not unrealistic combinations of GMs and GSDs. The bootstrap distributions assess the uncertainty due to random sampling variation but do not address uncertainties due to the lack of representativeness of the available study data. This can be assessed, to some extent, by comparing AER distributions from different studies in the same city.

Several bootstrap distributions were developed, one for each city-temperature-A/C combination. Examples of two of the bootstrap uncertainty distributions are provided in Figure 17 and Figure 18. Figure 17 shows the uncertainty distribution around the model input values GM=0.916 and GSD=2.451, which specify the distribution of AERs of residences in Houston without A/C when ambient temperatures are above 20 degrees C (24-hour average). Similarly, Figure 18 shows the uncertainty distribution for the AER distribution parameters for Los Angeles for residences without A/C when the ambient temperature is above 25 degrees C. Note that in these figures there is only one "original data" point (this is the APEX input value), indicated by the intersection of the cross-hairs in the figure. The clouds of points are all bootstrapped data. In the Monte Carlo uncertainty simulations, a GM, GSD pair is selected at random from the appropriate bootstrap uncertainty distribution, and used for input to APEX. (APEX then selects AER values randomly from the log-normal distribution with the bootstrap GM and GSD.)

We estimate the between-city variability by examining the variation of the GMs and GSDs across cities. Figure 19 shows the variation of GMs between the six cities or regions for which we have developed AER distributions, for the temperature ranges and A/C presence we are using to specify AER distributions in the inputs to APEX (Y means the residence has A/C, N

means it does not). Most of the cities modeled do not have city-specific AER distributions, and use AER distributions from a different city (Table 11). We use the city-to-city variability of the GMs and GSDs to characterize the uncertainty of applying city-specific AER distributions to a different city for which there are no AER data available. We model this uncertainty using a weighted bootstrap sampling of these GM,GSD pairs, with the weights based on similarity of the modeled city to the cities/regions for which AERs were developed. Thus, for Boston we assign higher weight to the New York distributions and lower weights to the Houston and Los Angeles area-specific distributions, as given in Table 12.

Non-Residential Air Exchange Rates

We are using a placeholder estimate for the uncertainty of the GM of the distribution of non- residential AERs used in APEX, assuming for now that this uncertainty is uniformly distributed within ±5 percent of the GM (5% of 1.109 = 0.06), and no uncertainty for the GSD. We plan to explore the literature to find a reasonable estimate for this uncertainty.

Uncertainty of Residential Air Conditioning Prevalence and Use

The AER distributions input to APEX are conditioned on the presence or absence of air conditioning, and estimates of residential air conditioning prevalence rates for each modeled area were obtained from the American Housing Survey of 2003. Appendix F of the Exposure Analysis TSD gives confidence intervals for the air conditioning prevalence rates, reproduced here in Table 13. We model the uncertainty of the prevalence rates with zero-mean normal distributions with standard deviations equal to the standard errors given in Table 13.

In addition to the uncertainty of prevalence rates, there is uncertainty about the amount of use of A/C given that a house or office has A/C. However, most of the studies of AERs that we used to develop AER distributions report presence or absence of air conditioning, and not whether the A/C was being used (Appendix A, Exposure Analysis TSD). Thus, the variability resulting from the use or non-use of A/C is built into the AER distributions, and is being taken into account. If, in the future, we have sufficient data to allow us to characterize AERs separately for conditions of use and non-use, then we can supply APEX with these distributions, as well as distributions for use vs. non-use. With the availability of such refined model inputs, the uncertainty of use vs. non-use will become more relevant.

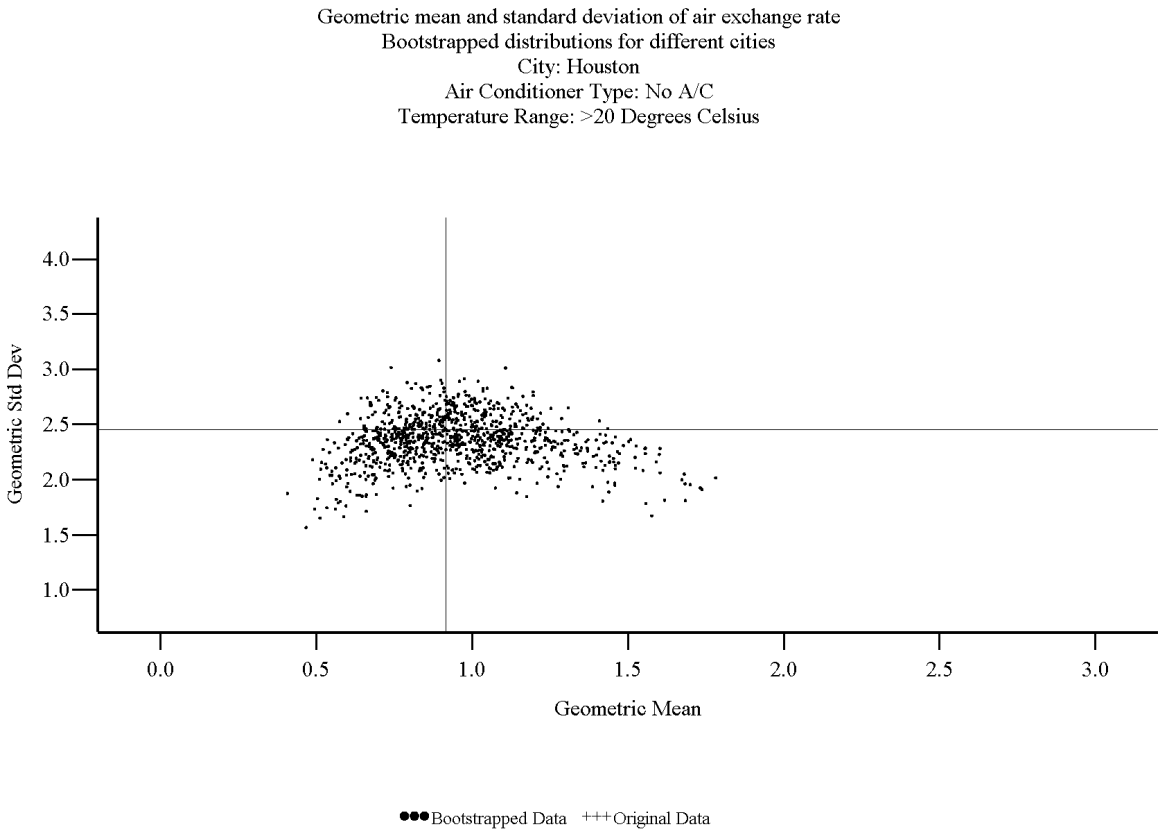


Figure 17. Bootstrap distribution of AER uncertainty for Houston, no A/C, >20 C

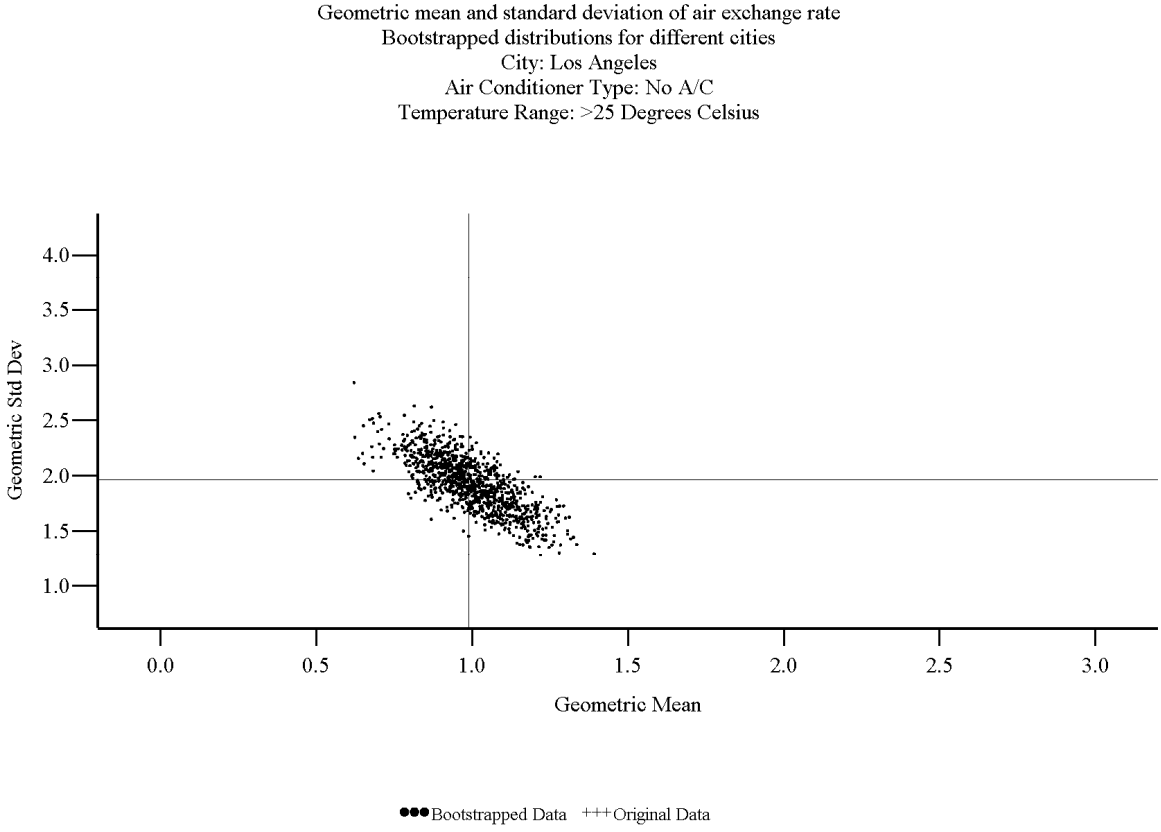


Figure 18. Bootstrap distribution of AER uncertainty for Los Angeles, no A/C, >25 C

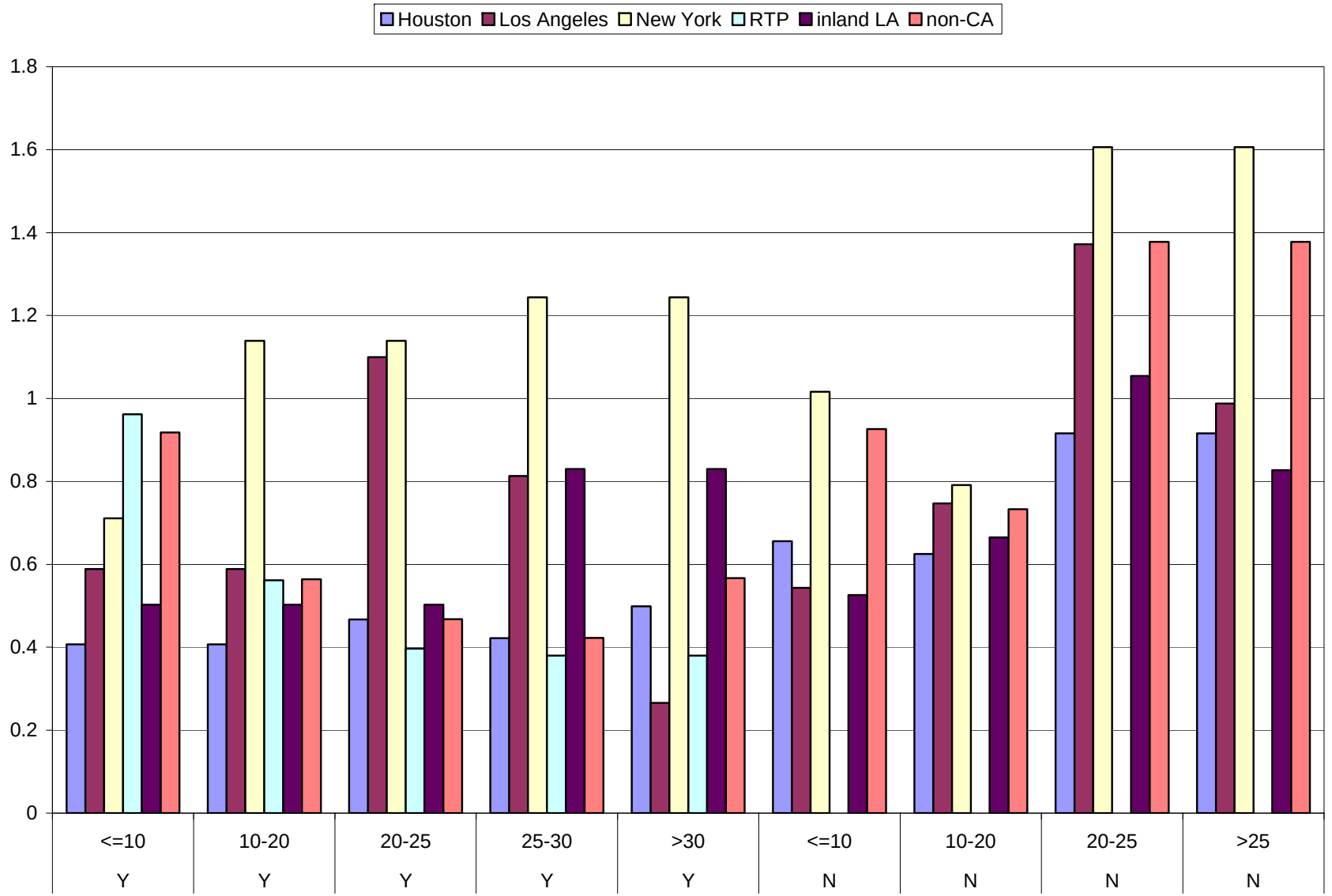


Figure 19. AER Geometric Means For Different Areas by Temperature Range (C) and A/C Presence (Yes/No)

Table 11. Assignment of residential air exchange rate distributions to modeled cities

Modeled city	Air exchange rate distribution
Atlanta, GA, A/C	Research Triangle Park, A/C only
Atlanta, GA, no A/C	All non-California, no A/C
Boston, MA	New York
Chicago, IL	New York
Cleveland, OH	New York
Detroit, MI	New York
Houston, TX	Houston
Los Angeles, CA	Los Angeles
New York, NY	New York
Philadelphia, PA	New York
Sacramento	Inland parts of Los Angeles
St. Louis	All non-California
Washington, DC, A/C	Research Triangle Park, A/C only
Washington, DC, no A/C	All non-California, no A/C

Table 12. Bootstrap sampling weights for Boston for uncertainty of the use of non-city-specific residential AER distributions

City/Region	Sampling weight
New York	0.6
Houston	0.0
Los Angeles	0.1
All non-California	0.2
Inland parts of Los Angeles	0.0
Research Triangle Park (A/C only)	0.1

Table 13. Uncertainty of air conditioning prevalence rates

City	Prevalence rate	Standard error	Lower 95% confidence bound	Upper 95% confidence bound
Atlanta, 2003	97.0	1.18	94.7	99.3
Boston, 2003	85.2	2.14	81.0	89.4
Chicago, 2003	87.1	1.39	84.4	89.8
Cleveland, 2003	74.6	3.38	68.0	81.3
Detroit, 2003	81.4	1.76	78.0	84.9
Houston, 2003	98.7	0.67	97.4	100.0
Los Angeles, 2003	55.1	1.70	51.7	58.4
New York, 2003	81.6	1.27	79.1	84.1
Philadelphia, 2003	90.6	1.30	88.1	93.2
Sacramento, 2003	94.6	1.93	90.8	98.4
St. Louis, 2003	95.5	1.67	92.3	98.8
Washington DC, 2003	96.5	1.00	94.5	98.4

Uncertainty of Deposition, Filtration, and Chemical Reaction Processes

The removal of ozone from a microenvironment due to deposition, filtration, and chemical reaction processes is modeled in APEX by a combined distribution of ozone decay rates. The rate of deposition of ozone to a surface depends on the material the surface is made of, the humidity, and the concentration of ozone. The rate of removal of ozone due to deposition in a specific microenvironment also depends on the dimensions, surface coverings, furnishings, and the ratio of surface area to volume in the microenvironment. The degree of ozone loss through filtration is a function of the HVAC system in the microenvironment. Other chemical processes that contribute to reduction in ozone concentrations indoors include reaction with NO_x emitted from gas stoves and reaction with VOCs from cleaning products.

The distribution of ozone decay rates used in the present study represents the decay rates measured in a study of 17 residences in Southern California (Lee et al., 1999). A lognormal distribution was fit to the measurements from this study, yielding a geometric mean of 2.5 and a geometric standard deviation of 1.5. These values are constrained to lie between 0.95 and 8.05 $hour^{-1}$. We estimate the uncertainty of this distribution using a bootstrap method described by Cullen and Frey (1999). This is a method for quantifying sampling uncertainty nonparametrically, but does not account for uncertainty resulting from nonrepresentativeness of the study in relation to the urban areas we are modeling. We found that the bootstrap-derived uncertainties can be adequately represented by independent normal distributions with zero means and standard deviations of 0.1 for the GM and 0.05 for the GSD.

We plan to review the literature on ozone loss in microenvironments due to deposition, filtration, and chemical reaction processes to estimate the uncertainty resulting from nonrepresentativeness of using the results of only one study. As a placeholder for this uncertainty, we assume that the GM of 2.5 is unbiased but could be off by 10 percent with 90 percent confidence, and represent this uncertainty with a normal distribution with a standard deviation of 0.15.

It is reasonable to assume that this uncertainty is independent of the sampling uncertainty, and therefore we can combine these uncertainties by summing their variances. Table 14 summarizes our preliminary estimates of the uncertainty of ozone decay rates.

Table 14. Uncertainty of lognormal distributions of ozone decay rates (per hour)

Source of Uncertainty	Geometric Mean	Geometric Standard Deviation
Finite sample	normal distribution, mean = 0, st. dev. = 0.1	normal distribution, mean = 0, st. dev. = 0.05
Nonrepresentativeness of the study[1]	normal distribution, mean = 0, st. dev. = 0.15	
Combined uncertainty	normal distribution, mean = 0, st. dev. = 0.18	normal distribution, mean = 0, st. dev. = 0.05

[1] Preliminary estimate of uncertainty (see text)

Uncertainty of Vehicle Penetration Factors

A vehicle penetration factor distribution (normal, mean 0.3, standard deviation 0.232, lower bound 0.1, upper bound 1.0) was developed with data from the Cincinnati Ozone Study (Johnson et al, 1995). This was a scripted study using three cars in one city in 1994, and therefore is not likely to be representative of general vehicle ventilation conditions. We plan to conduct a literature review and obtain available data to provide information on the uncertainty of vehicle penetration factors. We will complete Table 15 with this information, summarizing the results of studies which measured vehicle penetration factors or ratios of ozone concentrations inside and outside of vehicles. The range of the mean penetration factors in these studies will provide information on the uncertainty of these distributions (some studies are more representative of general conditions than others). For the current uncertainty analysis, we are using a placeholder estimate that the mean of the vehicle penetration factor distribution is likely to lie within ±0.2 of the base estimate, and may be biased low by 5 percent for vehicles traveling at higher speeds. We feel that this estimate is more realistic than the implied uncertainty of zero if we do not include this source of uncertainty due to a lack of data. We represent this uncertainty with normal distributions so that the mean values input to APEX are between 0.1 and 0.5 with 90 percent probability, with an average value of zero, for vehicles on local and urban roads, and mean values between 0.115 and 0.515 with 90 percent probability, with an average value of 0.015 (5% of 0.3) for vehicles on interstate highways. Table 16 gives the means and standard deviations of the normal distributions that represent the (additive) uncertainty of the

vehicle penetration factors input to the model. As noted above, this estimate of uncertainty is essentially a placeholder until we have further information.

Table 15. Summary of ozone vehicle penetration factor studies (incomplete)

Study description	Mean penetration factor
Cincinnati Ozone Study (Johnson et al, 1995). Scripted study using three cars in Aug.-Sept. 1994. 812 measurements.	0.30
RTP Patrol Cars study (Riediker et al., 2003). Ozone concentrations measured with Ogawa badges in vehicles and at the roadside. 25 measurements.	0.46

Table 16. Uncertainty of the means of vehicle penetration factor distributions

Vehicle class	Mean[1]	Standard deviation[1]
Traveling on local and urban roads	0.0	0.12
Traveling on interstate highways	0.015	0.12

[1] of normal distributions. These are placeholder estimates of uncertainty (see text).

Characterization of Population Demographics

Uncertainty of Demographic Model Inputs

Data from the 2000 Census provide the demographics of the modeled populations. When modeling a year close to the year of the Census, the uncertainty of the demographic mix of the population is relatively small, compared with the other uncertainties of APEX, and therefore we are not treating this as an explicit source of uncertainty in this analysis. The Census data input to APEX at a tract level are:

- age
- gender
- race (not used in this modeling analysis)
- home location (Census tract)
- work location (Census tract)
- employment probabilities (by age, gender, tract)
- between-tract commuting probabilities

However, we can quantify changes in the size of the total populations between the year of the Census (2000) and the year being modeled. Table 17 lists the percent increase in population from 2000 to 2002 and 2004 for the 12 modeled CSAs (calculated from the *Subcounty*

Population Estimates, April 1, 2000 to July 1, 2004, Population Estimates Program, U.S. Bureau of the Census Release dated June 30, 2005).

Table 17. Change in populations from 2000 to 2002 and 2004

Urban Area (CSA)	2000 to 2002 % change	2000 to 2004 % change
Atlanta, GA	5	10
Boston, MA	1	1
Chicago, IL	2	3
Cleveland, OH	0	0
Detroit, MI	0	1
Houston, TX	5	9
Los Angeles, CA	3	7
New York, NY	1	2
Philadelphia, PA	1	2
Sacramento, CA	6	11
St. Louis, MO	1	2
Washington, DC	3	5

The biases resulting from population changes likely cancel to a large degree when assessing relative differences between exposure and risk scenarios. These biases could be corrected for by increasing the counts of people exposed to ozone by these percentages.

Modeling People's Activity Patterns

The distributions of the variability of the activities of individuals are generated by random sampling of daily activity patterns in the Consolidated Human Activity Database (CHAD). CHAD consists of a collection of 24-hour "diaries" compiled from several studies. Each diary specifies the activities of an individual during the day, the locations of the individual during the activities, and the time period of each activity. The durations of the events in the diaries range from a few minutes to several hours.

Uncertainty of the Activity Pattern Data

The activity pattern database (CHAD) input to APEX is a very complex multivariate database which, due to its complexity, is less amenable than other model inputs to the Monte Carlo approach to uncertainty analysis. In particular, it would be very difficult to vary a set of characteristics of CHAD and generate different diary databases reflecting the varied

characteristics. In addition, we don't know a priori what the important characteristics of CHAD are with respect to uncertainties of exposure modeling. A further complication is that we must consider the uncertainties of CHAD in the context of the formation of a year-long activity sequence made up of diary days sampled from CHAD, for each individual simulated by APEX. The uncertainty that results from the method for assembling diary-days for each individual could also be important. The following are limitations of CHAD that result in uncertainties in modeling exposures.

- Diary errors, particularly the recall studies (72% of CHAD diaries are recall). There is extensive literature on diary errors; Takarangi et al. (2006) provide an instructive commentary on factors which conspire to produce inaccurate diary data.
- Incompatibility of the CHAD categories/codes with the coding schemes in the different studies in CHAD (each study's codes are mapped to the CHAD codes)
- Nonrepresentativeness of non-random studies
- Nonrepresentativeness of older studies (in CHAD 42% are pre-1990, 98% are pre-1995)
- Geographic (city-specific) nonrepresentativeness
- Sample size limitation. This is particularly important because of the stratification required for appropriate use of the data in exposure modeling.
- Longitudinal autocorrelation of activities is not characterized.
- Geographical locations of activities away from the home are unknown.

It is difficult to characterize the uncertainties in CHAD and to propagate these uncertainties to the model results, and we are taking two approaches to this problem, a multivariate statistical approach and a comparison with an independent activity database.

Multivariate Statistics Approach

In this approach we identify the few statistics (i.e., characteristics) of the activity database that are most influential in terms of the exposure results of interest, using the classification and regression trees (CART) method. We plan to try to estimate the uncertainty of these statistics, and from there quantify the uncertainty of the exposure modeling results due to uncertainty in the activity database. The diagram on the next page illustrates this approach, and the details will be filled in if this approach is successful. The success of this approach will depend on our ability to estimate the uncertainty of the CHAD statistics $\{\mathbf{X}_i\}$ (see diagram).

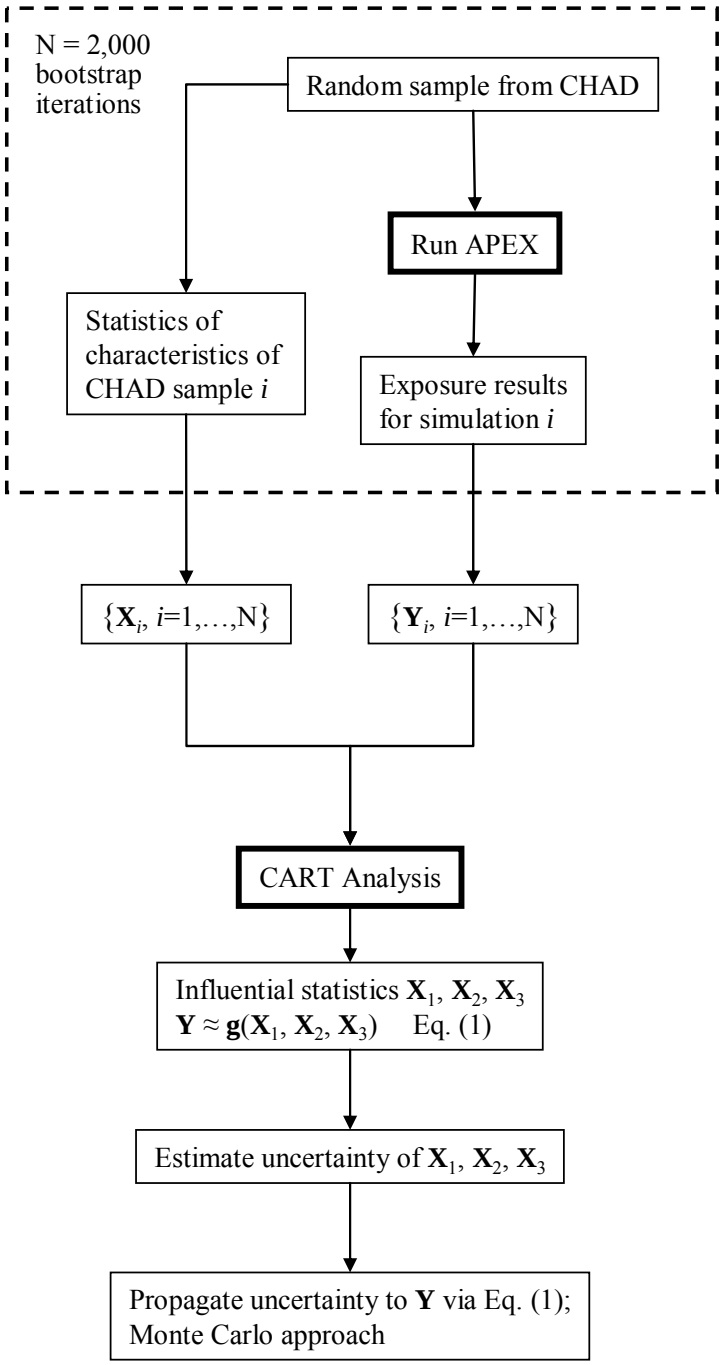


Diagram 1. Activity Data Uncertainty Analysis

Comparison with an Independent Activity Database

An excellent activity database is available for comparison with the CHAD data used for the exposure modeling. The Child Development Supplement (CDS) is part of the Panel Study of Income Dynamics (PSID), a longitudinal study of a representative sample of U.S. individuals and families which started collecting data in 1968. In 1997, PSID supplemented its main data collection with additional data on 0-12 year-old children and their parents. The CDS-I successfully completed interviews with 2,394 families (88%), providing information on 3,563 children. In 2002-2003, CDS recontacted families in CDS-I who remained active in the PSID panel as of 2001. CDS-II successfully reinterviewed 2,019 families (91%) who provided data on 2,907 children and adolescents aged 5-18 years. Time diary accounting was carried out for one randomly selected weekday and one weekend 24-hour period for each child. The *User Guide for CDS-II* (CDS, 2005) states:

> "The time diaries are one of the unique features of the CDS design. While the PCG [primary caregiver] and Child interviews include stylized questions about the children's structured and unstructured activities, and activities with parents and absent parents, the time diaries provide detailed accounting of the type, number, duration, and location of activities during sampled 24-hour days, beginning at midnight for one randomly sampled weekday and one randomly sampled weekend day. Using the time diaries, we additionally collected information on the social context of the activity by specifying with whom the child was doing the activity and who else was present, but not engaging."

The entire datasets are available from the Institute for Social Research at the University of Michigan at http://www.psidonline.isr.umich.edu.

We plan to run APEX for children aged 5-18 years using CHAD and using the CDS-II data for all 12 cities (with 2002 air quality data) and compare the two sets of model results. Since the CHAD data for children (3,075 diary-days for ages 5-18) are all older than 1995, and the CDS-II data (more than 5,000 diary-days for ages 5-18) are recent (2002-2003) and nationally representative, we can assume that the CDS-II data are significantly less uncertain than CHAD, and will attribute the differences in model results primarily to uncertainty due to CHAD.

Uncertainty of Longitudinal Diary Assembly

The method in APEX for assembling longitudinal diaries is intended to capture the tendency of individuals to repeat activities (this method is described in detail in the Exposure Analysis TSD). There are two model input parameters that control the strength of this tendency in the simulated individuals, a population diversity statistic (***D***) and a within-person autocorrelation statistic (***A***). For the current application, these statistics are based on the time a person spends outdoors each day, which is one of the most important determinants of exposure to ozone. The ***D*** statistic reflects the relative importance of within-person variance and between-person variance in the outdoor time. The ***A*** statistic specifies the day-to-day autocorrelation of outdoor time. The values used for this analysis (0.2 for ***D*** and 0.2 for ***A***) are

based on one study of school age children, and are considerably uncertain. To reflect this uncertainty in the Monte Carlo analysis, we allow ***D*** and ***A*** to vary independently, uniformly within a factor of two of their base values (varying from 0.1 to 0.4) Table 18 gives the distributions of (additive) uncertainty about the base values.

Table 18. Uncertainty of longitudinal diary parameters

Parameter	Distribution of uncertainty
population diversity statistic (***D***)	Uniform on [−0.1, 0.2]
within-person autocorrelation statistic (***A***)	Uniform on [−0.1, 0.2]

Modeling Physiological Processes

We plan to continue our review of the literature to quantify the uncertainties of these model inputs. This will then be included in the Monte Carlo assessment of uncertainty. Also see the discussion of the physiological model in APEX in the Model Uncertainty section below, which is relevant to this section.

Uncertainty of Physiological Model Inputs

The physiological model inputs to APEX are provided as parameters for distributions reflecting population variability. These have been recently updated by Isaacs and Smith (*New Values for Physiological Parameters for the Exposure Model Input File Physiology.txt*, December, 2005). The following distributions and parameters are input to APEX:

- Body mass (BM) (kg) distributions by age and gender
- Normalized maximal oxygen uptake (NVO_2max) distributions by age and gender
- Resting metabolic rate (RMR) (kcal/min) age- and weight-specific regression equations
- Metabolic equivalent (MET) distribution for each activity type (dimensionless). Distributions for a few activities are occupation- and age-dependent.
- Effective ventilation rate (EVR) cutpoints for specifying levels of exertion (e.g., 1-hour average EVR > 16 indicates moderate or greater exertion) (single values)
- Active PAI cutpoint (a person is characterized as "active" if their median daily PAI > 1.75) (single value)

Body Mass Distributions

The distributions of body mass come from the most recent data from the National Health and Nutrition Examination Survey (NHANES), compiled for the years 1999-2004 (CDC, 2005). The NHANES body mass data are sampled and weighted to provide unbiased national estimates of body mass. There will be some uncertainty due to regional/city differences. However, the uncertainty in the body mass distributions is small compared to the other uncertainties in the APEX input data, and we are treating it as insignificant.

NVO_2max Distributions

NVO_2max is used in the calculation of the maximum metabolic activity level that can sustained for about five minutes (maximum permitted MET value). These distributions were recently updated based on an extensive review of the literature and acquisition of data (Isaacs and Smith, 2005). Parametric fits to data were used to calculate the values input to APEX. We are considering the use of a bootstrap analysis of these fits to quantify the uncertainty of these inputs.

Resting Metabolic Rates

The uncertainty of the model for predicting resting metabolic rates is more relevant than the uncertainty of the coefficients input to APEX, and this is discussed below in the section on model uncertainty.

MET Distributions

The uncertainty of the MET distributions may turn out to be important. Johnson (2003, section 9.6) states:

> Perhaps the weakest link in the algorithm is the step which requires the analyst to provide a distribution of possible MET values for each activity code. These distributions are currently based on distributions provided by the developers of CHAD (McCurdy et al., 2000). Because available data were often insufficient to accurately define a distribution for each activity code, the developers tended to follow a conservative approach and over-estimate the variability of each distribution. Consequently, the Ve values produced by the ventilation rate algorithm may exhibit an excessive degree of variability.

McCurdy et al. (2000), in a paper describing the development of the METs distributions in CHAD, state:

> At this stage of development, the METs distribution assignment effort should be viewed as being preliminary in nature. More work is needed to better relate activity codes used in human activity pattern surveys to those long used by exercise physiologists and clinical nutritionists.

Most of the MET distributions in CHAD were developed based on Ainsworth (1993), which has been updated and revised in 2000 (Ainsworth, 2000, 2003). CHAD has not yet been updated with this newer information.

There is some uncertainty in the METS distributions related to the question of how well the MET distributions for defined activities represent the actual exertion during the discrete event duration. For example, a diary event for an hour may be coded "play basketball" (which has a relatively high MET value), but in reality the MET value may be much lower for the hour, since it is likely that the hour-long event contains periods of rest. Also, there is uncertainty due to the use of MET distributions for children, the elderly, and persons with compromised health,

since they were derived from healthy adults. Puyau et al. (2002) show that adult-derived MET cutpoints are not applicable to children.

There are several studies which report MET distributions, which might be able to be used to evaluate the distributions APEX assigns to specific population groups. For example, the Nurses' Health Study in 1992 obtained MET-hours/week for over 67,000 subjects (Kroenke et al., 2005). However, in most of these studies (including the Nurses' Health Study) MET values are not directly measured.

EVR Exertion Level Cutpoints

The EVR cutpoints input to APEX are selected for the risk calculations (discussed in the Staff Paper) and are not considered as uncertain here. (As opposed to the values of EVR calculated by APEX, which are uncertain.)

Active PAI cutpoint

In order to address the uncertainty of the PAI cutpoint used in the exposure modeling analysis, one must have a clear definition of what it means for a person to be characterized as active. Then one could assess the extent to which the PAI cutpoint classification is accurate. We do not have such a definition, and have essentially been using the PAI cutpoint as defining an active person. If this is our working definition of "active" then there is no uncertainty in this model input. We discuss this further in the section on model uncertainty below.

Convergence

APEX is a probabilistic model with numerous inputs and parameters defined in terms of probability distributions which reflect the natural variability of the physiology and activities of individuals and of physical processes. In order to realistically estimate distributions of population exposures, a sufficient number of individuals must be simulated by APEX to reflect these distributions. For this discussion we denote the number of simulated individuals in an APEX run by N_S. As N_S for a model run increases, the predicted exposure distributions converge to a limiting distribution. If too few individuals are simulated, then the results of simulations with identical inputs will differ because too few values from the input distributions are being sampled to properly characterize them.

To illustrate this phenomenon, we ran thousands of APEX simulations with identical inputs, but with varying N_S. From each APEX run we calculated statistics from the predicted distributions of exposures, for example, the fraction of the population who experience one or more hourly exposures greater than 0.12 ppm-hr. For runs with very few people simulated, these statistics are not stable and can vary widely; but for runs with many people simulated, the statistics have values that are closer together for the different model runs. This is illustrated in Figure 20, where we have plotted the spread of one statistic against N_S. The horizontal axis gives N_S, for 1000, 2000, up to 15,000, simulated in each APEX run. The vertical axis is the fraction of the population who experience one or more hourly exposures greater than 0.12 ppm-

hr, and the collection of those values for all runs with a given N_S is presented as a box plot. The bottom and top edges of a box indicate the 25th and 75th percentiles; whiskers are at the 5th and 95th percentiles; and squares indicate values outside this range. We see that for N_S = 1000, this statistic ranges from 0.172 to 0.242 (±17% from the median), while for N_S = 15,000 the range is only from 0.198 to 0.213 (±4% from the median).

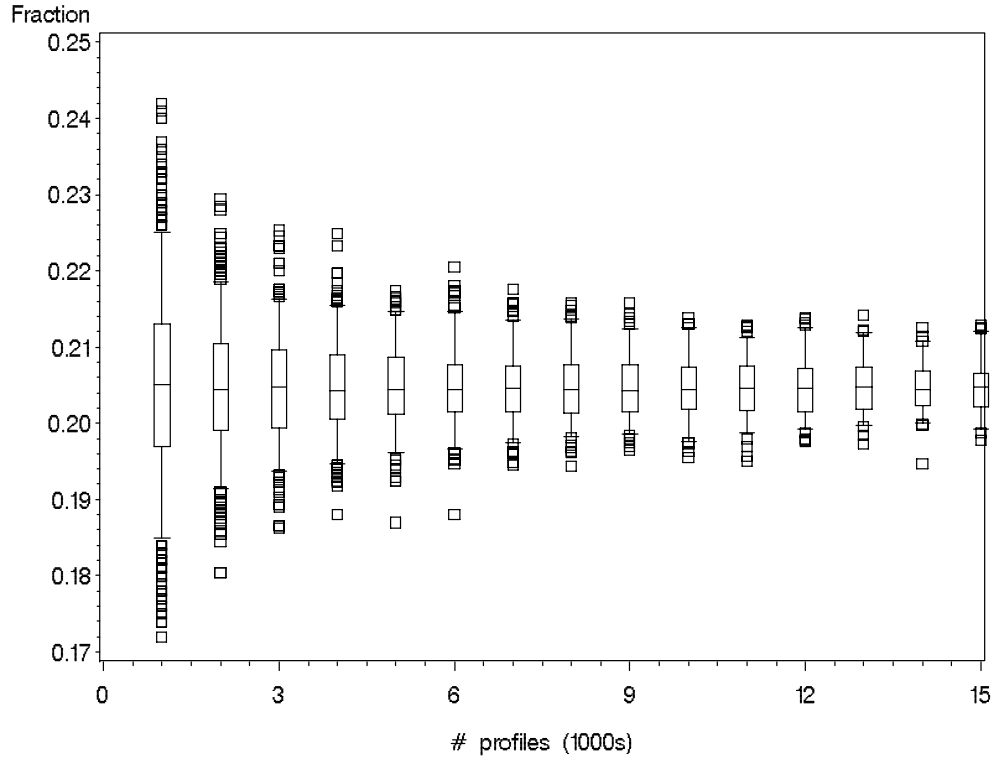


Figure 20. Distribution of the predicted fractions of population who experience any hourly exposures > 0.12 ppm-hr as a function of the number of profiles simulated

In practice, we model the distribution of exposures with a single simulation, and the deviation of this distribution from the limiting distribution (obtained with very large N_S) is an error, or uncertainty, due to lack of convergence. We could average together the results of 10 APEX runs, but we would be better off simulating 10 times as many individuals in one run. Since model run time is proportional to N_S, the N_S that one can simulate depends on the computing capacity and the time requirements. For the hundreds of APEX runs performed in support of the ozone NAAQS review, we simulated 60,000 individuals in each APEX run, to balance the desire for convergence with time limitations.

We have assessed the extent of "non-convergence uncertainty" for N_S = 60,000 for one city, Atlanta, for the 2002 base case scenario, by conducting several APEX simulations identical to the single simulation whose results are used in the exposure assessment. Figure 21 (children) and Figure 22 (all people) illustrate this uncertainty with the distributions of the number of people predicted by APEX who experience one or more 8-hour average exposures above 0.08 ppm-8hr, concomitant with moderate or greater exertion. This distribution is made up of the

predicted values for 1,268 APEX runs (one value from each run). We see that there is significant spread, even simulating as many as 60,000 individuals.

In the next four tables, we describe 12 such distributions; Table 19 and Table 20, respectively for children and all people, under moderate exertion, and Table 21 and Table 22 respectively for children and all people, under any exertion level. The last row in Table 19 corresponds to Figure 21 and the last row in Table 20 corresponds to Figure 22. For example, in the distribution in Figure 21, 90 percent of the values are within 4.5 percent of the median (the median should be close to the limiting value as N_S become large).

As expected, convergence is poorer for statistics that are in the tails of the distribution of population exposures. So, as the exposure cutoff level increases (e.g., going down any column in these tables) or as the population group looked at becomes smaller (e.g., children vs. adults), N_S needs to be larger to achieve the same level of convergence. This is illustrated in the summary provided by Table 23.

In these simulations conducted to assess convergence, we allow the starting seed of the sequence of random numbers generated by APEX to be picked randomly based on the date and time of the start of the run, so each simulation has a different starting seed. In the exposure simulations for the 12 cities described in the draft Staff Paper, we used different starting seeds for each city and year simulated, but used the same seed for all runs for a given city and year. For example, the same seed was used for the nine 2002 New York simulations (base case, current standard, 7 alternative standards). In this way the non-convergence uncertainty largely cancels out from the comparisons of the runs for a given city, although we have yet to assess the extent of this cancellation.

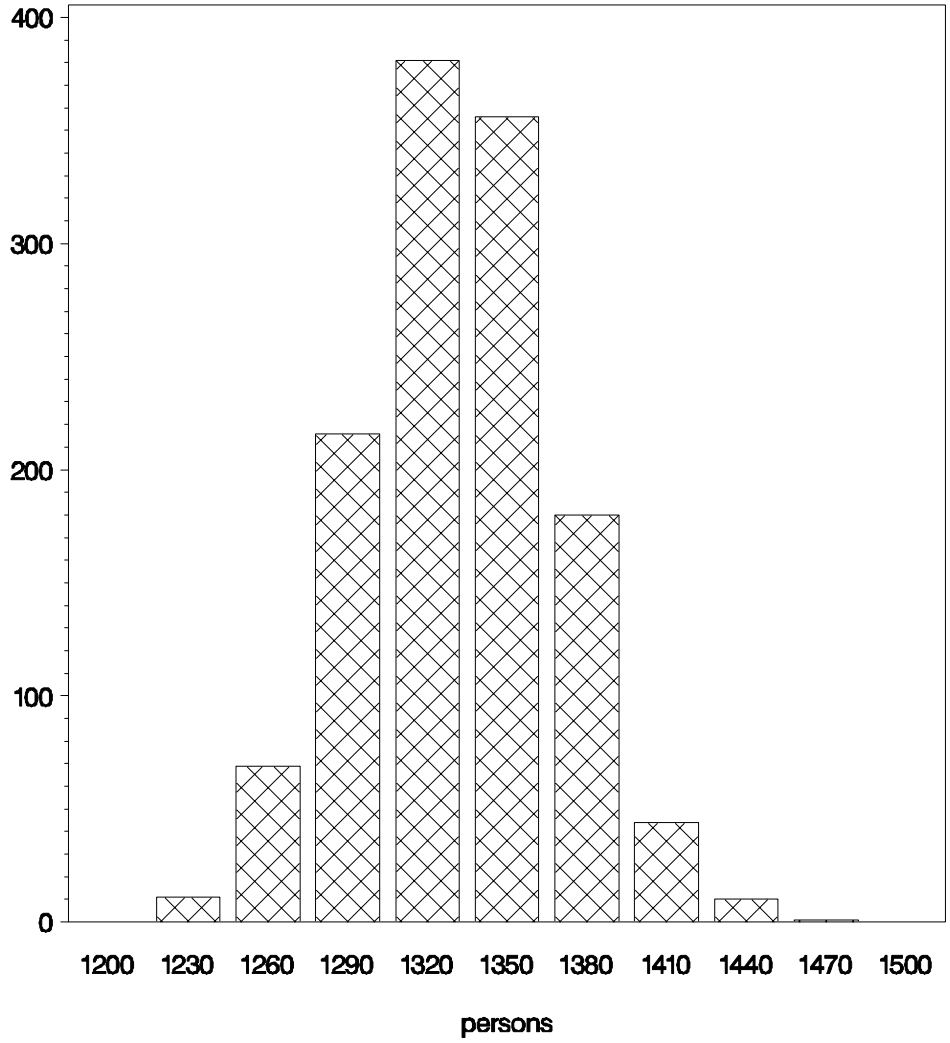


Figure 21. The distribution of the predicted number of children with at least one 8-hour exposure above 0.08 ppm-8hr at moderate or greater exertion for 1,268 repeated simulations of the Atlanta 2002 base case with 60,000 profiles

Table 19. Variability of replicate APEX simulations of 60,000 persons: Medians, 5th, 10th, 25th, 75th, 90th, 95th percentiles, and the percent differences of these from the medians of the number of persons with exposures above different daily maximum 8-hour exposure levels (ppm-8hr) – All children, moderate exertion

Exposure level	median	5th percentile		10th percentile		25th percentile		75th percentile		90th percentile		95th percentile	
0.06	7,873	7,727	(1.9%)	7,761	(1.4%)	7,815	(0.7%)	7,928	0.7%	7,977	1.3%	8,008	1.7%
0.07	4,277	4,169	(2.5%)	4,194	(1.9%)	4,234	(1.0%)	4,323	1.1%	4,361	2.0%	4,384	2.5%
0.08	1,332	1,272	(4.5%)	1,282	(3.8%)	1,306	(2.0%)	1,356	1.8%	1,378	3.5%	1,392	4.5%

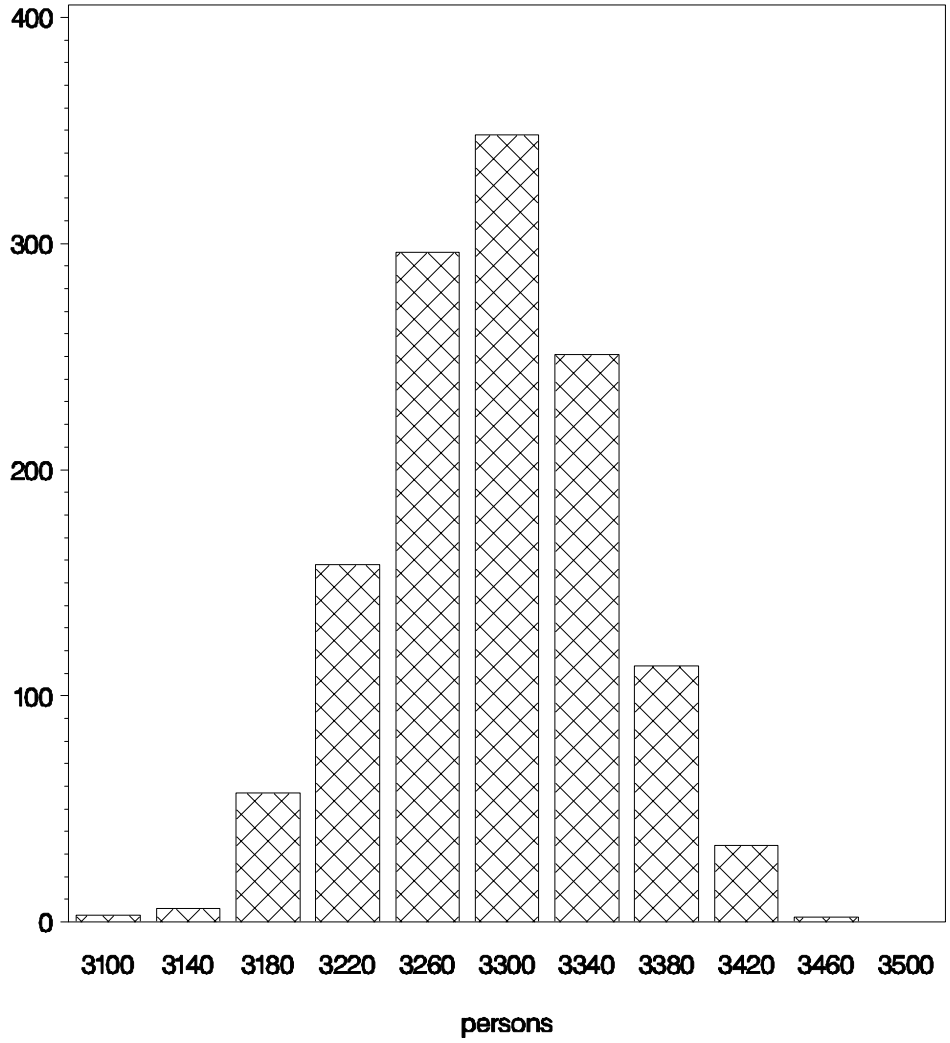


Figure 22. The distribution of the predicted number of people with at least one 8-hour exposure above 0.08 ppm-8hr at moderate or greater exertion for 1,268 repeated simulations of the Atlanta 2002 base case with 60,000 profiles

Table 20. Variability of replicate APEX simulations of 60,000 persons: Medians, 5th, 10th, 25th, 75th, 90th, 95th percentiles, and the percent differences of these from the medians of the number of persons with exposures above different daily maximum 8-hour exposure levels (ppm-8hr) – All people, moderate exertion

Exposure level	median	5th percentile		10th percentile		25th percentile		75th percentile		90th percentile		95th percentile	
0.06	21,816	21,622	(0.9%)	21,664	(0.7%)	21,734	(0.4%)	21,892	0.3%	21,968	0.7%	22,004	0.9%
0.07	10,804	10,642	(1.5%)	10,679	(1.2%)	10,740	(0.6%)	10,865	0.6%	10,931	1.2%	10,960	1.4%
0.08	3,294	3,199	(2.9%)	3,218	(2.3%)	3,254	(1.2%)	3,331	1.1%	3,364	2.1%	3,383	2.7%

Table 21. Variability of replicate APEX simulations of 60,000 persons: Medians, 5th, 10th, 25th, 75th, 90th, 95th percentiles, and the percent differences of these from the medians of the number of persons with exposures above different daily maximum 8-hour exposure levels (ppm-8hr) – All children

Exposure level	median	5th percentile		10th percentile		25th percentile		75th percentile		90th percentile		95th percentile	
0.06	10,405	10,253	(1.5%)	10,281	(1.2%)	10,344	(0.6%)	10,470	0.6%	10,521	1.1%	10,558	1.5%
0.07	6,373	6,237	(2.1%)	6,266	(1.7%)	6,317	(0.9%)	6,419	0.7%	6,465	1.5%	6,499	2.0%
0.08	2,082	2,011	(3.4%)	2,025	(2.7%)	2,052	(1.4%)	2,114	1.5%	2,142	2.9%	2,157	3.6%

Table 22. Variability of replicate APEX simulations of 60,000 persons: Medians, 5th, 10th, 25th, 75th, 90th, 95th percentiles, and the percent differences of these from the medians of the number of persons with exposures above different daily maximum 8-hour exposure levels (ppm-8hr) – All people

Exposure level	median	5th percentile		10th percentile		25th percentile		75th percentile		90th percentile		95th percentile	
0.06	44,107	43,912	(0.4%)	43,962	(0.3%)	44,030	(0.2%)	44,175	0.2%	44,242	0.3%	44,278	0.4%
0.07	25,819	25,613	(0.8%)	25,659	(0.6%)	25,736	(0.3%)	25,904	0.3%	25,974	0.6%	26,017	0.8%
0.08	9,463	9,322	(1.5%)	9,353	(1.2%)	9,403	(0.6%)	9,520	0.6%	9,570	1.1%	9,605	1.5%

Table 23. Summary of convergence statistics for the number of people predicted by APEX who experience one or more 8-hour average exposures above exposure levels of 0.06, 0.07, and 0.08 ppm-8hr: 90 percent confidence intervals around the medians

Exposure level (ppm-8hr)	Children, moderate exertion	Children, any exertion	All people, moderate exertion	All people, any exertion
0.06	± 1.8%	± 1.5%	± 0.9%	± 0.4%
0.07	± 2.5%	± 2.1%	± 1.5%	± 0.8%
0.08	± 4.5%	± 3.5%	± 2.8%	± 1.5%

APEX MODEL FORMULATION UNCERTAINTY

Uncertainties are inherent in modeled representations of physical reality due to simplifying assumptions and other aspects of model formulation. The methods for assessing input parameter uncertainty and model formulation or structure uncertainty are different. It is difficult to incorporate the uncertainties due to the model formulation into a quantitative assessment of uncertainty in a straightforward manner. The preferred way to assess model formulation uncertainty is by comparing model predictions with measured values, while having fairly complete knowledge of the uncertainty due to input parameters. Whence the importance of model evaluation and the availability of data suitable to model evaluation. In the absence of measurements that can be used to estimate model uncertainty, one must rely on informed judgment.

Our approach to assessing model formulation uncertainty is to partition this uncertainty into that of the components, or algorithms, of the model. For each of the algorithms within the model, we will discuss the simplifying assumptions and those uncertainties associated with the algorithms which are distinct from the input data uncertainties. Where possible, we will evaluate these algorithms by comparing their predictions with measured data. Otherwise, we will formulate an informed judgment as to a range of plausible uncertainties for the algorithms. We will assemble the different types of uncertainties to present an integrated assessment of model uncertainty.

» It should be noted that improvements to the algorithms in APEX are largely data-limited, in the sense that more and better data are needed as the basis for further improvements. Data collection efforts in the near future would best serve to reduce uncertainties by improving the inputs to the current algorithms and not to derive better algorithms. Uncertainty would be reduced significantly just by the use of better inputs. For example, APEX can model the dependence of AER distributions on hourly temperature, humidity, and wind speed, which are known to influence AERs, but data are not available to characterize these relationships. APEX has the flexibility to take advantage of much more data than are currently available.

There are several algorithms in APEX that involve simplifying assumptions that have the potential to introduce uncertainty into the model, including the following:

- demographic profiles model
- longitudinal diary construction model
- collapsing the numerous microenvironments in the diaries to 12 modeled microenvironments
- modeling movements of individuals (commuting, school, shopping, etc.)
- microenvironment concentration model – factors approach
- microenvironment concentration model – mass balance approach
- modeling near-roadway titration of ozone by NO_x
- model for assigning physiological characteristics to individuals
- MET model
- ventilation model

- dose model

The Treatment of Variability and Covariability in Apex

Assessment of the extent to which APEX correctly models variability and covariability is central to an understanding of the model uncertainty, and so we summarize here the approach APEX takes to this.

The APEX methodology essentially simulates individuals and then computes exposures to ozone concentrations for each of these simulated individuals. The individuals are selected to represent a random sample from a defined population. The collection of individuals represents the variability of the target population, and accounts for several types of variability, including demographic, physiological, and activities. Typically more than 50,000 individuals are modeled in order to capture the full range of variability.

APEX incorporates stochastic processes representing the natural variability of personal profile characteristics, activity patterns, and microenvironment parameters. In this way, APEX is able to represent much of the variability in the exposure estimates resulting from the variability of the factors effecting human exposure. APEX is also designed to account for covariability, or linear and nonlinear correlation, among the model inputs.

APEX models variability and covariability in two ways:

- **Stochastic**. The user provides APEX with probability distributions characterizing the variability of input parameters. These are treated stochastically in the model and the computed distributions of exposures reflect this variability. For example, the rate of decay of ozone in houses depends in a complex way on several factors which we are not able to explicitly model at this time. However, we can specify a distribution of decay rates which reflects observed variations in ozone decay rates. APEX randomly samples from this distribution to obtain values which are used in the mass balance model. Covariability is modeled through the use of conditional distributions. If two or more parameters are related, conditional distributions which depend on the values of the related parameters are input to APEX. For example, the distribution of air exchange rates (AERs) in a house depends on the outdoor temperature and whether or not air conditioning (A/C) is in use. In this case, a set of AER distributions is provided to APEX for different ranges of temperatures and A/C use, and the selection of the distribution in APEX is driven by the temperature and A/C status at that time.
- **Explicit**. For some variables used in modeling exposure, APEX models variability and covariability explicitly and not stochastically. For example, hourly-average ambient ozone concentrations and temperatures are used in model calculations. These are input to the model for every hour in the time period modeled, and in this way the variability and covariability of concentrations and hourly temperatures are modeled explicitly.

Each of these methods allows for linear and nonlinear relationships between variables to be modeled. Table 24 lists the components of exposure variability which are modeled by APEX.

Table 24. Components of exposure variability modeled by APEX

Parameter	Dimensions of Variation in APEX	Treatment in APEX
Population demographics (age, gender, race, employment, residence location, work location)	Individuals, by Census tract	Random samples from Census tracts
Commuting	Individuals, by Census tract	Random samples from Census tracts
Physiology (weight)	Individuals	Distributions by age and gender
Physiology (resting metabolic rate, maximum level of sustained metabolic activity, oxygen uptake per unit of energy expended)	Individuals	See section 4.3 in the APEX TSD.
Physiology (blood volume, lung diffusivity, endogenous CO production rate, amount of hemoglobin in the blood)	Individuals	See section 4.3 in the APEX TSD. Not used for modeling ozone.
Ambient pollutant concentrations	Space and time (hourly)	Hourly values at a set of locations are input; values from the closest location are used.
Ambient meteorological data	Space and time (hourly and daily)	Hourly values at a set of locations are input; values from the closest location are used; daily values are calculated in APEX.
Spatial concentration variability within microenvironments	Microenvironment type and geographical region	This variability can be incorporated into the variability of mass balance or factors model parameters.
Spatial concentration variability within air quality districts	Microenvironment type and geographical region	This variability can be incorporated into the variability of mass balance or factors model parameters.
Within-hour concentration variability	Microenvironment type and geographical region	This variability can be incorporated into the variability of mass balance or factors model parameters.
Microenvironment	Microenvironment type	APEX can model any number of user-defined microenvironments

There are also model inputs which are not tied to the individual which contribute to the variability of the modeling results. These include spatially and temporally varying air quality concentrations and meteorological variables, as well as a number of factors involved in the calculation of indoor and in-vehicle microenvironmental concentrations. The variability of air

quality and meteorological data is modeled by providing hourly average, spatially varying inputs to APEX. Variability for these inputs for time scales less than one hour can be modeled with parameters of the microenvironment model. The variability of other parameters is treated by specifying distributions for these parameters, from which APEX randomly samples values.

Correlations and non-linear relationships between variables input to the model can result in the model producing incorrect results if the inherent relationships between these variables are not preserved.

APEX has a sophisticated method for modeling linearly and non-linearly correlated input data. This is accomplished by providing inputs that enable the correlation to be modeled explicitly within APEX. For example, there are non-linear relationships between the outdoor temperature and rates of air exchange in homes (or automobiles). One factor that contributes to this is that windows tend to be closed more often when temperatures are low or high than when temperatures are moderate. This relationship is explicitly modeled in APEX by specifying different probability distributions of air exchange rates for different ambient temperatures.

Thus, the APEX formulation allows for relationships between input data to be modeled, provided that enough is known about these relationships to specify them. The degree to which these relationships are unknown contributes to the uncertainty of the results. For those relationships which APEX explicitly models the correlation, uncertainty arises from misspecification of the correlation in the model inputs.

Table 25 lists different types of covariability and how they are modeled in APEX. The center column of this table indicates whether or not APEX explicitly models this type of covariability.

Table 25. Components of covariability modeled by APEX

Type of Covariability	APEX?	Treatment in APEX / Comments
Within-profile correlations [1]	Yes	Activities, physiology, microenvironments
Between-profile correlations	No	Not important
Correlations between profile variables and microenvironment parameters	Yes	Profiles are assigned microenvironment parameters
Correlations between profile variables (age, gender) and activities	Yes	Age and gender are used in activity diary selection
Correlations between activities and microenvironment parameters	No	E.g., opening windows when cooking or smoking. Might be important, but do not have data.
Correlations among microenvironment parameters in the same microenvironment	Yes	Modeled with joint conditional variables

Type of Covariability	APEX?	Treatment in APEX / Comments
Correlations between demographic variables and air quality.	Yes	This is modeled with the spatially varying demographic variables and air quality input to APEX.
Correlations between meteorological variables and activities	Yes	Temperature is used in activity diary selection
Correlations between meteorological variables and microenvironment parameters	Yes	The distributions of microenvironment parameters can be functions of temperature
The consistency of the occupation (and time spent commuting) for an individual from one working day to the next.	No	Simulated individuals who are employed are assigned activity diaries without regard to occupation. This would be important for modeling outdoor workers.

[1] We use the term "correlation" to encompass linear and nonlinear relationships.

Errors in Coding

APEX has undergone fairly extensive testing, but has not been subjected to a rigorous, exhaustive test regime. Incorrect implementation of algorithms as documented falls into the realm of coding errors. We will not attempt to quantify the uncertainties in the model predictions that might be the result of coding errors.

Errors in Algorithms

The likelihood of errors in algorithms can be reduced by a scientific peer review of the documentation of the model algorithms. We will not attempt to quantify a likely range of uncertainties due to possible errors in algorithms. However, we present an example of such an error which resulted in increased uncertainty of our exposure modeling results.

In our review of the APEX modeling results, we have uncovered an error in the algorithm for estimating ventilation rates. This algorithm (section 2.5.1, Exposure Analysis TSD) included terms for uncertainty as well as variability. Since only variability should be reflected by the algorithm, this error erroneously inflates the variability, most noticeably for older adults. This error primarily affects the highest percentiles of the distributions of ventilation rates. For adults 70 years of age and older, the 99.9^{th} percentile of the ventilation rates distribution is a factor of two too high; for children, the difference is less than 1.5% at the 99.9^{th} percentile. Therefore, while the estimates of exertion levels are acceptable for children, they are too high for the general population. This has been corrected and the modeling will be repeated for the final Staff Paper.

Ambient Air Quality Concentrations

Ambient concentrations are not explicitly modeled by APEX; they are provided as input data. APEX is capable of using input data with highly resolved spatial and temporal resolution. Model uncertainty associated with ambient concentrations results from erroneous characterization of the levels and/or variability of concentrations in very localized areas, e.g., close to sources or sinks.

For ozone modeling, one important process that may not be adequately modeled is the effect on exposures of the decrease in ozone concentrations downwind of roadways due to titration by NO_x emitted by cars and trucks. APEX does simulate the decrease in ozone levels downwind of roadways, and the effect of this on exposures of people engaged in activities near roadways, but does not differentially model the affects on people in homes close to roadways (vs. homes not close to roadways).

As described above, we plan to quantify the potential impact of this uncertainty by performing an analysis separately modeling the population living near roadways (with concentration adjustments) and the remaining population, combining the results of these simulations, and comparing the predicted distribution of exposures to results of modeling without this special treatment.

Meteorological Data

Meteorological variables are not explicitly modeled by APEX; they are provided as input data. APEX is capable of using input data with highly resolved spatial and temporal resolution, and we do not consider model uncertainty associated with meteorological data to be an issue.

Modeling Concentrations in Microenvironments

There are two models in APEX for calculating concentrations in microenvironments, the mass balance and the factors models (see the APEX TSD for details):

$$\Delta C_{in} = \frac{dC(t)}{dt} = C_{ambient} \; x \; f_{proximity} \; x \; f_{penetration} \; x \; f_{air\,exchange} \; x \; f_{decay} \quad \text{(mass balance model)}$$

$$C_{hourly} = C_{ambient} \; x \; f_{proximity} \; x \; f_{penetration} \quad \text{(factors model)}$$

One can raise questions as to the appropriateness of the assumptions of the mass balance model in APEX for estimating concentrations in microenvironments, such as linearity assumptions and assumptions that parameters (e.g., air exchange rates, source strengths, infiltration factors, and deposition rates) can be treated as constant in time over an hour. However, of much greater importance for model uncertainty is how the inputs to the mass balance model (air exchange rates, decay rates, etc.) are modeled, so our discussion will focus on

these. The factors model formulation has no model uncertainty, by definition of that model's parameters.

Air Exchange Rate

APEX models the dependence of AERs on the microenvironment characteristics and temperature, but not the behavior of the occupants, which is known to influence AERs. The analysis of the uncertainties of the AER distributions input to APEX encompasses this aspect of model uncertainty.

Deposition Processes

The rate of deposition of ozone to some materials diminishes with cumulative exposure to ozone. This is not necessarily a small effect. In one study, 60 to 90 percent more ozone was scavenged by fiberglass insulation that had not been previously exposed to ozone, than by insulation with no previous exposure (Liu and Nazaroff, 2001; CD, Appendix AX3, page 179). This effect is not explicitly modeled by APEX. We will explore the potential impact of this model uncertainty by a sensitivity analysis.

Chemical Reaction Processes

Ozone reacts with a number of indoor pollutants, such as NO_x from gas stoves and VOCs from consumer products. Titration of ozone by NO_x from gas stoves reduces the concentration of ozone indoors. Lee et al. (1999) find ozone concentrations dropping by a factor of five within seven minutes of a gas stove being turned on. The inputs to APEX will be modified to take this into account before the final exposure modeling is performed in support of the ozone NAAQS review, and the uncertainties of those inputs (essentially the prevalence of gas stoves and the frequency of their use) and the algorithm will be incorporated into this uncertainty analysis. This modification will have the effect of slightly reducing some people's exposures.

Ozone reacts slowly with most other indoor pollutants, and this is a minor removal process compared to air exchange and surface removal (Weschler, 2000). Aside from the gas stove effect, the lack of a more refined treatment of indoor air chemistry is not considered to be a significant limitation of APEX for modeling ozone exposures.

Characterization of Population Demographics

The population demographics are taken directly from the 2000 Census and not modeled by APEX. Therefore there is no model uncertainty associated with this.

Modeling Activity Patterns

The following are population characteristics that contribute to the variability of exposures but which are not fully modeled in APEX. Of course, some of these are more important than others. Additional data collection will be required to assess whether or not these are limitations.

- Occupational category
- Life cycle (see, e.g., Zuzanek and Smale, 1992)
- Socio-economic status and educational level
- Longitudinal stability in occupation, exercise levels, and leisure activities
- Geographical locations of activities away from the home
- The specific microenvironments visited away from home

Even though some of these may influence exposures, they will not necessarily have much effect on the population distribution of exposures. In this case, there would be no reason to model them explicitly, unless one wanted to break out results by that variable. The uncertainty of the activity data input to APEX is likely larger than the uncertainty resulting from these limitations.

Behavior changes in response to ozone pollution or in response to air quality index (AQI) notification ("averting behavior") is not being taken into account in our exposure modeling. Eiswerth et al. (2005) find that increased ozone levels appear to influence the amount of time that asthmatic adults spend in different activities. In a national survey, Mansfield and Corey (2003) find a significant fraction of the people surveyed modifying their activities in response to ozone alerts. We do not feel that this is a relatively influential uncertainty at this time, however, this aspect of people's activities presumably will become more important in the future.

APEX uses a sophisticated model to sequentially (longitudinally) assign activity diaries to simulated individuals, which introduces a degree of realism into the ways that people tend to repeat certain activity patterns. We have performed sensitivity analyses to assess the impact of this treatment (Exposure Analysis TSD), and are including its parameters in the Monte Carlo uncertainty analysis. Additional data on longitudinal activity patterns are needed to evaluate this model.

Modeling Physiological Processes

Overview of the Physiological Model

The model in APEX of physiological processes that are relevant to inhalation exposure and dose is significantly improved over earlier (pre-2005) versions of APEX. APEX currently has a physiological model for ventilation rates (the primary driver of dose of ozone) which accounts for prior energy expenditure patterns (also known as oxygen debt [fatigue] and excess post-exercise oxygen consumption [EPOC]).

The physiological model produces two quantities which are used in this exposure assessment, an effective ventilation rate (EVR), which is used to characterize levels of exertion in compiling summary exposure tables, and a physical activity index (PAI_{med}), used to characterize simulated individuals as "active."

One of the key variables in this model is the "MET" (metabolic equivalent), defined as the ratio of the metabolic rate of energy consumption for an activity to the resting metabolic rate (RMR). For each simulated individual, APEX generates an event time-series of MET values from activity-specific MET distributions (some METS distributions are occupation/age dependent as well). Events are specified in the diaries, and last from 1 to 60 minutes. This time series of MET values is then adjusted for fatigue and excess post-exercise oxygen consumption. Then the oxygen consumption rate, VO_2, is calculated for each event as $VO_2 = MET_{adj} \cdot RMR \cdot ECF$, where ECF is a person-specific energy conversion factor and RMR is the person-specific resting (basal) metabolic rate. The expired ventilation rate Ve, is calculated by a stochastic function of VO_2, body mass, age, and gender. The effective ventilation rate EVR = Ve / BSA is averaged over 1- and 8-hours, and used to characterize levels of exertion. Body surface area (BSA) is currently modeled as a simple deterministic function of body mass (BM), and there is some uncertainty in the regression equation parameters.

Thus, EVR is a complex function of the activity-specific METs and person-specific RMR, ECF, BSA, and BM, which vary with age and gender. The person-specific parameters are modeled to reflect variability in the populations. For example, different 36-year old males will have different physiological parameters reflective of the variation observed in 36-year old males.

Once the final MET time series is calculated, a daily average physical activity index (PAI) for the simulated individual is calculated as the time-weighted average of MET values for each day. The median of the daily PAI values is calculated for each profile. This median daily PAI value (PAI_{med}) is used in the characterization of persons as "active" when creating the output exposure summary tables.

Uncertainty of the Physiological Model

As part of the next phase of this uncertainty analysis, we intend to review the recent literature to assess the appropriateness of the assumptions in this physiological model. There has been significant progress in modeling these physiological processes since the algorithms in APEX were developed, with the exception of the treatment of EPOC, which is state-of-the art. We conducted a quick literature search on the internet, which turned up the publications listed in Appendix A, along with either abstracts or the complete publication. Inspection of this list reveals a potential wealth of information for assessing the uncertainty of the physiological model in APEX, and then improving the model.

The physiological calculations do not directly affect APEX's estimation of exposures; rather, they are used to characterize the population according to exertion levels and "active" or not. These are important for exposure-based estimates of risk.

The Resting Metabolic Rate Model

The RMRs for individuals are estimated by a regression equation with coefficients specific to age and gender, which were developed by Schofield (1985). (See Johnson, 2003, Table 9-11.) Since then, studies have improved on this model. For example, Huang et al. (2004) find that the best predictive equation for RMR for obese adults include terms for age, gender, weight, height, and diabetes. Comparison with more recent models will provide information about the uncertainty of the Schofield model in APEX.

The Ventilation Rate Model

Ventilation rates are calculated in APEX, and are not input to the model. We plan to evaluate the APEX algorithm for calculating ventilation rates by comparing them with values in the literature. For example, Marty et al. (2002) develop parametric distributions of breathing rates for children and adults, which can be compared with the distributions predicted by APEX.

Classification of Individuals as Active

This is an area where a great deal of research is being done for both adults and children. Duke et al (2003) summarize nationally representative information about levels and types of physical activity among children aged 9–13 years. Puyau et al. (2002) show that adult-derived MET cutpoints are not applicable to children and can lead to erroneous conclusions regarding physical activity levels in children. Appendix A lists some of the recent work in this field.

APEX uses the PAI cutpoint to classify individuals as active or not active. There are two shortcomings of this method. First, it is not clear what the relevant classification of specific activities is in terms of levels of physical exertion. Second, given such a classification of activities, it is not clear how to best characterize a given individual as "active" or not.

There are various "definitions" or interpretations of how to classify levels of exertion in the literature. The CDC and the American College of Sports Medicine categorize physical activity levels in adults as *light*: < 3 MET, *moderate*: 3 to 6 MET, and *vigorous*: >6 MET. Reland et al. (2004) use low activity: < 4,185 kJ/week (1,000 kcal/week) high: > 8,370 (2,000) moderate: in between, where 1 MET = 4.185 kJ kg^{-1} h^{-1}. Marty et al. (2002) categorize activity levels according to ventilation rates (l/min per kg body weight), with different classifications for ages > 12 and ≤ 12 years. McCurdy and Graham (2004) present a survey of the exercise physiology literature of different measures used to define moderate and vigorous physical activity, and find many different ways that researchers are categorizing activity levels.

There is less research in the area of characterizing individuals (as opposed to activities) in terms of how active they are, particularly in the context of how it influences their health risk from exposure to ozone.

Sapkota et al. in their 2005 study on adult participation in recommended levels of physical activity, use a definition of "regular physical activity" given by CDC[1]. Moderate-intensity activity is described to respondents as any activity "that causes small increases in breathing and heart rate," and vigorous-intensity activity is described as any activity "that causes large increases in breathing or heart rate." Respondents are classified as active at the minimum recommended level if they report moderate-intensity activity at least 30 minutes per day, 5 or more days per week, or vigorous-intensity activity at least 20 minutes per day, 3 or more days per week. The Behavioral Risk Factor Surveillance System (BRFSS) survey for 2003 reports 46% of U.S. adults to be active by this definition (Sapkota et al., 2005).

APEX characterizes a person an active if their median daily average MET is greater than 1.75. One factor which contributes to the uncertainty of this model is the fact that the daily average MET is largely driven by the number of hours spent sleeping, which is not correlated with most definitions of active people. A better characterization might be the daily maximum 12-hour average MET, which would reflect levels of activity while not sleeping. In order to characterize the uncertainty associated with the estimation of exposures to an "active" population, we will use the CDC definition of "regular physical activity" for the definition of an active person.

Unknown Model Uncertainty

There are structural uncertainties of APEX of which we are currently unaware. We will attempt to characterize their uncertainties as they come to light. We are proceeding on two fronts to uncover additional uncertainties: peer review and diagnostic model evaluation.

Perhaps there is a correlation between the tendency of people to open windows and their tendency to engage in outdoor activities. If so, people who spend more time outdoors would tend to have higher AERs at home and work, and ignoring this could bias the modeled distribution of exposures. This is conjecture, but is an example of potential unknown model uncertainty.

UNCERTAINTY ANALYSIS RESULTS

As described above, we are using a Monte Carlo approach to produce quantitative estimates of the uncertainty of the APEX model results, based on estimates of the uncertainties of the model inputs. We are performing 1,000 simulations of the Boston 2002 base case, paired with 1,000 simulations of the 2002 Boston current standard scenario, incorporating the model input uncertainties described in this report. Each pair of simulations uses the same uncertain inputs and differs only by the air quality concentrations input to the model, so that we can assess the uncertainty of estimates of reductions in exposures as well as the uncertainty of the estimates of exposures. The results of these simulations will be available in August. We plan to also perform this analysis for one additional city.

1 http://www.cdc.gov/nccdphp/dnpa/physical/terms/index.htm

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APPENDIX A. RECENT PUBLICATIONS RELATED TO THE PHYSIOLOGICAL MODEL IN APEX

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