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Total Risk Integrated Methodology (TRIM) Air Pollutants Exposure Model Documentation (TRIM.Expo / APEX, Version 4)

Volume II: Technical Support Document

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CONTENTS

LIST OF TABLES

LIST OF EXHIBITS

LIST OF FIGURES

CHAPTER 1.   INTRODUCTION

1.1   TRIM and The APEX Model

The <u>A</u>ir <u>P</u>ollutants <u>E</u>xposure model (APEX) is part of EPA's overall Total Risk Integrated Methodology (TRIM) model framework (EPA, 1999), in particular the inhalation exposure component (TRIM.Expo$_{Inhalation}$). TRIM is a time-series modeling system with multimedia capabilities for assessing human health and ecological risks from hazardous and criteria air pollutants; it is being developed to support evaluations with a scientifically sound, flexible, and user-friendly methodology. The TRIM design includes three modules:

- Environmental Fate, Transport, and Ecological Exposure module (TRIM.FaTE);

- Human Exposure-Event module (TRIM.Expo); and

- Risk Characterization module (TRIM.Risk).

APEX is designed to estimate human exposure to criteria and air toxic pollutants at local, urban, and regional scales. The current release of the model is APEX4. Note that APEX has been extensively reviewed. Any changes to the computer code may lead to results that cannot be supported by this documentation. Model enhancements, bug fixes, and other changes are occasionally made to APEX, and thus users are encouraged to revisit the website http://www.epa.gov/ttn/fera/human_apex.html for notices of these changes.

1.2   Scope and Organization of This Document

The documentation of the APEX model is currently divided into two volumes. *Volume II: Technical Support Guide* (this document) is intended to be a reference on the scientific basis of the APEX model. The scientific background, original references, and equations for the APEX model algorithms are included in this volume. Topics covered include the methods implemented in APEX for sampling probability distributions, calculating microenvironmental concentrations, modeling ventilation, estimating exposure and dose, and assembling composite activity diaries. Other model algorithms, such as those for generating the study area and the simulated population are also described.

Volume I: User's Guide, is designed to be a hands-on guide to using APEX. It is applicable to all levels of expertise, from novice to advanced, and focuses on how to run the APEX computer model, develop the appropriate input files, and interpret the model output files.

1.3   Introduction to APEX

APEX estimates human exposure to criteria and toxic air pollutants using a stochastic, "microenvironmental" approach. That is, the model randomly selects data for a sample of hypothetical individuals from an actual population database and simulates each individual's movements over time, in different locations (e.g., at home, in vehicles) to estimate their exposure to (and, optionally, dose of) the modeled pollutants. APEX can assume people live and work in the same general area (i.e., that the ambient air quality is the same at home and at work) or

optionally can model commuting and thus exposure at the work location for employed individuals.

APEX is a multipollutant model. It can model the simultaneous exposure to any number of pollutants, assuming that the user can provide the necessary input air quality data and pollutant parameters.

The APEX model uses the personal profile approach to generate simulated individuals, for whom exposure time series are calculated. The *profile* is a description of the characteristics of an individual that may affect either their activities or the concentrations in the microenvironments. Typically, the profile includes demographic variables such as age, gender, and employment status, as well as physiological variables such as height and weight, and finally some situational variables such as possession of a gas stove or air conditioning. The demographic variables are used in the selection of *activity diaries* from EPA's Consolidated Human Activity Database (CHAD, McCurdy et al., 2000) to represent the individual, while the situational variables are used to help calculate the microenvironmental concentrations. The physiological variables are used in the calculation of pollutant dose.

An APEX model run consists of calculating the exposure (and optionally dose) time series for a user-specified number of profiles. The time series can be calculated on different temporal scales. Collectively, these profiles are intended to be a representative random sample of the population in a given study area. To this end, tables of demographic data from the decennial census are used, so appropriate probabilities for any given geographical area can be derived. In APEX the geographical units are called *sectors*. Using the standard input files provided with the model, each sector is a census tract. Ambient air quality and meteorological data for the study area are also required by the model; the area covered by an air quality monitor is called a *district*, and the area covered by a meteorological monitor is called a *zone*. APEX matches up each sector of the study area with an appropriate air quality district and meteorological zone to provide all the data necessary to simulate exposure and dose for an individual.

APEX can be thought of as a simulation of a field study that would involve selecting an actual sample of specific individuals who live in (or work and live in) a geographic area and then continuously monitoring their activities and subsequent inhalation exposures to a specific air pollutant during a specific period of time. The main differences between the model and an actual field study are that in the model:

- The sample of individuals is a "virtual" sample, created by the model according to various demographic variables and census data of relative frequencies, in order to obtain a representative sample (to the extent possible) of the actual people in the study area;

- The activity patterns of the sampled individuals (e.g., the specification of indoor and other microenvironments, the duration of time spent in each) are assumed by the model to be similar to individuals with similar demographic characteristics, according to activity data such as diaries compiled in EPA's Consolidated Human Activities Database (CHAD) (EPA, 2002; McCurdy et al., 2000);

- The pollutant exposure concentrations and doses are estimated by the model using temporally and spatially varying ambient outdoor concentrations, coupled with information on the behavior of the pollutant in various microenvironments; and

- Various reductions in ambient air quality levels due to potential emission reductions can be simulated by adjusting air quality concentrations to reflect the scenarios under consideration.

Thus, the model accounts for the most significant factors contributing to inhalation exposure—the temporal and spatial distribution of people and pollutant concentrations throughout the study area and among the microenvironments—while also allowing the flexibility to adjust some of these factors for regulatory assessments and other reasons.

Nomenclature. The following terms are used throughout this guide:

- Diary—a set of events or activities (e.g., cooking, sleeping) for an individual in a given time frame (e.g., a day).

- Air quality district—the geographical area represented by a given set of ambient air quality data (either based on a fixed-site monitor or output from an air quality model).

- Event—an activity (e.g., cooking) with a known starting time, duration, microenvironment, and location (usually home or work).

- Microenvironment—a space in which human contact with an environmental pollutant takes place.

- Profile—a set of characteristics that describe the person being simulated (e.g., age, gender, height, weight, employment status, whether an owner of a gas stove or air conditioner).

- Sector—the basic geographical unit for the demographic input to and output from APEX (usually census tracts).

- Study Area—the geographical area modeled.

- Study Area Population—total population of persons who live in the study area.

- Meteorological zone—the geographical area represented by a given set of meteorological data (either based on a meteorological station or output from a meteorological model.

Labeling Conventions. The labeling used in this document is as follows.

- *Input and output file names* are in italics.

- ***Model Variables*** are in bold italics, generally only when first used in a section.

- ***KEYWORDS***, which are used in the input files to identify variables and settings, are given in uppercase bold italics.

- `Input and output file excerpts` are in a box surrounded by a single line, indicating that the text inside the box is shown exactly as it exists in electronic form.

- This document also contains references to the APEX model code. Specifically, the discussions of the model algorithms include mention to the module and function or

subroutine in which they are implemented. The code locations are given in bold non-italic text in the format **Module:Subroutine** or **Module:Function.**

1.4 Strengths and Limitations of APEX

All models have strengths and limitations, and for each application it is important to carefully select the model that has the desired attributes. With this in mind, it is equally important to understand the strengths and weaknesses of the chosen model. The following sections provide a summary of the strengths and potential limitations of APEX.

1.4.1 Strengths

APEX simulates the movement of individuals through time and space to estimate their exposure to individual or multiple pollutants in indoor, outdoor, and in-vehicle microenvironments. Compared to conducting a field study that would involve identifying, interviewing, and monitoring specific individuals in a study area, APEX provides a vastly less expensive, more timely, and more flexible approach. The model also allows different air quality data, exposure scenarios, and other inputs and thus is very useful for decision making applications.

An important feature of APEX is its versatility. The model is designed with a great deal of flexibility so that different levels of detail in input data can be applied for different applications. The input data sets supplied with APEX contain information for several microenvironments, covering the needs of most applications. The air quality data input to the model can be in the form of monitoring or modeling data. The data can be for specific locations, on roadways, or geo-political units such as counties, or census units such as tracts, or the locations of air dispersion model receptors, or the grid cells of Eulerian model output. Criteria and hazardous air pollutants can be modeled by APEX.

A key strength of APEX is the way it 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.

Another strength of APEX is its ability to estimate exposures and doses on different timescales for all simulated individuals in the sample population from the study area. This ability allows for powerful statistical analysis of a number of exposure characteristics (e.g., acute and chronic exposure, correlations with activities and demographics), many of which are provided automatically by APEX in output tables.

APEX also estimates the exposures of workers in the areas where they work, in addition to the areas where they live. The pollutant concentrations in these respective locations may be very different from each other.

The use of APEX has been facilitated by the availability of model-ready input files which have been developed from the databases discussed above: national population demographics and commuting information from the 2000 U.S. Census; CHAD activity data; and microenvironment definitions.

1.4.2 Limitations

The following limitations of APEX have been identified:

- The population activity pattern data supplied with APEX (CHAD activity data) are compiled from a number of studies in different areas, and for different seasons and years. Therefore, the combined data set may not constitute a representative sample. Nevertheless, the largest portion of CHAD is from random-sample studies of national scope, which could be extracted by the user if desired to create a representative sample.

- The commuting data address only home-to-work travel; travel between sectors for other purposes is not modeled directly. APEX can model time spent in travel; however, based on the model settings, the ambient air quality during travel is assumed to be either 1) a composite of the air quality in all study area sectors or 2) a composite of the air quality in a randomly-selected group of sectors.

- APEX creates seasonal or year-long sequences of activities for a simulated individual by sampling human activity data from more than one subject in CHAD. Thus, uncertainty exists about season-long exposure event sequences. This approach can tend to underestimate the variability from person to person, because each simulated person essentially becomes a composite or an "average" of several actual people in the underlying activity data (which tends to dampen the variability). At the same time, this approach may overestimate the day-to-day variability for any individual if each simulated person is represented by a sequence of potentially dissimilar activities from different people rather than more similar activities from one person. These uncertainties have been partly removed with the implementation in APEX of an algorithm for combining diaries which addresses these limitations to some extent.

- The model currently does not capture certain correlations among human activities that can impact microenvironmental concentrations (e.g., cigarette smoking leading to an individual opening a window, which in turn affects the amount of outdoor air penetrating the residence).

- Certain aspects of the personal profiles are held constant, though in reality they change every year (e.g., age). This is only an issue for simulations spanning several years.

- At this point in time, no interactions between pollutants are modeled.

Other data and model limitations exist besides those identified above, including physiological, meteorological, and those associated with estimating concentrations in microenvironments. EPA will continue to refine the model and data to reduce these limitations to the extent possible. The uncertainties which result from these limitations of APEX have been characterized for an ozone assessment (Langstaff, 2007).

1.5 Applicability

APEX is an advanced air inhalation exposure model which can be used for a range of applications. APEX can be employed to model episodic "high-end" inhalation exposures that result from highly localized pollutant concentrations (e.g., residual risk assessments). APEX can also provide detailed probabilistic estimates of exposure for urban and greater metropolitan areas

(e.g. for regulatory analyses supporting national decisions such as NAAQS reviews). APEX is appropriate for assessing both long-term chronic and short-term acute inhalation exposures of the general population or of specific segments of the population. The model is designed to look at the range of inhalation exposures of different groups of people across a population, for a range of averaging times, in a single simulation. The current version of APEX produces results for flexible averaging times. By default APEX produces results for 1 hour, 8 hours, 24 hours, and annual time periods (or the length of a simulation, if shorter than one year). However, APEX can optionally model results for timesteps on a much smaller scale (e.g. ever 5 minutes) by setting optional run parameters and providing air quality data on the appropriate time scale.

Due to the computational demands (run time and disk space) of running APEX, it is not appropriate for national-level assessments of population exposure. However, this is not an inherent limitation in the model code or algorithms.

1.6 Brief History of APEX

APEX was originally derived from the probabilistic National Ambient Air Quality Standards Exposure Model (pNEM). The NEM series was developed to estimate exposure to the criteria pollutants (e.g., CO, ozone). In 1979, EPA began to develop NEM by assembling a database of human activity patterns that could be used to estimate exposures to outdoor pollutants (Roddin et al., 1979). The data were then combined with measured outdoor concentrations in NEM to estimate exposures to CO (Biller et al., 1981; Johnson and Paul, 1983). In 1988, OAQPS began to incorporate probabilistic elements into the NEM methodology, using activity pattern data based on various human activity diary studies in an early version of probabilistic NEM for ozone (pNEM/O_3). In 1991, a probabilistic version of NEM was developed for CO (pNEM/CO) that included a one compartment mass-balance model to estimate CO concentrations in indoor microenvironments (Johnson et al., 1992). A newer version of pNEM/O_3 was developed in the 1990's and applied to nine urban areas for the general population, outdoor children, and outdoor workers (Johnson et al., 1996a,b,c). During 1999-2001, an updated version of pNEM/CO (versions 2) was developed that relied on activity diary data from CHAD and enhanced algorithms for simulating gas stove usage, estimating alveolar ventilation rate (a measure of human respiration), and modeling home-to-work commuting patterns.

APEX evolved from pNEM to provide greater applicability, flexibility, and accuracy. The APEX model was substantially different than pNEM, particularly in the use of a personal profile approach rather than a cohort simulation approach. APEX introduced a number of new features including automatic site selection from large (e.g., national) databases, a series of new output tables providing summary statistics, and a thoroughly reorganized method of describing microenvironments and their parameters. Most of the spatial and temporal constraints were removed or relaxed in APEX. Several major improvements to APEX have been introduced in the most recent version, APEX4. Specifically, APEX4 includes:

- Multipollutant capability
- algorithms for the assembly of multi-day (longitudinal) activity diaries that model intra-individual variance, inter-individual variance, and day-to-day autocorrelation in diary properties.

- methods for adjusting diary-based energy expenditures for fatigue and excess post-exercise oxygen consumption

- new equations for estimation of ventilation

- the ability to model commuters leaving the study area

- the ability to model air quality and exposure on different time scales

- the ability to model person-to-person variability in air quality within an air district

- new output files containing diary event-level, timestep level, and hourly-level exposure, dose, and ventilation data, and hourly-level microenvironmental data

- the ability to model the prevalence of disease states such as asthma

- new output exposure tables that report exposure statistics for subpopulations such as children and active people under different ventilation levels.

- the ability to model inhaled dose for pollutants

- the inclusion of commuting data from the 2000 census

- expanded options for modeling microenvironments

- expanded location options for sampling ambient air quality

CHAPTER 2. OVERVIEW OF MODEL DESIGN AND ALGORITHMS

This chapter provides a brief outline of the key modeling steps, logic processes, and databases used in APEX.

APEX is designed to simulate population exposure to criteria and air toxic pollutants at local, urban, and regional scales. The user specifies the geographic area to be modeled and the number of individuals to be simulated to represent this population. APEX then generates a personal profile for each simulated person that specifies various parameter values required by the model. The model next uses diary-derived time/activity data matched to each personal profile to generate an exposure event sequence (also referred to as "activity pattern" or "composite diary") for the modeled individual that spans a specified time period, such as one year. Each event in the sequence specifies a start time, an exposure duration, a geographic location, a microenvironment, and an activity. Probabilistic algorithms are used to estimate the pollutant concentration and ventilation (respiration) rate associated with each exposure event. The estimated pollutant concentrations account for the effects of ambient (outdoor) pollutant concentration, penetration factor, air exchange rate, decay/deposition rate, and proximity to emission sources, depending on the microenvironment, available data, and the estimation method selected by the user. The ventilation rate is derived from an energy expenditure rate estimated for the specified activity. Because the modeled individuals represent a random sample of the population of interest, the distribution of modeled individual exposures can be extrapolated to the larger population.

The model simulation includes up to seven steps:

1. Characterize the study area - APEX selects sectors (e.g., census tracts) within a study area—and thus identifies the potentially exposed population—based on the user-defined center and radius of the study area and availability of air quality and weather input data for the area.

2. Generate simulated individuals - APEX stochastically generates a sample of simulated individuals based on the census data for the study area and human profile distribution data (such as age-specific employment probabilities). The user can specify the size of the sample. The larger the sample, the more representative it is of the population in the study area (but also the longer the computing time).

3. Construct a sequence of activity events - APEX constructs an exposure event sequence (activity pattern) spanning the period of simulation for each of the simulated persons (based on the supplied Consolidated Human Activity Database (CHAD) data, although other data could be used).

4. Estimate energy expenditures and ventilation – APEX constructs a time-series of energy expenditures for each profile based on the activity event sequence. These expenditures are adjusted for physiological realism, and then used to estimate a number of ventilation metrics that are later used in estimating dose and in identifying an active subpopulation of active persons for use in creating exposure summary tables.

5. Calculate timestep concentrations in microenvironments for each pollutant - APEX enables the user to define microenvironments that people in a study area would visit (e.g., by

8

grouping location codes included in the supplied CHAD database). The model then calculates timestep concentrations of each pollutant in each of the microenvironments for the period of simulation, based on the user-provided ambient air quality data. All the timestep concentrations in the microenvironments are re-calculated for each simulated individual.

6. Calculate exposures for each pollutant - APEX assigns a concentration to each exposure event based on the microenvironment occupied during the event and the person's activity. These values are averaged by timestep and by clock hour to produce a sequence of timestep and hourly-average exposures spanning the specified exposure period (typically one year). These hourly values may be further aggregated to produce daily, monthly, and annual average exposure values.

7. Calculate doses - APEX optionally calculates timestep, hourly, daily, monthly, and annual average dose values for each of the simulated individuals.

The model simulation continues until exposures are calculated for the user-specified number of simulated individuals. Figure 2.1 presents these steps within a schematic of the APEX model design. The following chapters provide additional detail on the algorithms used in each of the above simulation steps.

The above steps are largely self-contained in the APEX computer code and do not depend on subsequent steps. For example, the generation of simulated individuals (step 2) is independent of any other profile characteristics or modeling results. This means that the profile variables do not depend on the diaries assigned to that profile or to the properties of the microenvironments for that profile. The assignment of diaries to the profile (step 3) depends on the profile variables but not on the microenvironments, the exposure, the dose, or the properties of any other profile. The calculation of microenvironment concentrations (step 4) can depend on the profile variables through the use of conditional variables, but in APEX this step cannot depend on the contents of the selected activity diaries. Conceptually, this means that the microenvironments essentially have an existence of their own that is independent of the activities of the profile. For example, activities such as smoking and cooking can "occur" in a residence even when the person being profiled is not at home. In reality, the activities of the profiled person can have some effect on the microenvironments they visit, but this is not captured in the present version of the model. However, through the judicious use of source terms in microenvironments, APEX can simulate changes in concentrations due to the presence of the person (e.g., a "personal cloud" effect).

1. Characterize study area   **2. Characterize study population**   **3. Generate N number of simulated individuals (profiles)**

2000 Census tract-level data for the entire U.S. (sectors=tracts for the NAAQS ozone exposure application)

Sector location data (latitude, longitude)

Sector population data (age/gender/race)

Commuting flow data (origin/destination sectors)

Age/gender/tract-specific employment probabilities

Defined study area (sectors within a city radius and with air quality and meteorological data within their radii of influence)

Population within the study area

Stochastic profile generator

Locations of air quality and meteorological measurements; radii of influence

Age/gender-specific physiological distribution data (body weight, height, etc)

Distribution functions for profile variables (e.g, probability of air conditioning)

Distribution functions for seasonal and daily varying profile variables (e.g., window status, car speed)

A simulated individual with the following profile:
• Home sector
• Work sector (if employed)
• Age
• Gender
• Race
• Employment status
• Home gas stove
• Home gas pilot
• Home air conditioner
• Car air conditioner
• Physiological parameters (height, weight, etc.)

- National database

- Area-specific input data

- Intermediate step or data

- Data processor

- Output data

Figure 2.1a. Overview of APEX, Part 1

10

**4. Construct sequence of activity events
for each simulated individual**

Diary events/activities and personal information (e.g., from CHAD)

Activity diary pools by day type/temperature category

Selected diary records for each day in the simulation period, resulting in a sequence of events (microenvironments visited, minutes spent, and activity) in the simulation period, for an individual

Profile for an individual

Stochastic diary selector using age, gender, employment, and key diary statistic (for longitudinal diary assembly)

Stochastic calculation of energy expended per event (adjusted for physiological limits and EPOC) and ventilation rates

Each day in the simulation period is assigned to an activity pool based on day type and temperature category

Maximum/mean daily temperature data

Physiological parameters from profile

Sequence of events for an individual

Figure 2-1b. Overview of APEX, Part 2

11

5. Calculate concentrations in microenvironments for all events for each simulated individual

6. Calculate timestep / hourly exposures for each simulated individual

7. Calculate population exposure statistics

Microenvironments defined by grouping of CHAD location codes

Select calculation method for each microenvironment:
• Factors
• Mass balance

Input functions describing interpersonal, geographic, meteorological, and temporal variation in microenvironmental parameters

Timestep or hourly air quality data for all sectors

Calculate concentrations in all microenvironments

Average exposures for simulated person, stratified by ventilation rate:
•Timestep
•Hourly
•Daily timestep max
•Daily…

Population exposure indicators for:
• Total population
• Children
• Asthmatic children

Timestep concentrations and minutes spent in each microenvironment visited by the simulated individual

Concentrations for all events for each simulated individual

Calculate timestep concentrations in microenvironments visited

Sequence of events for each simulated individual

Repeat steps 5-7 for each pollutant in the simulation

Figure 2-1c. Overview of APEX, Part 3

12

CHAPTER 3.   USING PROBABILITY DISTRIBUTIONS IN APEX

APEX is a stochastic model. It makes use of random sampling from probability distributions to model variability in a number of input model parameters. Specifically, distributions are used:

1) **To model variability in MET (energy expenditures) for different activities.** Input MET distributions for each activity are defined in the *Activity-Specific MET* file.

2) **To model inter-person variability in physiological parameters**. Physiological parameter distributions are defined for each different age-gender cohort in the *Physiology* file.

3) **To model timestep, hourly, daily, geographic, or air quality variability in microenvironment parameters**.   Distributions for microenvironmental parameters are defined in the *Microparameter Descriptions* file.

4) **To model person-to-person variation in hourly air quality data within an air district.** Distributions for hourly air quality values can be defined in the *Air Quality Data* file. This is an optional feature of APEX.

This chapter gives direction on how to define distributions in these input files. In addition, each distribution available in APEX and its parameters are defined in detail.

3.1   The APEX Input Distribution Format

In all APEX input files, distributions are defined in the same manner, via a standard APEX format. This format consists of the following items:

- *Distribution Shape*. This variable gives the shape of the distribution.
- *Par1*. Parameter 1 of the distribution. Depends on shape.
- *Par2*. Parameter 2 of the distribution. Depends on shape.
- *Par3*. Parameter 3 of the distribution. Depends on shape.
- *Par4*. Parameter 4 of the distribution. Depends on shape.
- *LTrunc*. Lower truncation point of the distribution.
- *UTrunc*. Upper truncation point of the distribution.
- *ResampOut.*: Distribution resampling flag.

The distribution shape is a text keyword that defines the type of distribution to be used. The next four items (Par1-Par4) are numerical values defining the parameters of the distribution. The next two items (LTrunc and UTrunc) are the optional truncation limits for the distribution, and the last item is an optional character flag (ResampOut, set to either Y or N) indicating how sampled values outside of the truncation limits are handled. All the information is entered on a single line in the appropriate input file. Note that in each input file the distribution definition may be preceded on each line by additional data specific to that file; see sections on individual input files.

The probability distributions allowed in APEX are listed in Table 3.1. Equations for each of the distributions in the table are given in Section 3.2.

Table 3.1. Available Probability Distributions in APEX.

Distribution	APEX SHAPE KEYWORD	Par1	Par2	Par3	Par4	LTrunc (Optional)	UTrunc (Optional)	ResampOut (Optional)
Beta	BETA	Minimum	Maximum	Shape1 (s1) >0	Shape2 (s2) >0	Lower truncation limit	Upper truncation limit	Resample outside truncation? (Y/N)
Cauchy	CAUCHY	Median	Scale (b) > 0			Lower truncation limit	Upper truncation limit	Resample outside truncation? (Y/N)
Discrete	DISCRETE	This type of distribution has no parameters, rather the keyword is simply followed by a space-delimited list of up to 100 discrete values. The distribution returns each of these values with equal probability.						
Exponential	EXPONENTIAL	Decay constant, k > 0	Shift (a)			Lower truncation limit	Upper truncation limit	Resample outside truncation? (Y/N)
Extreme Value	EVALUE	Scale (b) > 0	Shift (a)			Lower truncation limit	Upper truncation limit	Resample outside truncation? (Y/N)
Gamma	GAMMA	Shape (s) > 0	Scale (b) > 0	Shift (a)		Lower truncation limit	Upper truncation limit	Resample outside truncation? (Y/N)
Logistic	LGT	Mean	Scale (b) > 0			Lower truncation limit	Upper truncation limit	Resample outside truncation? (Y/N)
Lognormal	LOGNORMAL	Geometric mean (gm) of unshifted dist	Geometric standard deviation (gsd) >1	Shift (a)		Lower truncation limit	Upper truncation limit	Resample outside truncation? (Y/N)
Loguniform	LUNIFORM	Minimum > 0	Maximum > 0			Lower truncation limit	Upper truncation limit	Resample outside truncation? (Y/N)
Normal	NORMAL	Mean	Standard deviation			Lower truncation limit	Upper truncation limit	Resample outside truncation? (Y/N)
OffOn	OFFON	Probability of being 0 (0-1)						
Pareto	PARETO	Shape (s) > 0	Scale (b) > 0	Shift (a)		Lower truncation limit	Upper truncation limit	Resample outside truncation? (Y/N)
Point	POINT	Point Value						
Triangle	TRIANGLE	Minimum	Maximum	Peak		Lower truncation limit	Upper truncation limit	Resample outside truncation? (Y/N)
Uniform	UNIFORM	Minimum	Maximum			Lower truncation limit	Upper truncation limit	Resample outside truncation? (Y/N)
Weibull	WEIBULL	Shape (s) > 0	Scale (b) > 0	Shift		Lower truncation limit	Upper truncation limit	Resample outside truncation? (Y/N)

Cells that are grayed out in the table correspond to items not needed for a particular distribution, and data entered in these locations will be ignored by APEX. In addition, the LTrunc, UTrunc, and ResampOut items are in general optional. (If LTrunc and UTrunc are defined but ResampOut is not, the default value of ResampOut=Y is used.) **Note however, that a placeholder period (".") must be used in the distribution definition for each item that is not used.**

Consider each of the examples below (one from each input file using distributions):

From the Activity-Specific MET file:

```
Row  Act     Age  Occ.      Shape        Par1  Par2  Par3  Par4  LTrunc UTrunc  ResampOut
  1  10000    0   ADMIN     LogNormal    1.7   1.45  0     .     1.4    2.7     Y
```

From the Physiology file:

```
!Variable  AgeMin AgeMax   Gen  Shape    Par1   Par2  Par3  Par4    LTrunc UTrunc  ResampOut
NVO2MAX       0      0      M    Normal   48.3   1.7   .     .       44.3   52.2    Y
```

From the Microparameter Descriptions file:

```
Block DType Season Area   C1  C2  C3   Shape       Par1   Par2  Par3 Par4  LTrunc UTrunc  ResampOut
1     1     1      1      1   1   1    Normal      2      0.5   0    .     0.111  10.111  Y
```

Note that in each case the distribution definitions follow the exact same format (starting with the Shape keyword). The only distribution type that does not follow this format is the Discrete distribution, see Section 3.2.4.

Distributions are read from the various input files and stored in **DistributionModule:ReadDist**.

3.2   Details of Distribution Sampling, Truncation, and Resampling

Probability density functions (PDFs) for each of the APEX distributions, parameterized in terms of their input APEX parameters, are given in this section (with the exception of the OffOn and Point distributions, which are trivial). In addition, real examples (of 10000 samples each) from APEX are shown for untruncated distributions and for truncated distributions using both ResampOut=Y and ResampOut=N.

When needed, stored distributions (which were read from the input files) are sampled in **DistributionModule:SampleDist.**

3.2.1   Resampling Options

ResampOut determines how truncated distributions are handed by the APEX sampling routines. If ResampOut = N, then any generated sample outside the truncation points is set to the truncation limit; in this case, samples "stack up" at the truncation points, and the probability associated with the area under the PDF outside the truncation bounds is associated with the truncation limit. If ResampOut = Y, then a new random value is selected from inside the valid

range. In this case, the probability outside the limits is spread over the valid values, and thus the probabilities inside the truncation limits will be higher than the theoretical untruncated PDF.

For each of the distributions defined in this section, the theoretical PDF is shown plotted against APEX results for each truncation case. (Note that the "untruncated" case is actually a truncated case with the truncation points set to the 0.1st and 99.9th percentiles where noted. These distributions had very long tails, and they were truncated so they would fit in the illustration).

3.2.2 Beta Distribution

The PDF for the beta distribution in terms of the APEX input parameters is

$$p(x) = \frac{(x-min)^{s1-1}(max-x)^{s2-1}\Gamma(s1+s2)}{\Gamma(s1)\Gamma(s2)(max-min)^{(s1+s2-1)}} \tag{3-1}$$

where Γ indicates the gamma function and S1 and S2 are shape parameters. See Table 3.1 for assignment of the parameters in this equation to the APEX parameters Par1-Par4. The theoretical PDF for the beta distribution is illustrated in Figure 3.1 along with real examples obtained from APEX using the different sampling options.
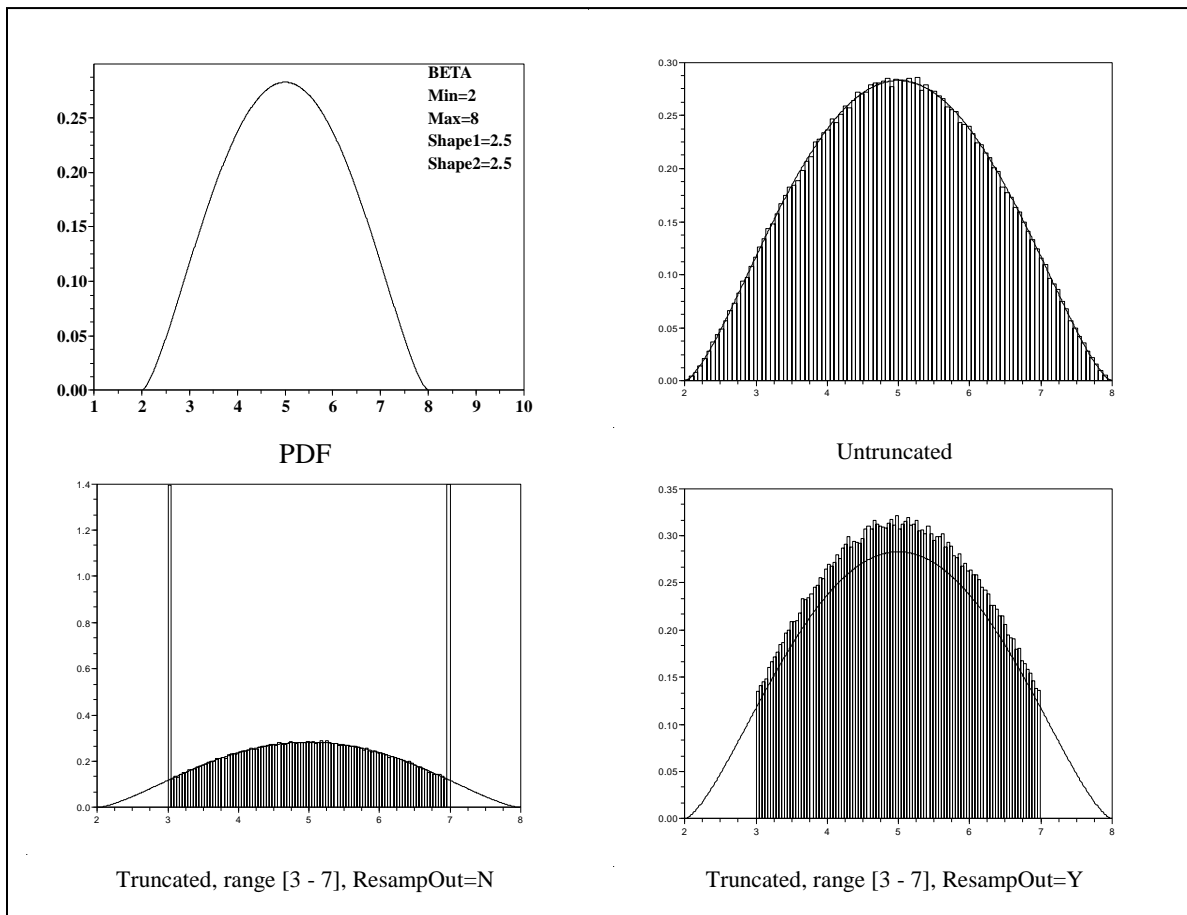
Figure 3.1. The Beta Distribution in APEX.

16

3.2.3   Cauchy Distribution

The PDF for the Cauchy distribution in terms of the APEX input parameters is

$$p(x) = \frac{1}{b\pi \left(1 + \dfrac{(x - median)^2}{b^2} \right)}$$

(3-2)

where b is a scale parameter. See Table 3.1 for assignment of the parameters in this equation to the APEX parameters Par1-Par4. The theoretical PDF for the Cauchy distribution is illustrated in Figure 3.2 along with real examples obtained from APEX using the different sampling options.

Figure 3.2. The Cauchy Distribution in APEX.

17

3.2.4   Discrete Distribution

The discrete distribution is a custom form of APEX distribution. Rather than being defined by the regular 7 parameters, the discrete distribution is just given as a space-separated list of up to 100 values. APEX will return all values with equal probability.

An example of a discrete distribution having 6 values is shown in Figure 3.3.

Figure 3.3 The Discrete Distribution in APEX

3.2.5 **Exponential** Distribution

The PDF for the exponential distribution in terms of the APEX input parameters is

$$p(x) = ke^{\left(\frac{a-x}{k}\right)} \qquad \text{for } x > a$$
$$p(x) = 0 \qquad \qquad \text{for } x < a$$

(3-3)

where a is a shift parameter and k is the decay constant. See Table 3.1 for assignment of the parameters in this equation to the APEX parameters Par1-Par4. The theoretical PDF for the exponential distribution is illustrated in Figure 3.4 along with real examples obtained from APEX using the different sampling options.

Figure 3.4. The Exponential Distribution in APEX.

3.2.6 Extreme Value Distribution

The PDF for the extreme value distribution in terms of the APEX input parameters is

$$p(x) = \frac{1}{b} e^{\left(\frac{a-x}{b} - e^{\frac{a-x}{b}} \right)}$$

(3-4)

where a is a shift parameter and b is a scale parameter. See Table 3.1 for assignment of the parameters in this equation to the APEX parameters Par1-Par4. The theoretical PDF for the extreme value distribution is illustrated in Figure 3.5 along with real examples obtained from APEX using the different sampling options.

Figure 3.5. The Extreme Value Distribution in APEX.

3.2.7 Gamma Distribution

The PDF for the gamma distribution in terms of the APEX input parameters is

$$p(x) = b^{-s}(x-a)^{s-1}\frac{e^{\frac{a-x}{b}}}{\Gamma(s)} \qquad (3\text{-}5)$$

where a is a shift parameter and b is a scale parameter. See Table 3.1 for assignment of the parameters in this equation to the APEX parameters Par1-Par4. The theoretical PDF for the gamma distribution is illustrated in Figure 3.6 along with real examples obtained from APEX using the different sampling options.

Figure 3.6. The Gamma Distribution in APEX.

3.2.8 Logistic Distribution

The PDF for the logistic distribution in terms of the APEX input parameters is

$$p(x) = \frac{e^{\frac{a-x}{b}}}{\left(1 + e^{\frac{a-x}{b}}\right)^2}$$

(3-6)

where a is a shift parameter and b is a scale parameter. See Table 3.1 for assignment of the parameters in this equation to the APEX parameters Par1-Par4. The theoretical PDF for the logistic distribution is illustrated in Figure 3.7 along with real examples obtained from APEX using the different sampling options.
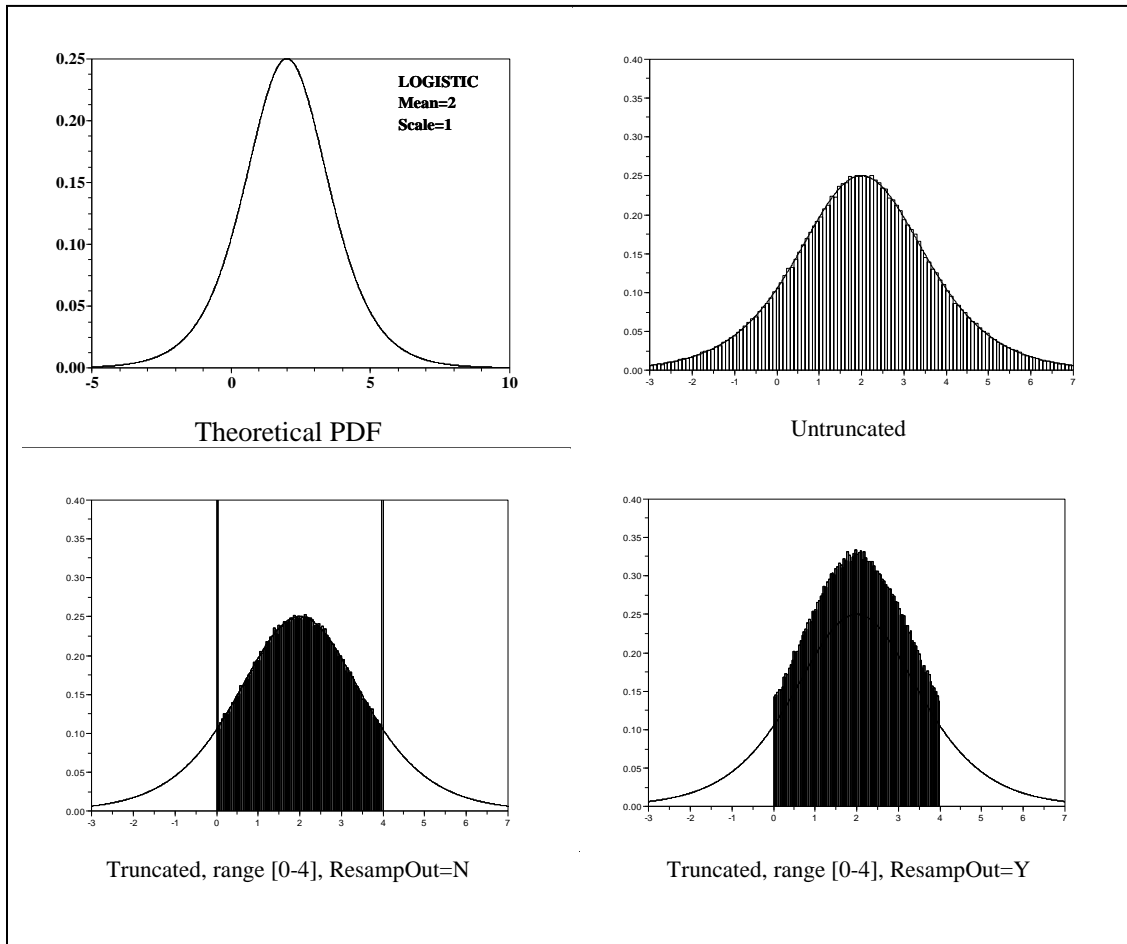
Figure 3.7. The Logistic Distribution in APEX.

3.2.9 Lognormal Distribution

The PDF for the lognormal distribution in terms of the APEX input parameters is

$$p(x) = \frac{1}{\sqrt{2\pi}(x-a)\log(GSD)} e^{-\frac{1}{2}\left[\frac{\log\left(\frac{x-a}{GM}\right)}{\log(GSD)}\right]^2} \tag{3-7}$$

where a is a shift parameter, GM is the geometric mean, and GSD is the geometric standard deviation. See Table 3.1 for assignment of the parameters in this equation to the APEX parameters Par1-Par4. The theoretical PDF for the lognormal distribution is illustrated in Figure 3.8 along with real examples obtained from APEX using the different sampling options.


LOGNORMAL
GM=1
GSD=1.5
Shift=2

Theoretical PDF

Untruncated

Truncated, range [2.5-4], ResampOut=N

Truncated, range [2.5-4], ResampOut=Y

Figure 3.8. The Lognormal Distribution in APEX.

23

3.2.10 Loguniform Distribution

The PDF for the loguniform distribution in terms of the APEX input parameters is

$$p(x) = \frac{1}{log\left(\frac{max}{min}\right)x} \tag{3-8}$$

where min and max are the minimum and maximum values of the untruncated distribution, respectively. See Table 3.1 for assignment of the parameters in this equation to the APEX parameters Par1-Par4. The theoretical PDF for the loguniform distribution is illustrated in Figure 3.9 along with real examples obtained from APEX using the different sampling options.
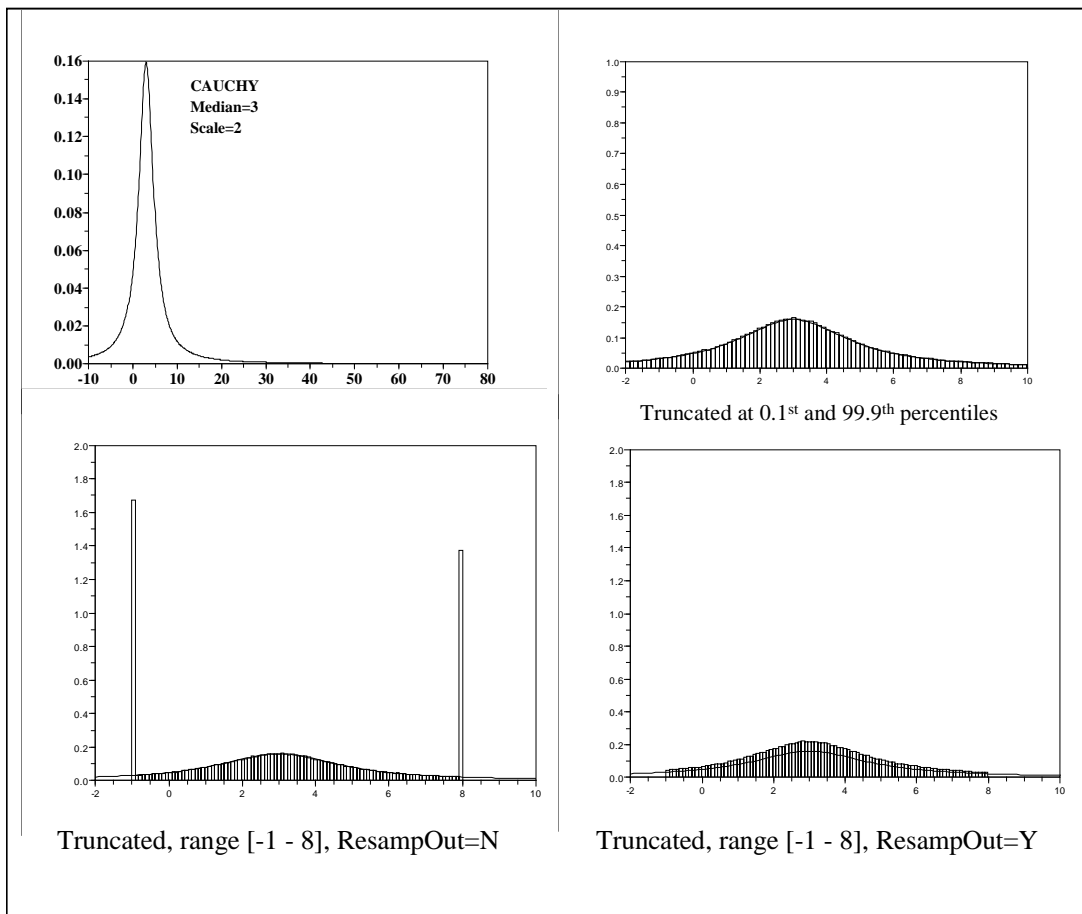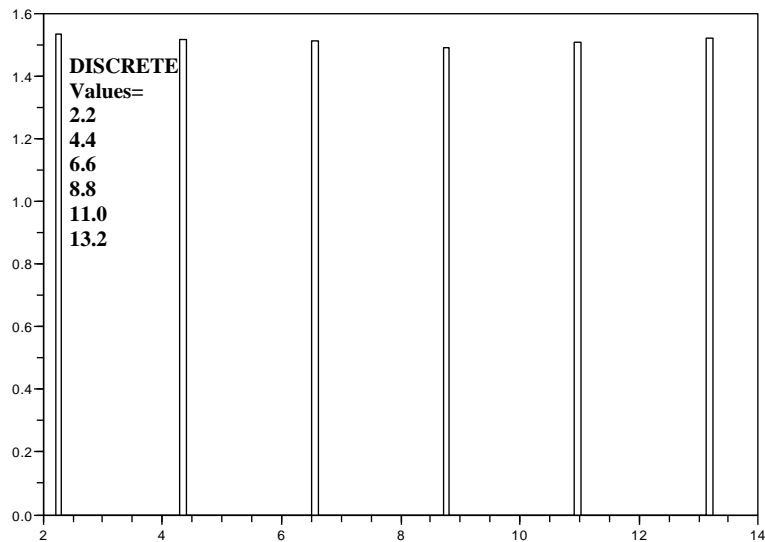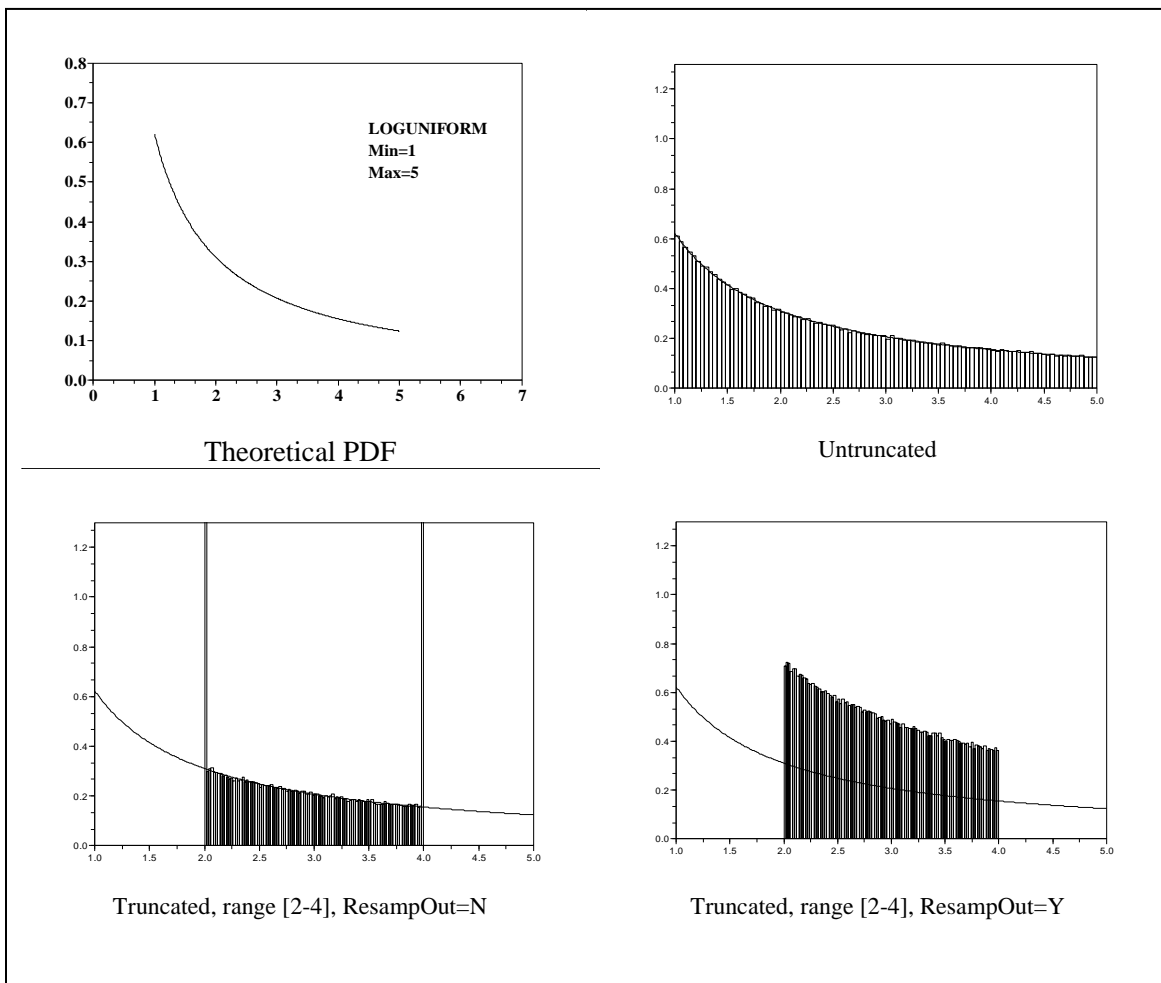

Figure 3.9. The Loguniform Distribution in APEX.

3.2.11 Normal Distribution

The PDF for the normal distribution in terms of the APEX input parameters is

$$p(x) = \frac{1}{SD\sqrt{2\pi}}\, e^{\frac{-(x-mean)^2}{2SD^2}} \tag{3-9}$$

where mean is the mean of the untruncated distribution and SD is the standard deviation. See Table 3.1 for assignment of the parameters in this equation to the APEX parameters Par1-Par4. The theoretical PDF for the normal distribution is illustrated in Figure 3.10 along with real examples obtained from APEX using the different sampling options.

Figure 3.10. The Normal Distribution in APEX.

3.2.12 Pareto Distribution

The PDF for the Pareto distribution in terms of the APEX input parameters is

$$p(x) = \frac{sb^s}{(x-a)^{s+1}} \tag{3-10}$$

where a is a shift parameter and b is a scale parameter. See Table 3.1 for assignment of the parameters in this equation to the APEX parameters Par1-Par4. The theoretical PDF for the Pareto distribution is illustrated in Figure 3.11 along with real examples obtained from APEX using the different sampling options.
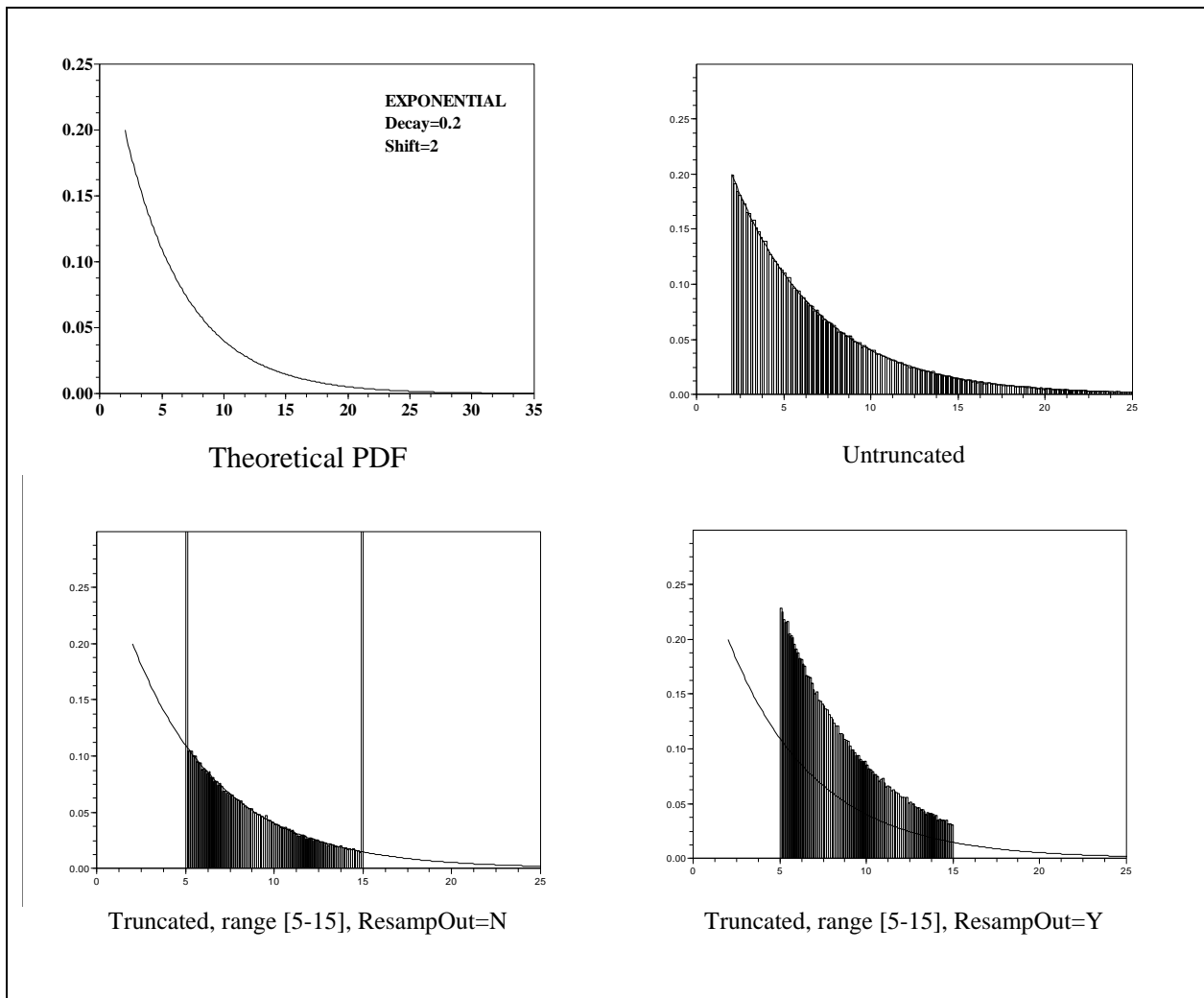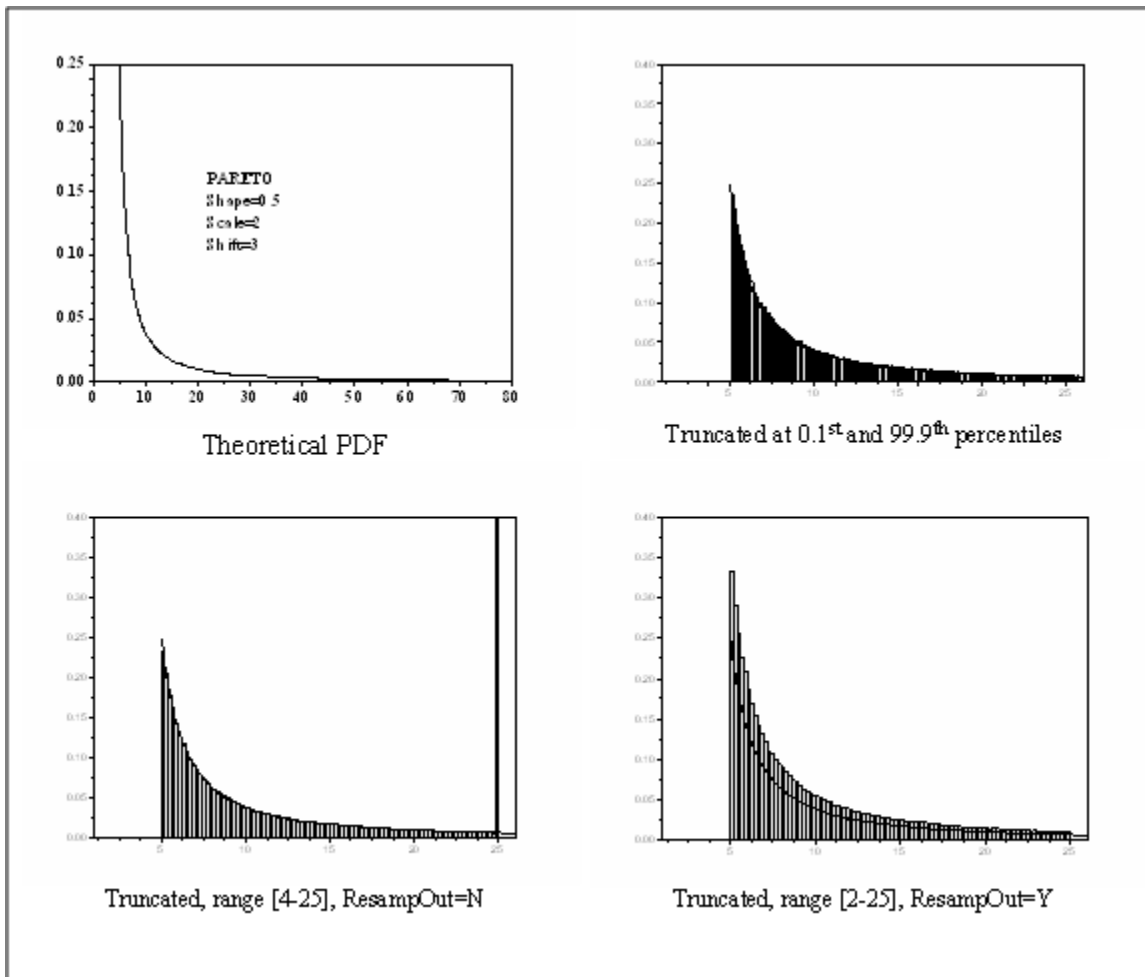

Figure 3.11. The Pareto Distribution in APEX.

3.2.13 Triangle Distribution

The PDF for the triangle distribution in terms of the APEX input parameters is

$$p(x) = \frac{2(x - min)}{(peak - min)(max - min)} \qquad min \leq x \leq peak \qquad (3\text{-}11)$$

$$p(x) = \frac{2(max - x)}{(max - min)(max - peak)} \qquad peak \leq x \leq max$$

where min, max, and peak are the minimum, maximum, and peak of the untruncated distribution, respectively. See Table 3.1 for assignment of the parameters in this equation to the APEX parameters Par1-Par4. The theoretical PDF for the triangle distribution is illustrated in Figure 3.12 along with real examples obtained from APEX using the different sampling options.
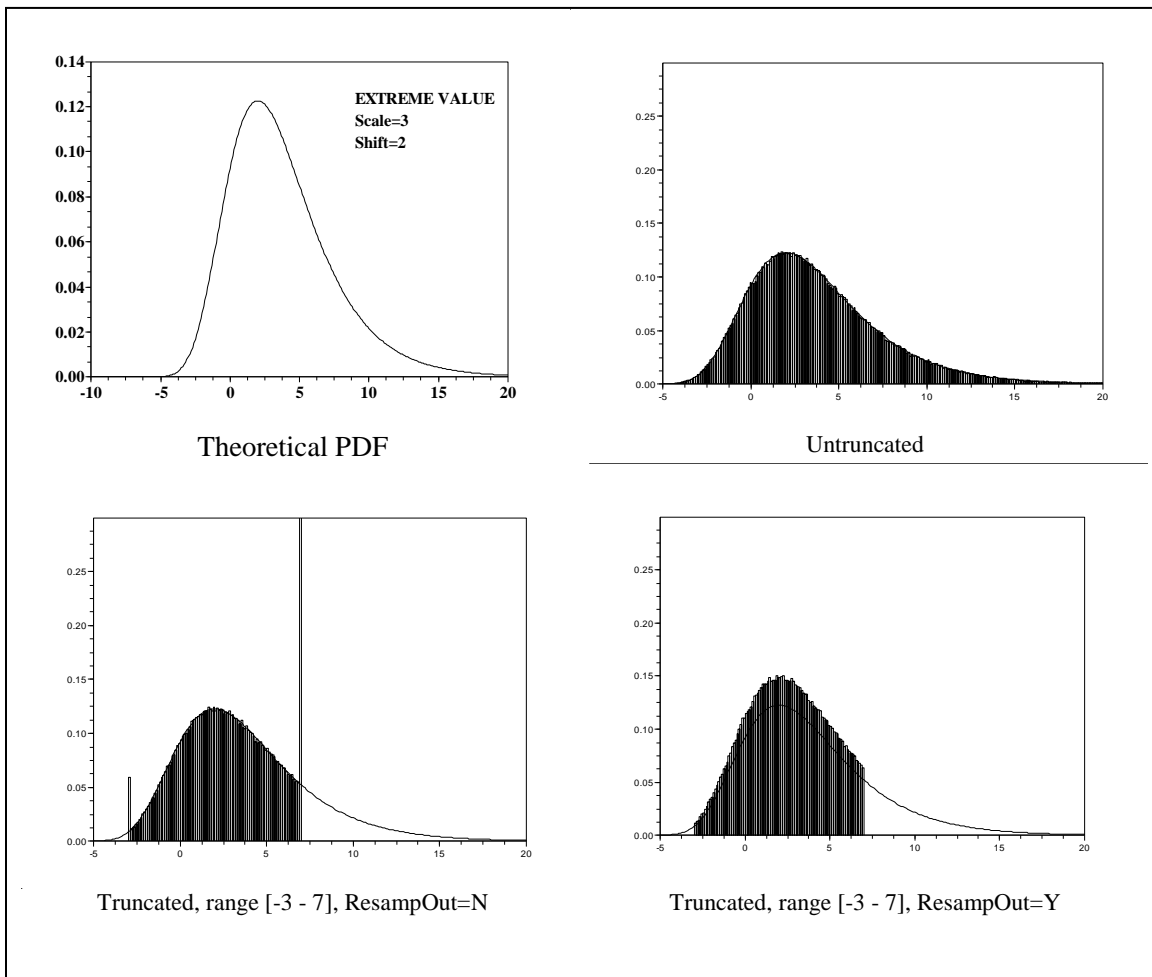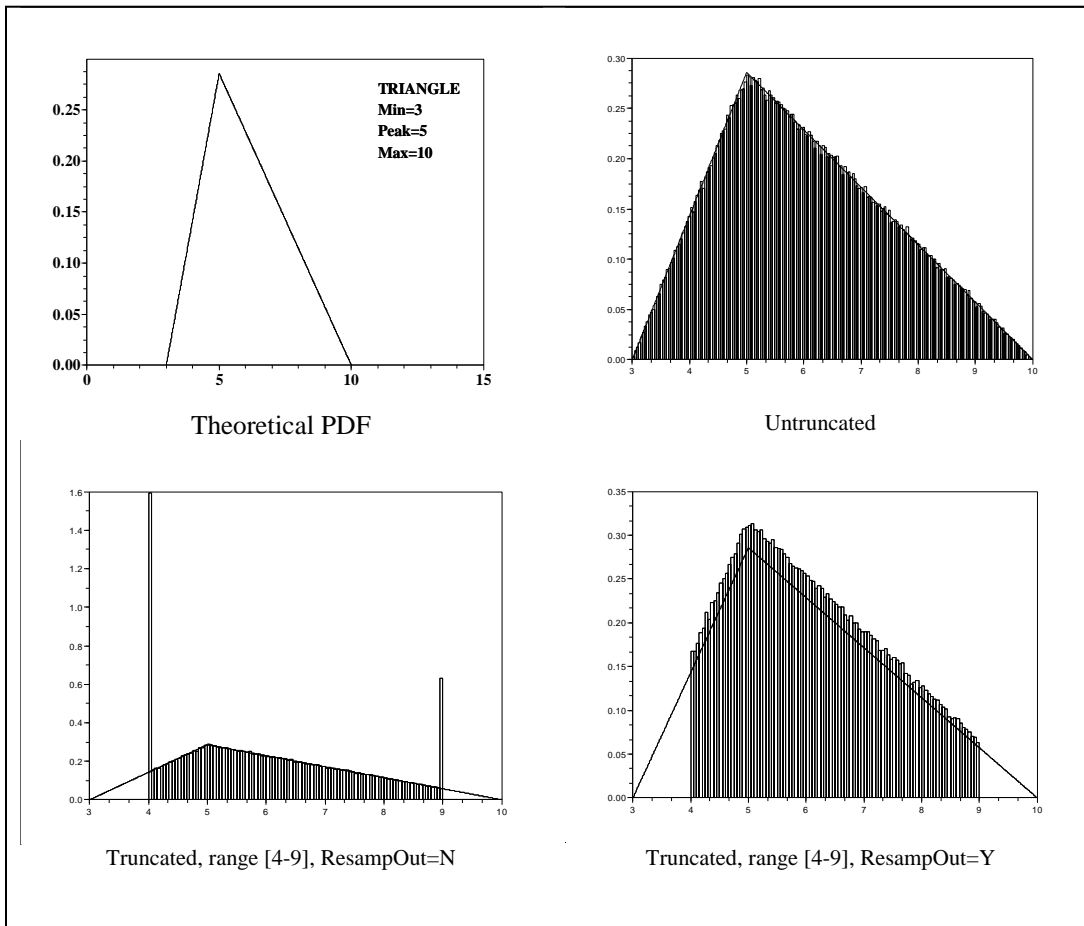

Figure 3.12. The Triangle Distribution in APEX.

3.2.14 Uniform Distribution

The PDF for the uniform distribution in terms of the APEX input parameters is

$$p(x) = \frac{1}{(max - min)} \tag{3-12}$$

where min and max are the minimum and maximum values of the untruncated distribution, respectively. See Table 3.1 for assignment of the parameters in this equation to the APEX parameters Par1-Par4. The theoretical PDF for the uniform distribution is illustrated in Figure 3.13 along with real examples obtained from APEX using the different sampling options.
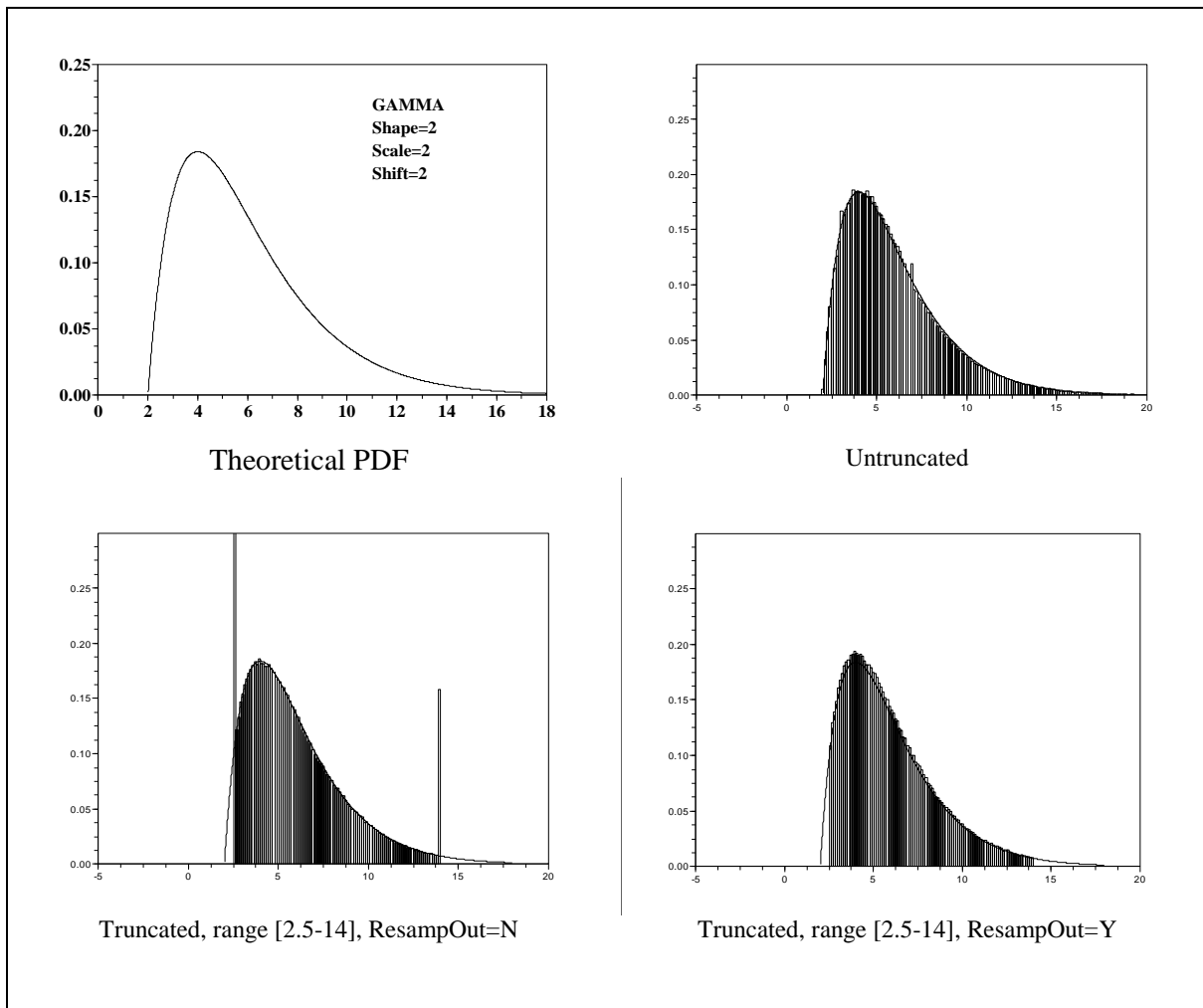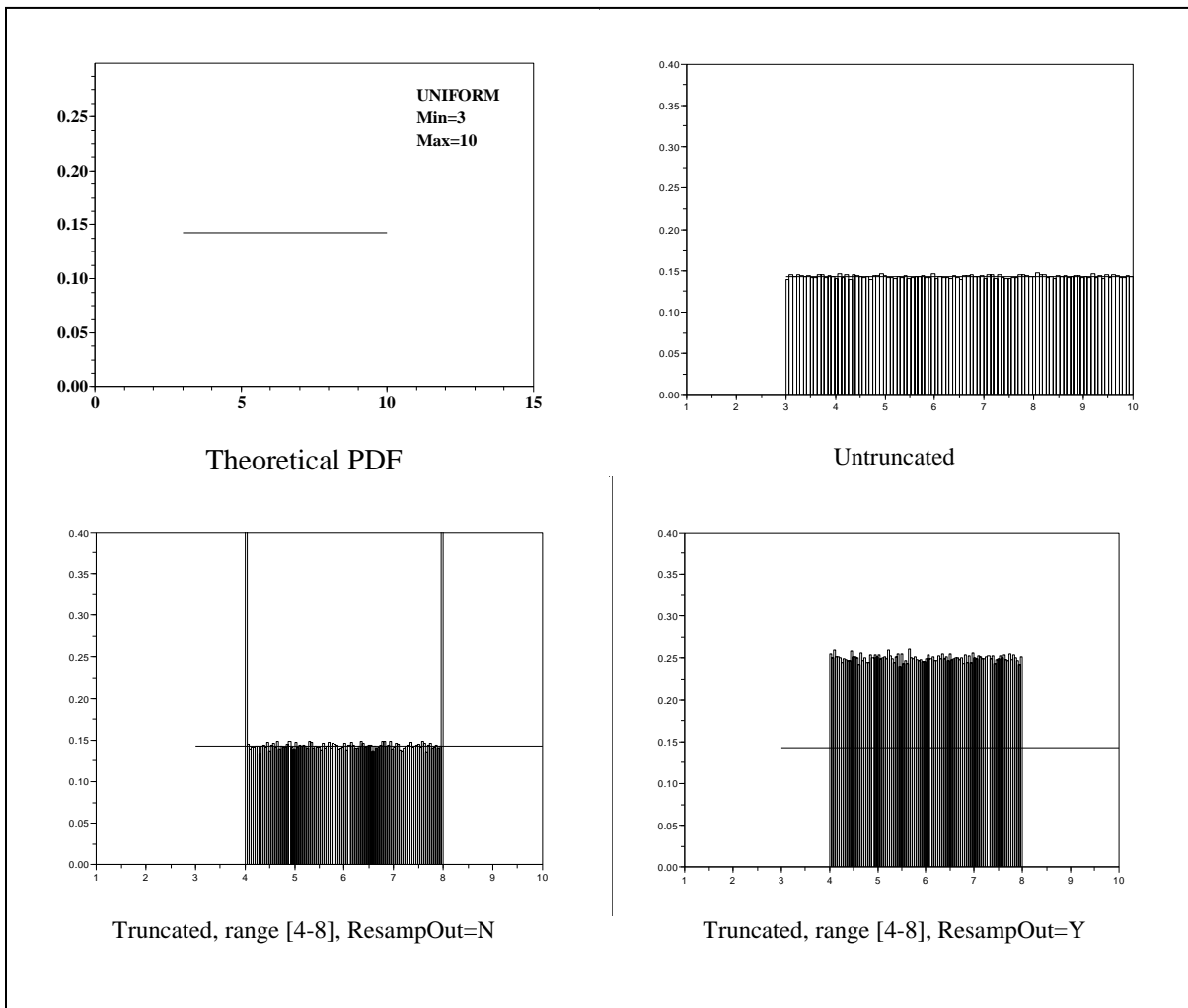

Figure 3.13. The Uniform Distribution in APEX.

3.2.15 Weibull Distribution

The PDF for the Weibull distribution in terms of the APEX input parameters is

$$p(x) = sb^{-s}(x-a)^{s-1}e^{-\left(\frac{x-a}{b}\right)^{s}}$$

(3-13)

where a is a shift parameter and b is a scale parameter. See Table 3.1 for assignment of the parameters in this equation to the APEX parameters Par1-Par4. The theoretical PDF for the Weibull distribution is illustrated in Figure 3.14 along with real examples obtained from APEX using the different sampling options.
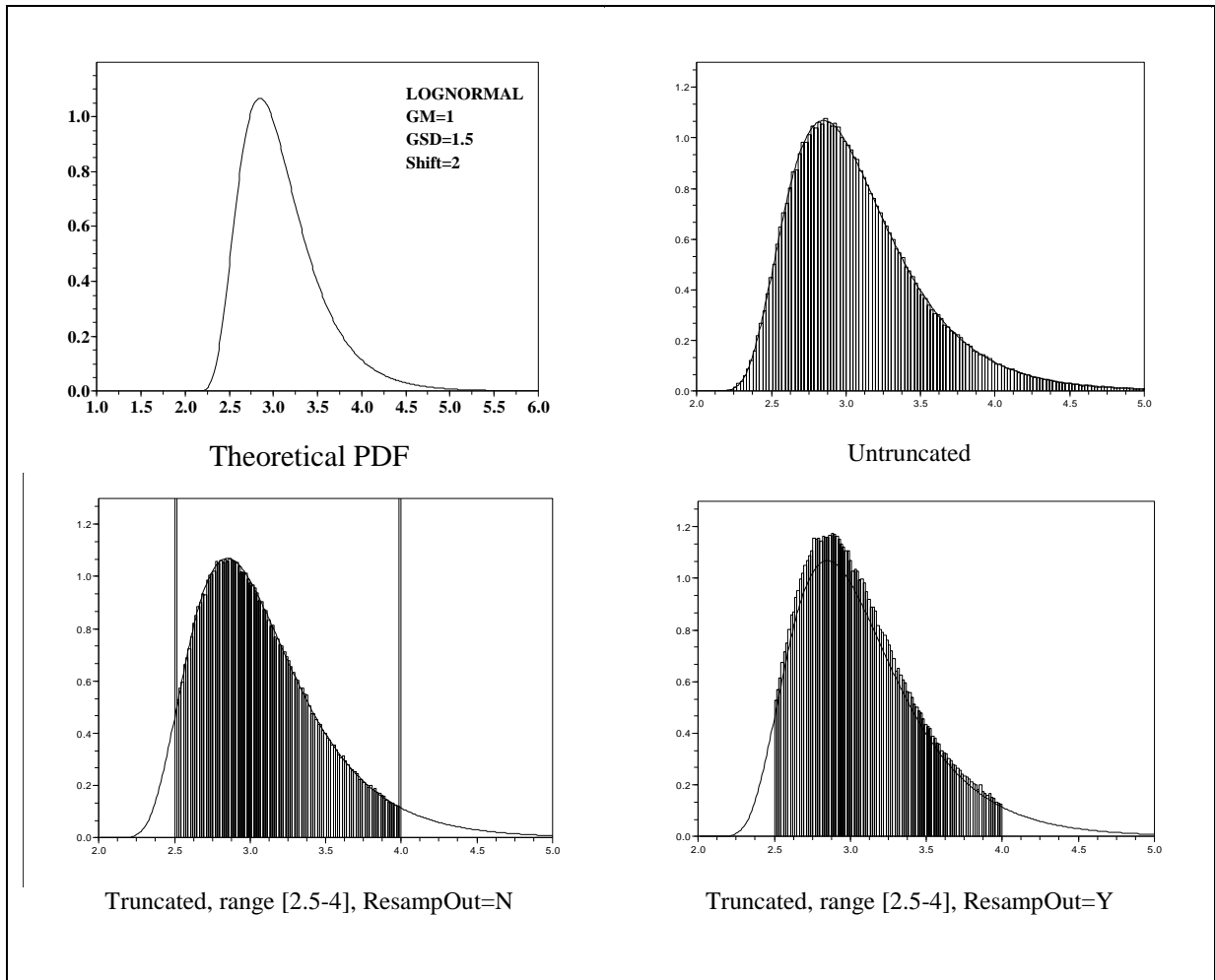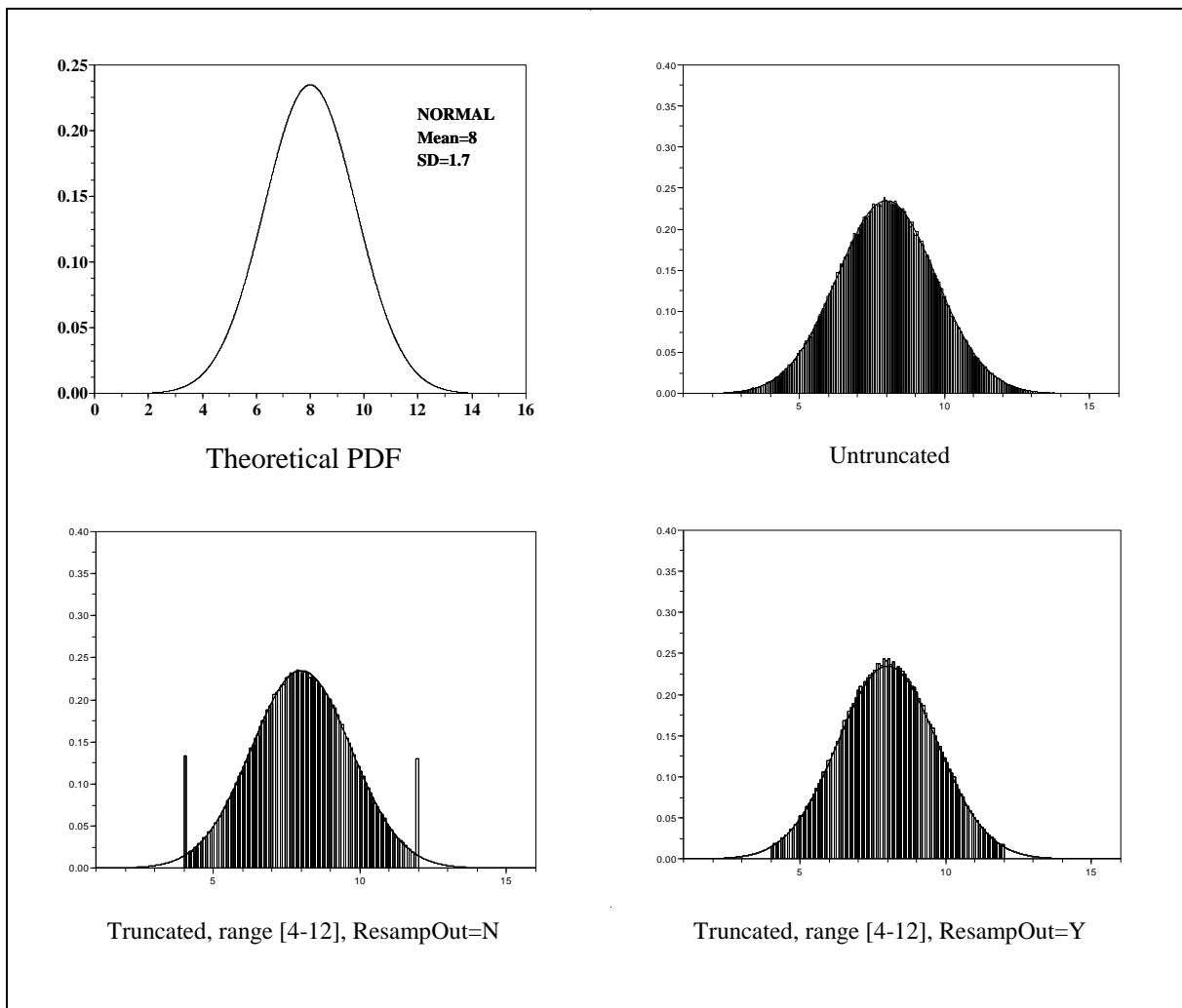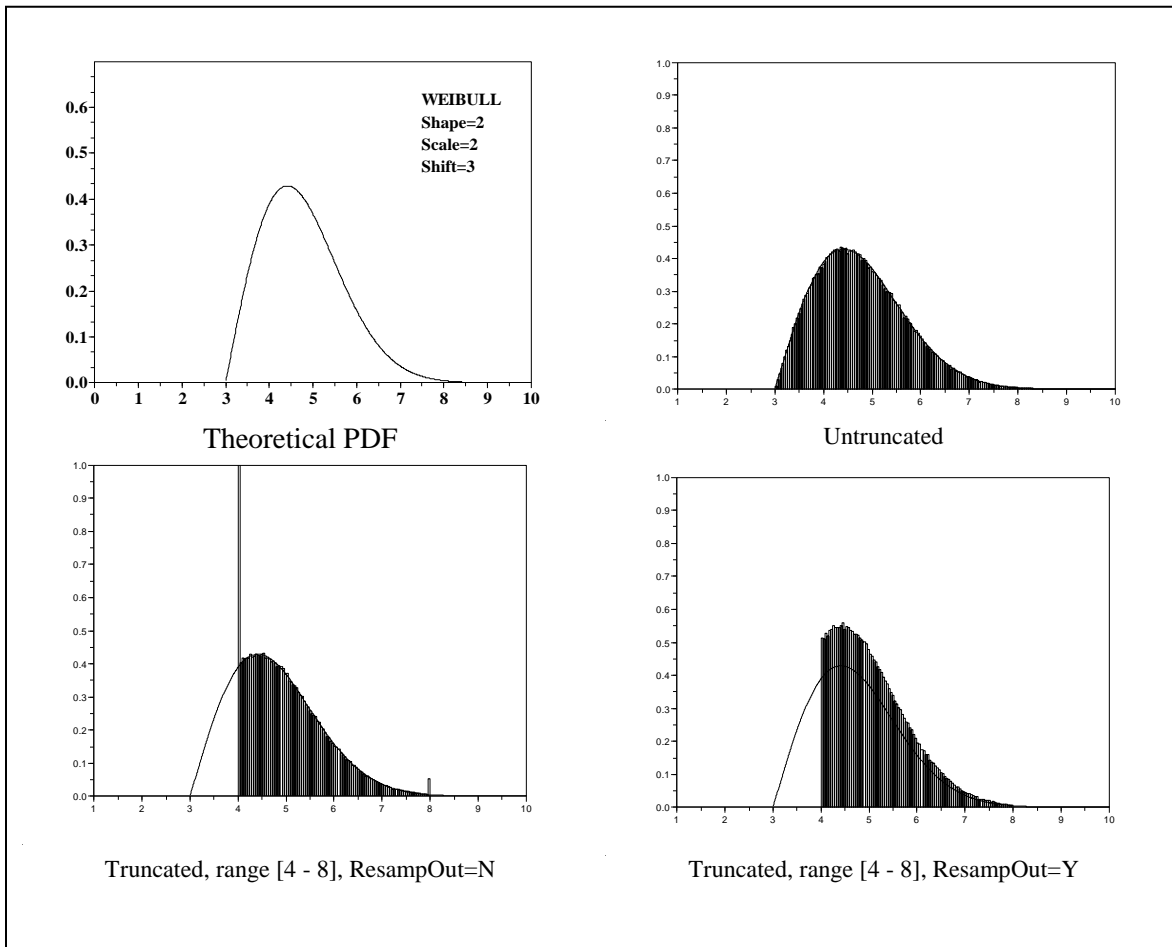

Figure 3.14. The Weibull Distribution in APEX.

CHAPTER 4.   CHARACTERIZING THE STUDY AREA

An <u>initial study area</u> in an APEX analysis consists of a set of basic geographic units called <u>sectors,</u> typically defined as census tracts. (See **Nomenclature**, section 1.3)   The user provides the geographic center (latitude/longitude) and radius of the study area. APEX calculates the distances to the center of the study area of all the sectors included in the sector location database, and then selects the sectors within the radius of the study area. One can also provide a list of counties or census tracts as part of the specification of the initial study area. APEX then maps the user-provided timestep <u>air quality district</u> and hourly <u>meteorological zone</u> data to the selected sectors. The sectors identified as having acceptable air and meteorological data within the radius of the study area are selected to comprise a <u>final study area</u> for the APEX simulation analysis. This final study area determines the population make-up of the simulated persons (profiles) to be modeled.

The following sections describe in more detail how a final study area is determined in an APEX simulation analysis.

4.1   APEX Spatial Units

4.1.1   Initial Study Area

The APEX study area has typically been the neighborhood around an emission source or on the scale of a city or larger metropolitan area. Larger study areas are possible to simulate, depending on computing capabilities, available data, and the desired precision of the run.

The user defines an initial study area by specifying the latitude and longitude of a central point (referred to here as the *study area central location*), together with a radius. The user also has the option of providing a list of counties or census tracts to be modeled. If present, this list further restricts the area to be modeled to the counties or tracts to be modeled which are within the specified study area radius. The final study area is a function of the availability of the user-supplied demographic data, pollutant concentration data, and the meteorological data within the initial study area, as determined respectively by population sectors, air quality districts, and meteorological zones. Figure 4.1 and the subsections below provide additional details about these geographical units.

4.1.2   Sectors

The demographic data used by the model to create personal profiles is provided at the sector level. For each sector the user must provide demographic information allowing the determination of age, gender, race, and work status. This is most commonly done by equating sectors with census tracts and providing input files with counts at the tract level for each age, gender, and race combination. The current release of APEX includes input files that already contain this demographic and location data for all census tracts in the 50 states and D.C., based on the 2000 Census. One of the APEX input files (generically named *Sector Location* file in this guide) lists the sector ID and location for all sectors that have associated population data. The supplied *Sector Location* file has been prepared listing all the census tracts in the 2000 U.S. Census. Corresponding *Population* files have been supplied as well. This allows the user to

model any desired study area in the country without having to make any changes to these input files.
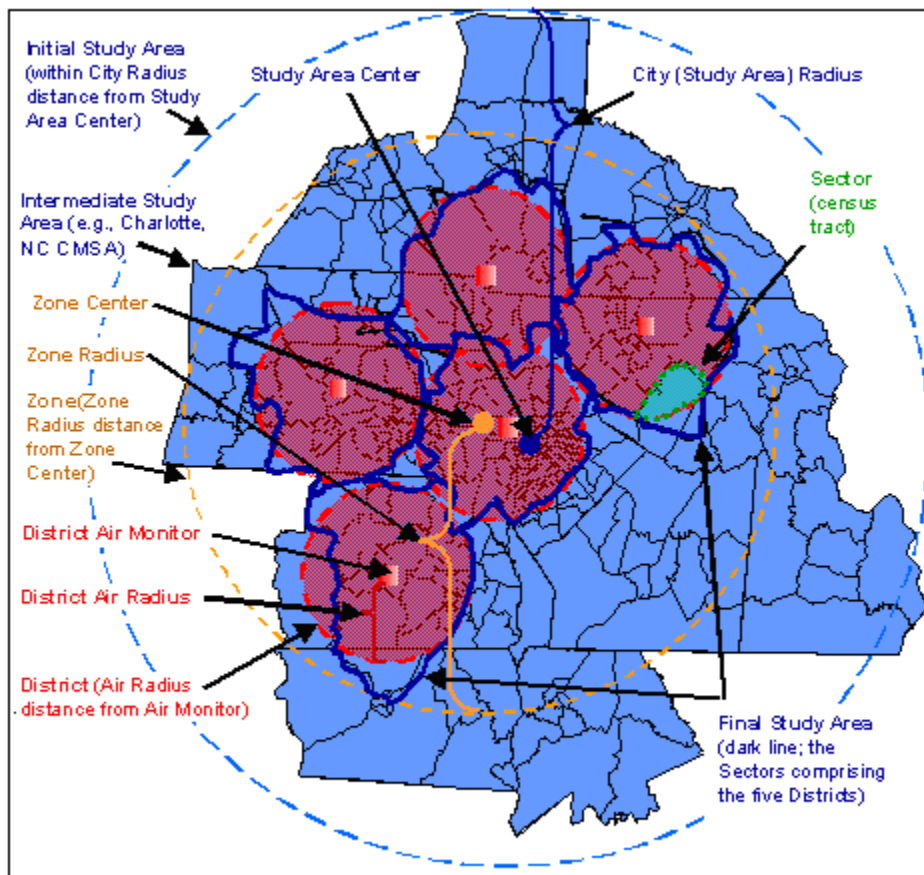
Figure 4.1. Example of Study Areas, Air Quality Districts, Meteorological Zones, and Sectors

If available, finer scales such as census block groups could be used instead. Also, data could be aggregated to larger regions such as counties if fewer sectors were desired. Regardless of the specific meaning for sectors, in APEX the shape of sectors is irrelevant in the sense that the model only uses the central location each sector, determined by the latitude and longitude for some representative point.

In the *Simulation Control* file for an APEX run, the user specifies the area to be modeled by specifying the latitude and longitude of a central location for the study area, along with a radius (the *CityRadius* parameter). Optionally, the user may also provide a list of counties or census tracts to be modeled. If present, this list further restricts the study area.

For each model run, APEX selects the sectors that meet the study area conditions in the following way. First, the sector location must be within the specified distance (radius) of the designated center of the study area. Second, if the user provided a specific list of counties identified by their FIPS codes (using *CountyList* and *County* in the Control file) , then the sector

31

must belong to one of these counties. This is achieved using the first five characters of the sector ID, which should contain the FIPS code for the county in which the sector is located. The user may also provide a list of census tracts (sectors) using the **TractList** and **Tract** variables. If no county or tract list is provided, the initial study area is roughly circular, consisting of all sectors with sector locations within the specified radius. The final study area consists of the subset of sectors in the initial study area for which air quality and meteorological data are available. This is discussed under the next two subsections (4.1.3 and 4.1.4).`

One way to exert greater control over the selection of sectors is to edit the Census input files to eliminate any undesired sectors. However, the *Sector Location* file and the various *Population* files must all have the same set of sectors in them, so consistent editing is necessary. The *Sectors* and *Population* files provided with the current release of APEX contain data for all census tracts in the 50 states and D.C. from the 2000 Census.

The sectors are read in **SpaceTimeModule:ReadSiteLists**.

4.1.3   Air Quality Districts

The spatial units for ambient air quality data are called air quality districts. Ambient air quality data are provided as timestep (e.g. hourly) time series at specific locations. These locations could be monitoring sites, or political units such as counties, or census units such as tracts, or receptor locations or grid points as used by some air quality models. As with sectors, each air quality district has a nominal central location consisting of a latitude and a longitude. The air quality district locations are stored in the *Air Quality District Location* input file. The user designates the maximum representative radius of the air quality districts as a modeling parameter called **AirRadius**. If desired, the user can specify a different **AirRadius** for each district using the *Districts* file. The same set of air quality districts must be used for each pollutant. Users can also specify roadway concentrations in the *Air Quality District Location* file. These data will be used for microenvironments set to "R (Road)" or "RW (Road Work)" in the *ME Mapping* file instead of using the ambient AQ data for the person's Home or Work district.

The model checks each air quality district listed in the *Air Quality Data* input files (one for each pollutant) to determine if the district has data covering the entire simulation period. Note that each air quality district may have a different period of operation (i.e., different start and/or stop dates), but there can be no missing data or gaps between the simulation start and stop dates. If the user is supplying monitoring data as inputs, for example, then any missing values within each monitoring period must be filled in. The monitoring period can exceed the simulation period for the model run because APEX extracts the portion of the input data that corresponds to the simulation period. If the monitoring period does not cover the entire simulation period, the air quality district is deleted in its entirety.

APEX calculates the distance from each sector location to each air quality district center, and assigns the sector to the nearest air quality district, provided it is within the maximum representative air quality radius. If there is no air quality district within range (that is, all air quality district centers are further than **AirRadius** from the sector center), the sector is deleted from the study area and is not modeled. It is possible and perhaps even likely that some air quality districts in the *Air Quality Data* input files will have no sectors assigned to them. Such air quality districts are not used. This feature allows the user to prepare an input file in the

simplest manner, perhaps containing more air quality districts than are necessary. For example, one might prepare a single *Air Quality Data* input file for a pollutant for all air quality districts in the state of Texas. This same input file could then be run on a study area around Houston, or Dallas, or some other location in Texas, without having to alter the input file. In principle, although the file would be very large, a single nationwide *Air Quality Data* file could be prepared and used for any pollutant of interest.

By default, APEX will assign each person within a sector the corresponding appropriate ambient values from the sector's matching air district. Thus, for each timestep in the simulation, all persons within the same district will have the same air quality value. However, APEX can optionally model person-to-person variation in air quality within an air district. In this case, an optional form of the Air Quality Data file is provided, which lists air quality distributions for each hour for each air district. Each person in the district is assigned a randomly sampled value from the appropriate hourly distribution. See *Volume I* for details on using this option. Note that this option can only be used when the APEX timestep is equal to 1 hour (the APEX default).

The air quality districts are read in from the input file in **SpaceTimeModule:ReadSiteLists**. The actual air quality is read from the *Air Quality Data* files in **SpaceTimeModule:ReadAirQuality.** If the *Air Quality Data* file uses hourly distributions for each district (an optional feature of APEX, see *Volume I*), then the air data for each simulated individual is sampled in **SpaceTimeModule: GenerateAirQuality.**

4.1.4   Meteorological Zones

Another spatial unit in APEX is the *meteorological zone*, which is the equivalent to air quality districts but for meteorological data. Most of the rules that apply to air quality districts also apply to meteorological zones. Each meteorological zone is associated with a central location (specified by latitude and longitude), a maximum representative radius given by *ZoneRadius*, a *Start Date*, and a *Stop Date*. The start and stop dates may differ for each meteorological zone, and must encompass the entire simulation period or else the meteorological zone is deleted. There can be no missing data between the start and stop dates of the simulation.

APEX calculates the distance from each sector location to each meteorological zone center, and assigns each sector to the nearest meteorological zone if within range (*ZoneRadius*), or deletes the sector otherwise.

The meteorological zone locations are read in from the *Meteorological Zone Location* input file in **SpaceTimeModule:ReadSiteLists**. The actual meteorological data is read from the *Meteorology Data* file in **SpaceTimeModule:ReadMeteorologyData.** When the data are read in, daily maximum and average temperatures are calculated for later use.

4.2   Determining the Final Study Area

4.2.1   Matching Sectors, Air Quality Districts, and Meteorological Zones

The APEX code for reading the locations of sectors, air quality districts, and meteorological zones, and for pairing the sectors to the nearest air quality districts and meteorological zones, is found in **SpaceTimeModule: SelectSites**.

The final study area consists of all the sectors within *CityRadius* of the study area central location, restricted to the listed counties or tracts (if provided), that have both an air quality district and a meteorological zone within range. If both tracts and counties are listed, then the resulting study area is the union of the two lists. Sectors for which a valid air quality district (one within *AirRadius*) or a valid meteorological zone (one within *ZoneRadius*) cannot be found are discarded from the final study area. The study area population is the total population in the input *Population* files that reside in these sectors.

The **SelectSites** subroutine makes use of the function **SpaceTimeModule: Distance** which calculates the distance between two points given their latitudes and longitudes. It is discussed below.

4.2.2 The Distance Algorithm

APEX uses a computational algorithm (implemented in **SpaceTimeModule:Distance**) to calculate the distances (e.g. study center to sector center, sector center to air quality district center) required to determine the final study area. The method is accurate, simple in terms of program code, and works well everywhere on the globe. It calculates the distance between two points based on their latitudes and longitudes. It is based on projecting the points onto a **sphere**, rather than onto a plane, using the following steps:

- The latitude and longitude of the two points (locations) in question are identified
- The two sets of angles, (θ_1, ϕ_1) and (θ_2, ϕ_2), subtended at the Earth's center by the radial vectors to the two points are calculated
- The net angle between these two radial vectors is found
- The Earth's radius at the average latitude of the two points is calculated
- The results from the previous 2 steps are multiplied to give the distance between the points, D

All angles are measured in radians. In step 1, the angles ϕ subtended by the radial vectors at the Earth's center are the same as the longitudes of the points in question. However, calculating the θ from latitude is more complicated since it is affected by the flattening of the poles. The intersection of the Earth's surface with a plane through the poles is an ellipse. Let the eccentricity of the ellipse be given by e. Latitude measures the angle between the polar axis and a locally horizontal surface such as sea level (a tangent surface to the Earth). For a point on an ellipse at an angle θ from the semimajor axis, the tangent line has slope s:

$$s = -(1 - e^2)\cot(\theta) \tag{4-1}$$

where the square of the eccentricity of the earth is $e^2 = 0.00672265$.

This slope is equal to the negative cotangent of the latitude. Hence

$$\theta = \tan^{-1}\left[(1 - e^2)\tan(lat)\right] \tag{4-2}$$

When applied to both points, this gives angles θ_1 and θ_2.

The radius of the Earth varies with latitude but not with longitude. At an angle theta relative to the semimajor axis, the distance from the center to a point on the ellipse is given by

$$R = A\sqrt{\frac{1-e^2}{1-e^2\cos^2(\theta)}} \qquad (4\text{-}3)$$

where A is the semimajor axis length, A = 6378.388 km. For purposes of the distance calculation, θ is set to the average of θ_1 and θ_2.

For two points at (θ_1, ϕ_1) and (θ_2, ϕ_2) on a sphere of radius R, the arc length of the great circle connecting them, the distance D, is given by the product of the radius and the net angle between them:

$$D = R\cos^{-1}\left[\cos(\theta_1)\cos(\theta_2)\cos(\phi_1-\phi_2) + \sin(\theta_1)\sin(\theta_2)\right] \qquad (4\text{-}4)$$

which follows from the formula for the dot product of the radial vectors, expressed in spherical coordinates.

All of the above formulas are exact. The only approximation being made is in claiming that the arc of the Earth's surface between the two points lies exactly on a sphere. In most practical cases, the error resulting from this approximation is in the range of one to ten parts per million.

4.3   Modeling Commuting

APEX models commuting by assigning a work sector to each employed modeled individual based on commuting data for the individual's home sector from the 2000 Census. Two files with commuting data are required for the model: nationwide files of (1) commuting flow data (the *Commuting Flow* file) and (2) commuting time data (the *Commuting Time* file). Both are supplied with APEX. The nationwide *Population Data* and both *Commuting* input files use census tracts as the sectors. The *Population Data* files contain year 2000 tract-level U.S. Census counts, tract locations, and national employment probabilities by age. The *Commuting Flow* file contain adult commuting patterns based on the 2000 Census. The *Commuting Time* file contains adult commuting times for each tract based on the 2000 Census. As part of step 2 (Figure 2-1), APEX can extract the flows for the selected home sectors from the *Commuting Flow* file and derive profile level commuting times from the *Commuting Times* file. The development of the commuting files are described below.

4.3.1   Nationwide Commuting Flow Database for 2000

A national commuting database was generations from a set of US Census files listing the number of persons living in one tract and working in another. The original files, derived from the 2000 Census, are distributed by the US DOT Bureau of Transportation Statistics at their web site http://transtats.bts.gov/. The data used were collected as part of the Census Transportation Planing Package (CTPP). The files used are from CTPP Part 3-The Journey To Work files. They contain counts on individuals commuting from home to work locations at a number of geographic scales. Tract-to-tract data were used for the commuting databases.

One concern identified from these data was that some home-work pairs are very widely separated geographically. For example, some people live in Alabama but work in Alaska. This may be the case for either military personnel, or others who are stationed in remote workplaces for weeks or months at a time, but in APEX the need is for daily commuting flows and there is no way to determine from these data which workers commute on a daily basis. A preliminary analysis of the home-work counts showed that a graph of Log(flows) versus Log(distance) had a near-constant slope up to somewhere around 100 kilometers. Beyond 150 kilometers the slope is also fairly constant but flatter, meaning that flows were not as sensitive to distance. Between these two distances there is a smooth transition from one slope to the other. A simple interpretation of this result is that at distances below 100 km the vast majority of the flow was due to persons traveling back and forth daily, and the numbers of such persons decrease fairly rapidly with increasing distance. At large distances the majority of the flow are persons who stay at the workplace for extended times, in which case the separation distance is not as crucial in determining the size of the flow.

To apply the home-work data to commuting patterns in APEX, a simple rule was chosen. It was assumed that all persons in home-work flows up to 120 km are daily commuters, and no persons in more widely separated pairs commute daily. This meant that the list of destinations for each home tract can be restricted to only those work tracts that are within 120 km of the home. In practice, this cutoff has little impact in an APEX model run since persons who live and work more than 120 km apart are not likely to have both their home and work sectors inside the same study area.

The resulting database contained a total of 64,958 distinct home sectors, and 65,075 work sectors, based on data from 117,792,172 persons. The home-work tract pairs were sorted by the home tract ID, and for each home tract the possible destinations were listed, one per line. The flows were converted to fractions of the home tract total, and then expressed as cumulative fractions since this is the form that will be needed by APEX. The work sectors were sorted by decreasing fraction of the home tract total, and the information was written to an ASCII text file. Every record in this file contains three variables: a tract ID, a flow fraction, and a distance. A convention was used that the flow fraction and distance were set to -1.0 to indicate a home tract. The first three records on the nationwide ASCII file are as follows:

```
01001020100 -1.00000 -1.0
01001020700 0.10412  5.5
01101000100 0.20097  19.6
```

The first record contains the ID of the first home tract by sort order, followed by two placeholder values. The second record contains ID for the first destination tract for the current home tract. The destination tracts are sorted in order of decreasing commuting fraction. The number 0.10412 indicates that the largest percentage of commuters of the commuters who live in this home tract (around 10.4%) commute to tract 01001020700. The third number on each line is the separation distance in kilometers between the home and work tracts. The third record shows the second destination tract for this same home tract, followed by a cumulative fraction of 0.20097. This

means that about 9.7% of the workers in that home tract go to second work tract, despite the two being greater than 19 kilometers apart. Further examination of this file reveals that this particular home tract has 38 destination tracts to which workers commute. Note that fractions down to 0.00001 (one in one hundred thousand) are reported. Fractions that round to zero at this precision are deleted from the database.

The number of destinations per home tract is not constant. There are two ways to know when the last destination for a given home tract has been reached. First, the cumulative flow fraction for the last destination is always 1.00000. Second, the next record in the file has negative flow and distance indicators as placeholders, indicating that the record contains the ID of the next home tract. The mean number of associated work tracts per home tract is 79, with a minimum of 1 and a maximum (within 120 km) of 413. Overall, this file has over 5.2 million records and occupies 131 megabytes of disk space.

4.3.2   Census year 2000 Nationwide Commuting Time Database

As part of the 2000 Census, travel time to work was recorded via the long-form questionnaire of adults in ages 16 and older. This question was asked of all people who indicated that they worked at some point during the reference week. This travel time is an estimate of the usual amount of time in minutes it took for the respondent to get from home to work each day. This time includes not only time in motor vehicles, but also time spent waiting for public transportation, carpooling, walking to the bus, etc. These data are available online via the US Census data portal (http://dataferrett.census.gov/) and are found in Table P31, variables P031001-P031015.

The first column in the data file lists the census tract, followed by the total number of workers, the total number of non-home workers, and thirteen time bins. These bins are as follows: <5, 5-9, 10-14, 15-19, 20-24, 25-29, 30-34, 35-39, 40-44, 45-59, 60-89, 90-120, and 0 minutes (at-home workers). APEX processes the raw data into cumulative probability distributions for later use. These time bins are hard coded into APEX, and cannot be modified. At 4.3 megabytes, the file is not large; it contains one record for each census tract in the US (65443 tracts).

4.3.3   Implementation of Commuting in APEX

The APEX model only extracts the commuting data that pertains to the selected study area. For each sector in the study area (home sector) APEX reads in a list of possible work sectors, the cumulative probabilities associated with each, and the distances to each sector. The cumulative probabilities range from 0 to 1; the work sectors having higher probabilities are associated with a larger "range" of this interval. For each worker (each profile with Employed=YES), a uniform random number R from zero to one is generated. This random number is used to select a corresponding work sector (the one that is associated with smallest cumulative probability that is $\geq R$) for the profile. With the selection of the work sector, the distance to this work sector is also recorded.

When a profile's activity diary events are read from the *Diary Events* file, they are characterized as occurring in one of three places: "Work", "Home" or "Other" based on the CHAD location

and activity codes. For profiles who are commuters, all "Work" events will use the work sector's air quality data when calculating microenvironmental concentrations. "Home" events will use the home sector data; "Other" events will use an average of data from different sectors (either all sectors in the area or a random selection, based on the APEX input settings). See Section 8.2.1 for more information on home, work, and other locations.

It is likely that some profiles will commute to sectors outside of the final study area. The user may choose to include these profiles in the analysis or discard them by setting the *Simulation Control* file variable ***KeepLeavers***. If KeepLeavers=YES, the air quality data for the work sector is unknown. Therefore, it is assumed to be related to the average concentration over all of the study area air quality districts at the same point in time. Calling this average C_{avg}, the ambient concentration C for the person is:

$$C=LeaverMult*C_{avg}+LeaverAdd \tag{4-5}$$

where ***LeaverMult*** and ***LeaverAdd*** are also set in the *Simulation Control* file. If KeepLeavers = NO, then these individuals are not modeled.

Diaries are weighted by commuting time, so that people with long commute distances also have long commute durations. For each tract included in the simulation, APEX uses the list of all possible destinations to calculate a cumulative probability distribution of commuting distances. By comparing a person's home-work distance with the tract-specific probability distribution, the person's commute distance is ranked relative to all other possible destinations in the tract.

For weighting to occur, commuting time must be estimated for each individual. Tract-level commuting time is assigned based on the commuting distance cumulative distribution function: if a person is in the 75th percentile of commuting distance, that person is also in the 75th percentile of commuting time. The midpoint of the commuting distance bin is matched to a commuting time bin. This distance midpoint is linearly interpolated within the time bin to estimate the commute time.

For example, the commuting distance for an individual is 1.1 miles. If the 4th through 10th distance percentiles of people in the tract have a 1.1 mile commutes, then APEX will look at the commuting time bins for the same tract and find in which bin the midpoint, 7th percentile, lies. In this example, the 7th percentile lies in the 10 – 14 minute time bin. To select a time out of this range, APEX linearly scales within the bin. In our example, 10 and 14 minutes correspond to the 4th and 12th time percentiles. So the 7th percentile commuting time is 14 - 4 × (12-7) / (12-4) = 11 minutes.

Additionally, if modeling commuting, commuting time is a required input on the CHAD *Diary Questionnaire* file. By modifying the *Diary Questionnaire* file, users have the option to use any method of assigning commute time to diaries they wish. In the version of the *Diary Questionnaire* file included with APEX, we defined commuting time as the total time spent in travel locations or activities before and after work activity. Commuting time is calculated on all weekdays for all employed people in CHAD. Work activities are defined in CHAD by the activity codes 10000 – 10300 and 18100. Travel activities are defined by either the 18000 or 18200 activity codes, or the location codes 31000 – 32000. An exception was made to allow for people walking (activity code 17131) short (<10 minute) amounts of time between work and

travel activities. To match the Census bins, a cap of 120 minutes (240 minutes total for the day) was placed on the computed daily commute time.

Since commuting time both is a personal variable and a parameter on the Diary Questionnaire file, we are now able to weight diaries based on commuting time. Previous versions of APEX weighted on three categories: gender, employment, and age. Commuting time is the fourth category. However, weights are only applied for employed individuals on weekdays; diary selection for unemployed people is not affected by the change.

The user has the option to set two commuting time windows. All diaries within the first time window are weighted at 100%. Diaries within the second window, diaries outside both windows are weighted at a level determined by the user using keywords in the *Control File*. These variables may be modified to match the desired strength of the correlation to commuting time. For no correlation, all weights can be set to 1.0. These windows are in units of minutes (as opposed to a percentage of the target time) so that matching of diaries applies equally well for both low and high targets.

CHAPTER 5.   GENERATING SIMULATED INDIVIDUALS (PROFILES)

APEX stochastically generates a user-specified number of simulated persons to represent the population in the study area. Each simulated person is represented by a "personal profile." The personal profile (see step 2 in 2-1) is a set of parameters that describe the person being simulated. The simulated person has a specific age, a specific home sector, a specific work sector (or does not work), specific housing characteristics, specific physiological parameters, and so on.

The profile does not belong to any particular real person, instead it is a fictional or simulated person. A single profile does not have much meaning in isolation, but a collection of profiles represents a random sample drawn from the study area population. This means that statistical properties of the collection of profiles should reflect statistical properties of the real population in the study area.

APEX generates the simulated person or profile by probabilistically selecting values for a set of profile variables. The profile variables fall into five categories:

- Demographic variables, which are generated based on the census data;

- Residential variables, which are generated based on sets of user-defined distribution data;

- Physiological variables, which are generated based on age- and gender-specific distribution data; and

- Daily varying variables, which (in most cases) are based on distribution data that change daily during the simulation period.

- Modeling variables, which can have a variety of meanings, and are usually defined by the user. The individual profile variables are given in

- Table 5.1.

The profile variables do not depend on the results for any other profile, and in general do not depend on any results (diary selection, microenvironment concentrations, exposure, or dose) for the current profile. The exception is the person's physical activity index (PAI), which is calculated using the activity diary.

At present, APEX does not allow the user to select which variables are part of the personal profile. If such an enhancement were included, the user would be able to assign (say) a family size to each profile using input files rather than by reprogramming the source code.

The process by which APEX generates the personal profile is illustrated in Figure 5.1. The demographic and residential variables are set in **ProfileModule:GenerateProfiles,** the physiological variables are generated in **ProfileModule:GeneratePhysiology**, and the daily-varying variables are set in **ProfileModule:GenerateDailyVars**.

The following subsections describe the different categories of profile variables in more detail.

Table 5.1. Profile Variables in APEX

Variable Type	Profile Variable	Description
Demographic variables	Index	Internal APEX profile index
	Gender	Male/Female
	Race	White, Black, Native American, Asian, and Other
	Age	Age (years)
	Profile Group	A user generated profile factor that can vary by age, gender, and sector.
	Home sector	Sector in which a simulated person lives
	Work sector	Sector in which a simulated person works
	Home District	Air quality district assigned to home sector
	Work District	Air quality district assigned to work sector
	Meteorological zone	Meteorological zone assigned to home sector
	Employment Status	Indicates employment outside home
	Commuting Distance	Distance (km) from home to work
	Commuting Time	One-way home-work commuting time (min)
Residential variables	Gas stove	Indicates presence of gas stove
	Gas pilot	Indicates presence of gas pilot light
	Home air conditioning	Indicates type of home ventilation/air conditioning system
	Car air conditioner	Indicates presence of air conditioning in the simulated person's car
Physiological variables	Blood volume	Blood volume of a simulated person (ml)
	Body Mass	Mass of simulated person (kg)
	Body Mass Index	Body Mass Index (lbs/in^2)
	Weight	Body weight of a simulated person (lbs)
	Height	Height of a simulated person (in)
	Resting metabolic rate	Resting metabolic activity rate (kcal/min)
	Body surface area	Surface area of the body (m^2)
	Maximum permitted MET value	Maximum metabolic activity level (multiple of resting metabolic rate) that can obtained by the individual

Variable Type	Profile Variable	Description
		(dimensionless)
	Energy conversion factor	Oxygen uptake per unit of energy expended (liters/kcal)
	Lung CO diffusivity	Lung CO diffusivity parameter used in COHb calculation (ml/min/torr)
	Endogenous CO production rate #1	Endogenous (internally produced) CO production rate #1 (ml/min)
	Endogenous CO production rate #2	Endogenous CO production rate #2 (ml/min) used only for women between ages of 12 and 50 for half the menstrual cycle
	Hemoglobin altitude factor	Correction for blood hemoglobin density at high altitudes
	Recovery Time	Time to recover a maximum oxygen deficit (hours)
	Ventilation slope	Slope term for MET to ventilation conversion
	Ventilation intercept	Intercept term for MET to ventilation conversion
	Ventilation residual	Residual term for MET to ventilation conversion
	Hemoglobin density in the blood	Amount of hemoglobin in the blood (g/ml)
	Normalized maximum oxygen consumption	Maximum rate of oxygen consumption by the individual, normalized to body mass (ml of oxygen/min/kg)
	Starting day of menstrual cycle	The day during the first 28 days of the simulation period that menstruation begins; used for calculating endogenous CO
	Disease status	Whether or not the person has the disease. Probability is determined by the input *Prevalence* file.
	$\beta 1 - \beta 7$	Model parameters for the $\%\Delta FEV1$ ozone model
	Variance of U	Model parameter for the $\%\Delta FEV1$ ozone model, describes the variability in the effect on an individual
	$\%\Delta FEV1$ – age slope	The slope of the age - $\%\Delta FEV1$ relationship

Variable Type	Profile Variable	Description
	%ΔFEV1 – age y-intercept	The y-intercept of the age - %ΔFEV1 relationship
	Maximum oxygen deficit	Maximum oxygen deficit obtainable by profile (ml/kg)
Daily varying variables	Daily endogenous CO production rate	Daily endogenous CO production rate in the simulation period (ml/min)
	Diary number	Index for the selected diary for the day
	First event #	Index of the first event for the day in the composite activity diary
	Diary ID	CHAD (or other database) ID for the diary selected for the day
	Diary age	Age of the CHAD diary selected for the day
	Diary employment	Employment status of the CHAD diary selected for the day
	Last event #	Index of the last event for the day in the composite activity diary
	Residence window position	Daily residence window position (open or closed) during the simulation period
	Car window position	Daily car window position (open or closed) during the simulation period
	Daily average car speed category	Daily average car speed category during the simulation period
	Daily Conditional variable # 1	Generic user-defined daily conditional variable # 1
	Daily Conditional variable # 2	Generic user-defined daily conditional variable # 2
	Daily Conditional variable # 3	Generic user-defined daily conditional variable # 3
	PAI	Daily physical activity index (MET, dimensionless)
	Diary key statistic	Key diary statistic (such as outdoor time of vehicle time) for the day. Used for constructing longitudinal activity diary. Equal to 0 if not using longitudinal assembly.
Modeling Variables	Number of diaries	Number of different activity diaries used to construct the composite activity diary for the person.
	Profile Conditional Variable #1	Generic user-defined conditional variable # 1.
	Profile Conditional Variable #2	Generic user-defined conditional

Variable Type	Profile Variable	Description
		variable # 2.
	Profile Conditional Variable #3	Generic user-defined conditional variable # 3.
	Profile Conditional Variable #4	Generic user-defined conditional variable # 4.
	Profile Conditional Variable #5	Generic user-defined conditional variable # 5.
	Regional Conditional Variable #1	Regional user-defined conditional variable # 1.
	Regional Conditional Variable #2	Regional user-defined conditional variable # 2.
	Regional Conditional Variable #3	Regional user-defined conditional variable # 3.
	Regional Conditional Variable #4	Regional user-defined conditional variable # 4.
	Regional Conditional Variable #5	Regional user-defined conditional variable # 5.
	AQ Conditional Variable #1	User-defined conditional variable #1 that depends on AQ during event
	AQ Conditional Variable #2	User-defined conditional variable #2 that depends on AQ during event
	AQ Conditional Variable #3	User-defined conditional variable #3 that depends on AQ during event
	AQ Conditional Variable #4	User-defined conditional variable #4 that depends on AQ during event
	AQ Conditional Variable #5	User-defined conditional variable #5 that depends on AQ during event

```
        ┌─────────────────────────┐
        │  Select population type │
   ┌───▶│  (Race/Gender combination)│
   │    └─────────────────────────┘
   │                │
   │                ▼
   │    ┌─────────────────────────┐
   │    │    Select home sector   │
   │    └─────────────────────────┘
   │                │
   │                ▼
   │    ┌─────────────────────────┐
   │    │ Select age group within │
   │    │       home sector       │
   │    └─────────────────────────┘
   │                │
   │                ▼
   │    ┌─────────────────────────┐
   │    │ Assign age within age   │
 NO│    │         group           │
   │    └─────────────────────────┘
   │                │
   │                ▼
   │    ┌─────────────────────────┐
   └────│  Check if age within    │
        │  range set in Simulation│
        │     Control file        │
        └─────────────────────────┘
             YES │
                 ▼
```
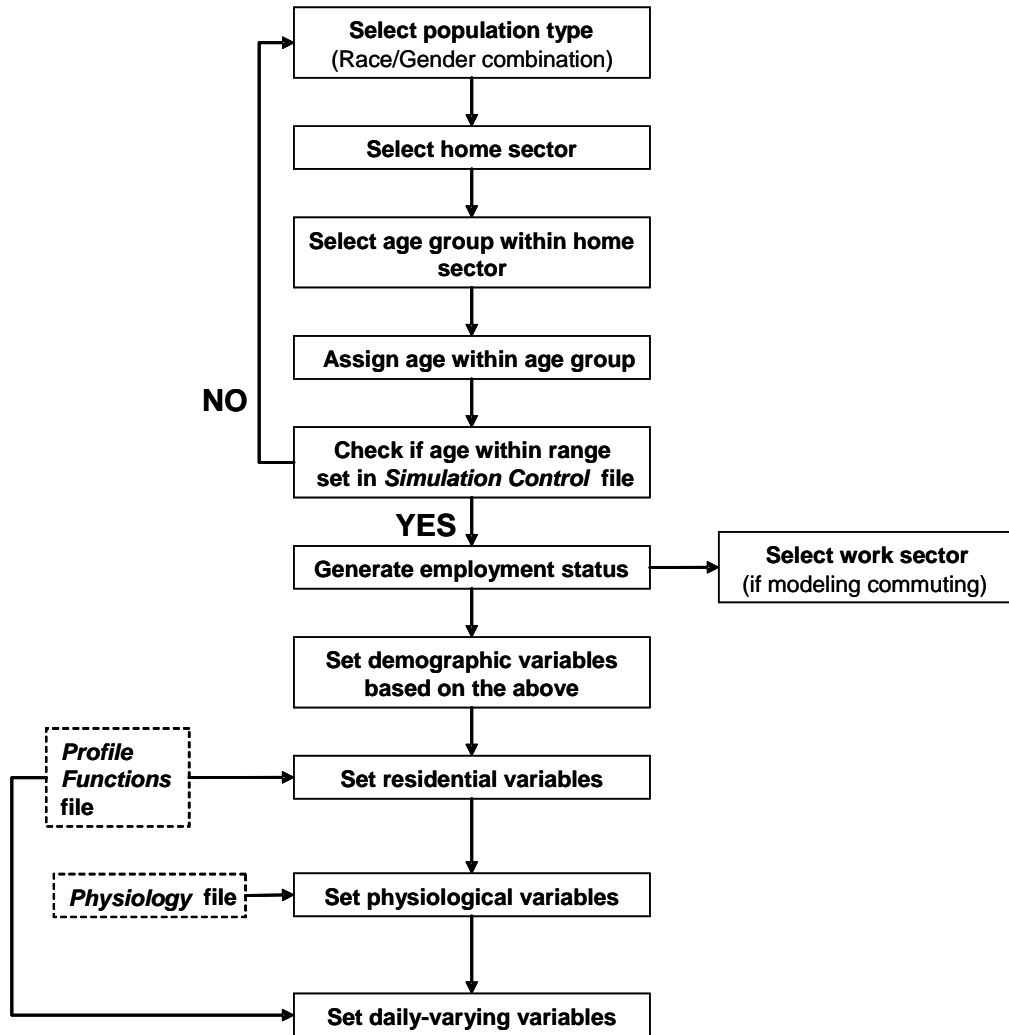
Figure 5.1. Generating a Simulated Profile

5.1 Demographic variables

The following are the profile variables of a demographic nature:

- **Age:** Age in years (integer)

- **Employed:** YES if employed outside home, NO otherwise

- **Gender:** Male or Female

- **Profile Factor Group:** A user defined group that can be flexibly defined to be any factor that varies by location, age and gender, and which may include occupation.

- **HomeD:** Number of air quality district assigned to home sector

- **HomeSec:** Number of home sector for this profile

45

- **Race:** White, Black, Native American, Asian, Other

- **WorkD:** Number of air quality district assigned to work sector

- **WorkSec:** Number of work sector (if any)

- **Index:** Sequential number indexing the set of profiles

- **Zone:** Number of meteorological zone for home sector

- **CommDist**: The distance from the home to the work tract

- **CommTime**: The time it takes the person to commute between home and work.

The values of demographic variables (gender, age, etc.) for a simulated profile are selected probabilistically according to the following steps (see Figure 5.1):

- The fractions of people in each of the gender/race combinations ("population types") in the final study area are calculated and then used as probabilities to randomly select a gender/race type for a simulated individual.

- The fractions of the selected population type in each sector within a study area are found and then used as probabilities to randomly select a home sector for the simulated person.

- The fractions of people in each age group in the selected population type in the selected sector are calculated and then used as probabilities to randomly select an age group for the simulated person.

- A specific age within the selected age group is randomly selected, assuming a uniform distribution.

- The employment probability for the selected age group (for the home sector) is used to randomly determine whether a simulated person will work.

- Is the user specifies a profile factor, the profile factor probability for the selected age group will be used to randomly determine the group of the individual.

- If the commuting option is used and a simulated person works, use the fractions of people commuting to each of the work sectors for the selected home sector to randomly select a work sector that a simulated person will commute to. If the commuting option is not used, assume a person who works does so in their home sector.

- When the commuting option is used, along with the commuting distance (the distance from the home to work tract) APEX estimates the commuting time. The commuting time is based on the length of the individual's commute compared to all commuters in their home tract. Longer commute lengths lead to longer commute durations.

5.2 Residential Variables

The residential variables are set after the demographic variables described above. The residential variables are categorical variables that are used to indicate whether a residence or a car associated with a simulated person has a specified appliance or component that may affect

exposure. The rules for assigning these four variables are specified by the user in the *Profile Functions (Distributions)* input file (see *Volume I*). The residential variables are:

- **AC_Home:** An integer indicating the type of home ventilation systems (e.g., central air, attic fan, window unit, no A/C).

- **AC_Car:** YES if has air conditioning in car, NO otherwise

- **HasGasStove:** YES if has gas stove in home, NO otherwise

- **HasGasPilot:** YES if has gas pilot for gas stove in home, NO otherwise

APEX randomly determines the result for the variable based on the probabilities specified in the input files. For example, suppose a user specifies probabilities of 0.3 for not having a car conditioner (AC_Car= NO) and 0.7 for having a car air conditioner (AC_Car=YES). APEX randomly generates a value in the range of 0 to 1, assuming a uniform distribution. If this value is larger than 0.3, the simulated person will own an air conditioner, otherwise not.

These variables may be used as conditional variables for calculating concentrations in microenvironments (see Chapter 8).

5.3 Physiological Profile Variables

The physiological variables are used for estimating ventilation, calculating dose (as described in Chapters 7 and 10) and classifying profiles in reporting results. This section covers the calculation of these variables. The profile variables relating to physiology are as follows:

- **Blood:** Volume of blood (milliliters)

- **BM:** Body mass (kilograms)

- **BSA:** Body surface area (m^2)

- **Diff:** Lung CO diffusivity(ml/min/torr)

- **ECF:** Energy conversion factor (liters of oxygen per kcal)

- **Endgn1:** Endogenous CO production rate #1 (ml/min)

- **Endgn2:** Endogenous CO production rate #2 (ml/min)

- **Height:** Body height (inches)

- **Hemfac:** Hemoglobin altitude adjustment

- **Hmglb:** Hemoglobin density (grams per milliliter of blood)

- **METmax:** Maximum obtainable MET value (unitless)

- **MOXD:** Maximum obtainable oxygen debt (ml/kg body mass)

- **NVO2max:** Maximum normalized oxygen consumption (milliliter of oxygen per minute per unit body mass)

- **PAI:** Median daily physical activity index (MET, dimensionless)

- **RMR:** Resting metabolic rate (kcal/min)

- **RecTime:** Oxygen debt recovery time (hours)

- **Start:** Starting day (phase) for menstrual cycle (if applicable)

- **VeSlope:** Slope for MET to ventilation rate conversion

- **VeInter :** Intercept for MET to ventilation rate conversion

- **VeResid :** Residual for MET to ventilation rate conversion

- **Weight:** Body weight (pounds)

- **Ill:** Flag indicating whether or not a person has the disease that is modeled in the *Prevalence* input file.

- **BMI:** Body Mass Index (lbs/in^2)

- **B1 – B7:** Model parameters used in the calculation of %ΔFEV1

- **FEVU:** A variance term describing an individual's responsiveness to ozone (used for %ΔFEV1)

- **FEVE1 & FEVE2:** Terms that describe error involved in %ΔFEV1 measurements

- **FEVSLP:** The slope of the linear regression relating %ΔFEV1 and age

- **FEVINT:** The y-intercept of the linear regression relating %ΔFEV1 and age

The physiological profile variables do not affect the exposure calculations for individuals in any way, as none of them affect either the selection of diaries or the concentrations in the various microenvironments. However, the physiology of a profile affects the ventilation calculations and thus influences (1) the calculation of dose (see Chapter 10) and (2) the calculation of exertion level, which is used to group exposure results in the output *Tables* file (see *Volume I*).

The physiological variables are calculated from input data. The *Physiology* input file contains distributions that are used to set the physiological profile variables and parameters for each simulated person. Specifically, the physiology file contains distributions for the following variables and parameters for each age and gender cohort (see *Volume I* for more information):

- **NVO2max:** normal distributions for NVO2max in ml O_2/min/kg (Isaacs and Smith, 2005)

- **BM** lognormal distributions for BM in kg (Isaacs and Smith, 2005)

- **RMRSLP, RMRINT,** and **RMRERR:** Point distributions for regression coefficients for RMR (slope, intercept, and error) as a function of BM in MJ/Day (Johnson et al., 2000, adapted from Schofield, 1985)

- **BLDF1** and **BLDF2:** Point distributions for blood volume factors for calculation of volume (ml) from height and weight (Johnson et al., 2002)

- **HMG**: Normal distributions for blood hemoglobin density (g/lm of blood) (Johnson et al., 2002)

- *HTSLP, HTINT,* and *HTERR*: Point distributions for regression coefficients for height in inches (slope, intercept, and error) as a function of age (children 0-17) or body mass (adults) (Johnson et al., 2000)

- *BSAEXP1* and *BSAEXP2*: Point distributions for exponential parameters for calculating body surface area (m^2) as a function of body mass (Burmaster, 1998)

- *MOXD*: Normal distributions for maximum obtainable oxygen debt in ml per kg body weight (Isaacs et al., 2007). MOXD is used in the adjustment of MET values; see section 7.2.

- *ECF*: Uniform distributions for the energy conversion factor for the person. Liters of oxygen per kcal. (Johnson et al., 2000, adapted from Esmail et al., 1995)

- *RecTime*: Uniform distributions for the time required to recover a maximum oxygen deficit (hours). (Isaacs et al., 2007) RecTime is used in the adjustment of MET values; see section 7.2.

- *Endgn1* and *Endgn2*: Point distributions for endogenous CO production rates in ml/min. (**ENDGN2** is used for women in 2nd half of menstrual cycle).

- $\beta 1 - \beta 7$, **FEVU, FEVE1, FEVE2:** Distributions for model parameters used by the %ΔFEV1 ozone calculations.

- *FEVSLP* and *FEVINT*: Point estimates describing the linear regression relationship between %ΔFEV1 and age.

The *Ventilation* input file contains data for a set of regression parameters used by APEX to estimate the ventilation-related profile variables VeSlope, VeInter, and VeResid. See *Volume I* for an example of the *Ventilation* file; see Graham and McCurdy (2005) for the derivation of these parameters. The file contains the following parameters for 5 age groups:

- *VEB0* and *VEB0SE*: Mean and standard error for regression parameter b0

- *VEB1* and *VEB1SE*: Mean and standard error for regression parameter b1

- *VEB2* and *VEB2SE*: Mean and standard error for regression parameter b2

- *VEB3* and *VEB3SE*: Mean and standard error for regression parameter b3

- *VEEB*: Interpersonal variance

- *VEEW*: Intrapersonal variance

Note: the standard error terms defined in the *Ventilation* file are not currently used by APEX, but could be used for future uncertainty analyses.

Once the above parameters are read/set by APEX, the physiological profile variables are formulated as follows in **ProfileModule:GeneratePhysiology** using the appropriate parameter values for the profile age and gender. First, *NVO2max, BM, RMR, HMG, BLDF1, BLDF2, HTSLP, HTINT, HTERR, MOXD, ECF, RecTime , BSAEXP1, BSAEXP2, Endgn1, Endgn2, β1-β7, FEVU, FEVSLP,* and *FEVINT* are sampled from the appropriate input distribution (using the APEX sampling methods, Section 3.2) for the profile's age and gender. Then the other profiles variables are calculated as follows:

$$Weight = 2.2046\,(BM) \tag{5-1}$$

where weight is given in pounds (lbs.). BMI in pounds per inches is calculated as:

$$BMI(lbs\;in^{-2}) = \frac{703\;Weight\;(lbs)}{Height^2\;(in^2)} \tag{5-2}$$

Body surface area (in m^2) (Burmaster, 1998) is calculated as

$$BSA = e^{BSAEXP1}\,BM^{BSAEXP2} \tag{5-3}$$

Resting metabolic rate (Johnson et al., 2000) is given in units of kcal/min by

$$RMR = 0.166[(RMRSLP)(BM) + RMRINT + RMRERR] \tag{5-4}$$

where 0.166 is the conversion factor for converting MJ/day to kcal/min.

The maximum MET value an individual can obtain is given by their personal maximum energy expenditure divided by their RMR. Personal maximum energy expenditure is simply maximum oxygen consumption converted to kcals via ECF, and thus METmax can expressed as:

$$METmax = \frac{(0.001)(BM)(NVO2max)}{ECF * RMR} \tag{5-5}$$

where 0.001 is the conversion factor for ml to liters O$_2$ such that METmax is a unitless number. The lower bound for METmax is 5, and the higher bound is 20; values outside of this range are set to the corresponding bound.

For children under the age of 18, height (in inches) is a function of age (in years):

$$Height = HTINT + age * HTSLP + HTERR \quad \text{(children under 18)} \tag{5-6}$$

for adults, height (in inches) is a function of body weight (in pounds):

$$Height = HTINT + ln(weight) * HTSLP + HTERR \quad \text{(adults 18 and older)} \tag{5-7}$$

Alion staff fit these equations for height, and derived the accompanying coefficients.

Several physiological variables are calculated differently for males and females, including lung CO diffusivity in ml/min/torr (Johnson et al., 2000). This variable is only used in the APEX CO dose algorithm.

$$Diff = 0.361(Height) - 0.232(Age) + 16.3 \qquad \text{(males)} \tag{5-8}$$

$$Diff = 0.556(Height) - 0.115(Age) - 5.97 \qquad \text{(females)} \tag{5-9}$$

where height is in inches and age in years. Blood volume in milliliters (Johnson et al., 2000) is calculated as:

$$Blood = BLDF1(Weight) + BLDF2(Height)^3 - 30 \tag{5-10}$$

where weight is in pounds and height in inches. For males, VeInter is calculated as

$$VeInter = Intterm - [VEB3] \qquad \text{(males)} \tag{5-11}$$

and for females

$$VeInter = Intterm + [VEB3] \qquad \text{(females)} \tag{5-12}$$

where

$$Intterm = VEB0 + Z(VEEB) + [VEB2][ln(1 + Age)] \tag{5-13}$$

where Z is a number drawn from a normal distribution ranging from -4 and 4.

For both genders

$$VeSlope = VEB1 \tag{5-14}$$

$$VeResid = VEEW \tag{5-15}$$

The variables VeSlope, VeInter, and VeResid are used in the APEX ventilation algorithm (see Chapter 7 and Graham and McCurdy, 2005).

5.4 Daily-Varying Variables

The daily varying variables are generated for each day in the model simulation for each profile in **ProfileModule:GenerateDailyVars**. There are eight daily-varying profile variables:

- *DailyConditional1* User-defined daily conditional variable #1
- *DailyConditional2* User-defined daily conditional variable #2
- *DailyConditional3* User-defined daily conditional variable #3
- *Endgn* Endogenous CO production rate on given day (ml/min)
- *PAI* Daily physical activity index (MET, dimensionless)
- *SpeedCat* Category for average vehicle speed on given day
- *WindowRes* Residence window status (open or closed) for given day
- *WindowCar* Car window status (open or closed) for given day
- *DiaryID* ID of the activity diary selected for the day (as it appears in the *Diary Questionnaire* and *Diary Events* files).
- *DiaryEmp*. Employment status of the activity diary selected for the day.
- *DiaryAge*. Age of the activity diary selected for the day.

- ***Stat.*** Value of the key diary statistic for the activity diary selected for the day.

The rules for defining WindowRes, WindowCar, SpeedCat, DailyConditional1, DailyConditional2, and DailyConditional3 are provided by the user in the *Profile Functions (Distributions)* input file. These variables may be used as conditional variables for use in calculating the concentrations in microenvironments. The *Profile Functions* file and conditional variables are covered in detail in *Volume I*. Conditional variables are also explained further in the Microenvironments chapter (Chapter 8) of this Volume.

The variable Endgn is used in the evaluation of the blood COHb level. Even though it is stored in an array of daily values, for males it always has the same value from day to day, that is, it is always set to the physiological profile variable Endgn1. For females it may have one of two values (the physiological profile variables Endgn1 and Endgn2) depending on the phase of the menstrual cycle.

The variable PAI is calculated as the time-averaged MET value for the entire simulation day. As it depends on the daily activity diaries, it is not set in the profile module, but rather later, in the ventilation subroutine **ExposureDoseModule:Ventilation**.

The variables DiaryID, DiaryAge, and DiaryEmp are mainly for QA of the diary selection and diary assembly methods. The variable Stat contains the value for the key diary variable, which is used to construct the longitudinal diary, and thus is usually a variable important to exposure (such as time spent outdoors or time spent in vehicles). See Section 6.3. These variables are all set in **DiaryModule:CompositeDiary**.

5.5 Modeling Variables

The remaining profile variables are general modeling variables. They are:

- ***Number of diaries***. Number of different activity diaries used to construct the composite activity diary for the person.

- ***Profile Conditional Variable #1-5.*** Generic user-defined profile conditional variables. Can be defined by the user model any property of the simulated person (for example, behavior or residential properties) that may affect microenvironmental parameters.

- ***Regional Conditional Variable #1-5***. Regional user-defined conditional variables. Can be defined by the user model any property of the simulated person (for example, behavior or residential properties) that vary by county or sector.

- ***Air Quality Variable #1-5***. User-defined conditional variables that depend on the ambient air quality during the event, and are recalculated with each timestep.

The number of diaries is a convenience variable that is set during the diary assembly process, in **DiaryModule:CompositeDiary**. It depends on the number of appropriate diaries available in

CHAD for the person, the diary pools, and other factors. It gives the modeler an idea of the heterogeneity in the diary selection for the person.

The profile and regional conditional variables are defined by the user in the *Profile Functions* file (see *Volume I*). They are set in ***ProfileModule:GenerateProfiles.***

CHAPTER 6.   Constructing a Sequence of Diary Events

APEX probabilistically creates a composite diary for each of the simulated persons by selecting a 24-hour diary record—or diary day—from an activity database for each day of the simulation period. The Consolidated Human Activity Database (CHAD) has been supplied with APEX for this purpose. A composite diary is a sequence of events that simulate the movement of a modeled person through geographical locations and microenvironments during the simulation period.   Each event is defined by geographic location, start time, duration, microenvironment visited, and activity performed. Events crossing a time step boundary will be separated into two distinct events.

The APEX model generates sets of exposure time series, one for each simulated individual, and both mean exposures over time and variation in exposures are important. The ability to realistically reproduce these exposure metrics depends on the method used to construct the composite activity diaries for the simulated population. APEX provides three methods of assembling composite diaries. The first (basic) method, which is adequate for estimating mean exposures, simply involves randomly selecting an appropriate activity diary for the simulated individual from the available diary pool. The second method is a more complex algorithm for assembling longitudinal diaries that realistically simulates day-to-day (within-person) and between-person variation in activity patterns (and thus exposures). The third method uses a Markov-chain clustering algorithm to recreate realistic patterns of day-to-day variability. All methods are covered in this chapter.

As all methods of composite diary assembly require the creation of diary pools, their construction is covered first.

6.1   Constructing the Diary Pool

6.1.1   Diary Data

The composite diary is created by concatenating individual one-day activity diaries from the CHAD database. APEX currently provides this database as two files: a file containing personal information of the studied individual, and one containing the actual diary events (see *Volume I* for more information). The *Diary Questionnaire (DiaryQuest)* file contains the following variables, in this order, as comma-separated values:

- CHAD ID
- Day of the week (e.g., Monday)
- Gender (M/F)
- Race
- Status of employment (Y/N)
- Age (years)
- Maximum hourly temperature on day of study (°F)

- Average temperature on day of study (°F)

- Occupation

- Count of missing time in minutes (when activity and/or location codes are missing from the activity file)

- Number of events

- Commuting time (in minutes; only required for simulations modeling commuting)

The *Diary Events* file contains the following variables as comma-separated values:

- CHAD ID

- Start time (of the event)

- Duration (minutes)

- Activity code

- Location code

See *Volume I* for a description of the CHAD activity and location codes. The events file contains a record for each of the events indicated by the number of events in the diary questionnaire file. Note that while CHAD data are provided with APEX, other activity data could be used instead, as long as the input file formats are followed and the CHAD coding conventions are used.

Diary Occupation is an optional file in which users can specify new occupations for each individual. These occupations overwrite those found in the *Diary Questionnaire* file. This file consists of two columns, CHAD ID and a string containing the occupation of the individual. This file may be useful for matching via occupation group.

The APEX diary input files are read by **DiaryModule:ReadDiaries**.

6.1.2   Grouping the Available Diaries into the Diary Pools

A diary pool is a group of CHAD diaries, appropriate for a given simulation day, from which a daily diary may be drawn. The criteria for creation of the Diary Pools are defined using the DiaryPool variable in the *Profile Functions (Distributions)* input file (see *Volume I*). Briefly, the user can define different pools for different combinations of ranges of maximum temperature, average temperature, and day of the week. Thus, the definition of a diary pool for a single (hypothetical) simulated day may be something like "all CHAD activity diaries for a weekend day for which the maximum temperature was between 70 and 80 degrees, and the average temperature was between 50 and 80 degrees." The idea behind this logic is that temperature and day of the week affect the type of activities people perform, and thus it is important to match these real properties of the activity diaries to corresponding simulated days. It should be noted that in APEX, CHAD diaries that are missing temperature data are thrown out (ie. not assigned to any diary pool.)

The number of diary pools that are defined affects the number of diaries that available for selection on a given day. Therefore, it is important not to define the pools too narrowly, as it could result in the same activity diaries being selected over and over again, or could result in pools with no diaries in which case APEX will fail with a fatal error.

The diary pools are created in **DiaryModule:ReadDiaries**.

6.2 Basic (Random) Composite Diary Construction

Basic (random) composite diary construction is implemented in **DiaryModule:CompositeDiary**. In basic composite diary construction, APEX develops a composite diary for each of the simulated individuals (profiles) in the following manner:

Once the diary pools have been created (based on temperature and day of the week as described above), a selection probability for each diary within the pool is calculated based on age/gender/employment similarity of the simulated person to the "real" diaries. If desired, the user can use the Profile Factor Groups to match diaries by occupation as well. The probabilities are calculated in **DiaryModule:DiaryProbabilities**. The selection probability is a product of several probabilities between 0 and 1, one each for age, gender, and employment (and occupation, if selected). The gender and employment probabilities are straightforward: if the gender or the employment status of the diary matches that of the profile, then the probability for these factors is set to 1. If they do not match, the probability is set to 0. The exception is for the employment probability for children under 16. Since APEX does not model employment status for children under sixteen (the employment profile variable will always be 0), then the employment probability is always set to 1 for this age group. This prevents APEX from discarding the CHAD activity diaries for children under age 16 that had an employment status=YES. Matching by occupation is similar to matching via employment and gender. However, any occupation listed on a diary that is not listed as one of the input occupation groups is automatically set to missing (*X*).

The age selection probability is a bit more complicated. APEX provides the user with the option of using activity diaries that have an age close to that of the simulated profile, although it may not match exactly. This range is controlled by the *Simulation Control* file setting *AgeCut2Pct* (see *Volume I*). Ages in this range will be given a probability of 1. In addition, APEX allows for the use of "shoulder ages," which are the age ranges (of width *AgeCutPct*) above and below the main age window. These ages are given reduced probability equal to the value of the *Simulation Control* file setting the variable *Age2Prob*.

If the employment status, occupation, gender, or age for an activity diary is missing, then the selection probability for that variable is determined directly from the *Simulation Control* file variables *MissEmpl*, *MissOcc*, *MissGender*, and *MissAge*, respectively.

The final selection probability for each diary is the product of the age, gender, employment, and occupation selection probabilities. Then, on each day of the simulation period, APEX randomly selects a diary day from the appropriate diary pool, based on selection probability value.

6.3   D&A Longitudinal Activity Diary Assembly

The second method of multi-day diary construction in APEX, which is required for characterizing within-person and between-person exposure variability, is a longitudinal diary assembly algorithm that constructs multi-day diaries based on reproducing realistic variation in a user-selected key diary variable. The variable may reflect any diary property, and is provided to APEX in the *Diary Statistics* input file. It is assumed that the key variable has a dominant influence on exposure. The APEX release provides *Diary Statistics* files for outdoor time and vehicle time, which were constructed by summing the total time associated with "outdoor" and "vehicle" CHAD location codes for each diary (see *Volume I*). For some scenarios, the key variable might be travel time or time performing a particular activity. The key variable could also be a composite formed from several different variables, for example, a weighted average of diary variables. The necessary condition for implementing the method is that every single-day diary be assigned a numeric value for this key variable. This allows the set of available diaries in every diary pool to be ranked in terms of this key variable, from lowest to highest. The method uses this key variable to preferentially select appropriate diaries from the available pool on the different days in order to produce a final longitudinal activity diary that has specific statistical properties. The method is primarily contained within **DiaryModule:DiaryRanks**, which is called from **DiaryModule:DiaryProbabilities**.

The longitudinal diary construction method targets two statistics, D and A. The D statistic reflects the relative importance of within-person variance and between-person variance in the key variable. The A statistic quantifies the lag-one (day-to-day) variable autocorrelation, which characterizes the similarity in diaries from day to day. Desired D and A values for the key variable are selected by the user and set in the *Simulation Control* file, and the algorithm constructs a longitudinal diary that preserves these parameters. See Section 6.3.2 for guidance on selecting appropriate D and A values for a particular simulation.

6.3.1   The D&A Longitudinal Diary Assembly Algorithm

The longitudinal diary selection method is based on the scaled rank, or "x-score" for the key variable for each diary. The x-scores are calculated within diary pools. First, a pool is sorted from lowest to highest on the key variable and given a corresponding rank, R. If there are K diaries in a pool, and each diary has equal statistical weight then the x-score for the diary at rank R is

$$x = \frac{\left(R - \frac{1}{2}\right)}{K} \qquad (6\text{-}1)$$

If the diaries have unequal statistical weight, then the x-scores will not be evenly spaced from 0 to 1 (as some diaries will correspond to a greater "interval" on the 0 to 1 scale). In APEX, eq. 6-1 is not used, but rather the x-scores are assigned to each diary by sorting the diary pool on the key statistic, and then applying the age, gender, and employment probabilities as described in Section 5.2. The diaries are then assigned to days in the simulation based on their x-scores by the algorithm described below.

An overview of the longitudinal diary method is shown in Figure 6.1. For each simulated person, the following steps are performed:

1. An individual target x-score T_i is selected from a beta distribution (β_1) that depends on the value of D.

2. For each day in the simulation, a daily scaled x-score (scaled rank) is generated. It is picked from a different beta distribution (β_2) having a peak near T_i.

3. An individual target correlation A_i is sampled from a beta distribution (β_3) having a peak near the population autocorrelation A.

4. The independently sampled daily x-score values are re-ordered to induce the target autocorrelation A_i.

5. Diaries are assigned from the diary pool according to the final time-series of daily x-score values.
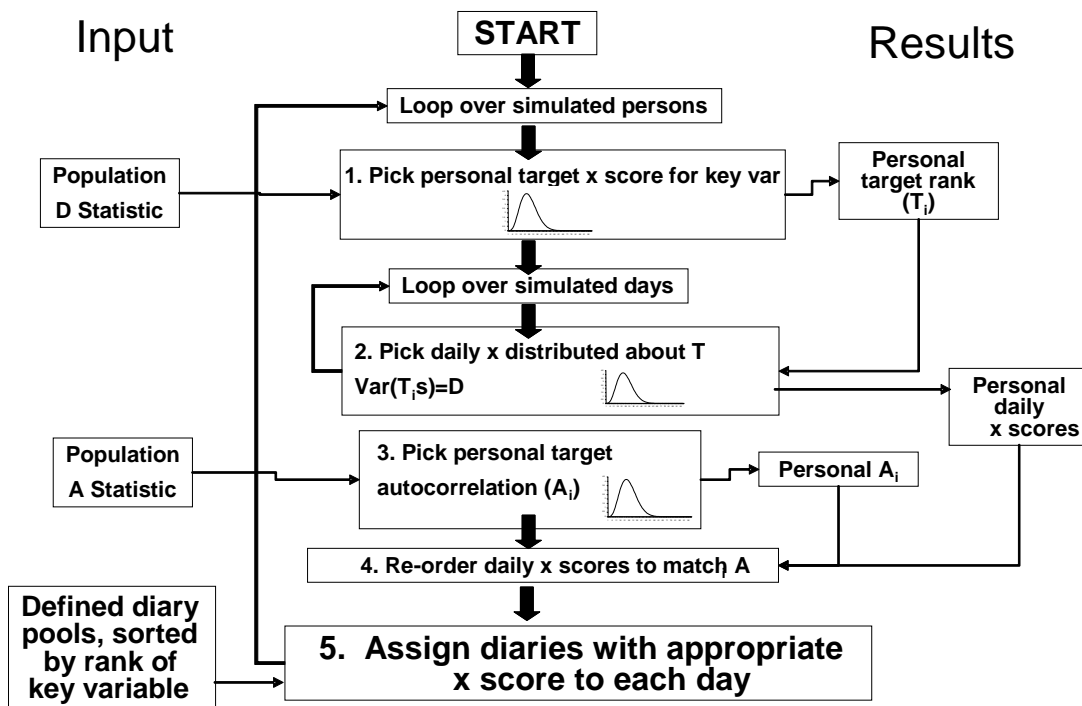
Figure 6.1. Overview of the Longitudinal Diary Assembly Algorithm

All of the random number generation in the new method involves drawing numbers from Beta distributions, with bounds of min=0, max=1. All of the random number distributions are bounded both above and below, which is a natural property of the Beta distribution. Given these fixed end points, the Beta distribution has two shape parameters which allow a great variety of forms. Both shape parameters (for all the distributions) are positive. The means and shape parameters for each of the Beta distributions were formulated to 1) properly reproduce D for the population, while 2) producing unbiased x-scores across the population. The resulting equations

for the parameters are given below. See Glen et al. (2007) for the derivation of these equations. Each of the above steps of the algorithm is described in detail below:

1. An individual target x-score T_i is selected from a uniform distribution that depends on the value of *D*. The distribution of T_i depends on the value of *D*, and is chosen from a uniform distribution described as:

$$T_i = Uniform((1 - \sqrt{D})/2, (1 + \sqrt{D})/2) \tag{6-4}$$

2. For each day in the simulation, a daily x-score is generated. To generate daily scores, a beta distribution (β_2) dependent on *D* with a peak near the target value T_i is constructed. Since each individual has a personal value of T_i, each will have a unique β_2. As *D* approaches zero, β_2 flattens into a uniform distribution. As *D* approaches one, β_2 narrows to a spike at T_i. One x value is selected randomly from the PDF for each day in the simulation, plus a few extra (15 extra is sufficient for a one-year simulation). Since the β_2 for two individuals differ, the between-person variance does not go to zero as the number of draws becomes large. The shape parameters a and b for β_2 are a function of T_i and *D*:

$$a = \frac{2T_i}{(1-D)} \tag{6-5}$$

$$b = \frac{2(1-T_i)}{(1-D)} \tag{6-6}$$

Thus for each day in the simulation, an x-score is generated as

$$x = \beta_2 = \beta(a,b) \tag{6-7}$$

3. An individual target correlation A_i is sampled from a different beta distribution (β_3) having a peak near the population autocorrelation *A*. The width of this distribution is w_2:

$$w_2 = min(2 - 2|A|, 1) \tag{6-8}$$

The personal target for *A*, A_i, is then generated as:

$$A_i = A + w_2 (\beta(2.625, 2.625) - 0.5) \tag{6-9}$$

4. The independently sampled daily x-scores are re-ordered to induce the target autocorrelation A_i. This is done with a single pass, from first simulation day to the last. The reordering process involves selecting each x-score in the time series from another beta distribution (β_4) that is a function of both the individual autocorrelation target A_i and the previous x-score. The "extra" diaries come into play here; they allow the avoidance of undesirable forced selections. The shape parameters c and d for β_4 for day j are:

$$c = s\left(\frac{1-A_i}{2} + A_i x_{j-1}\right) \tag{6-10}$$

$$d = s\left(\frac{1+A_i}{2} - A_i x_{j-1}\right)$$ (6-11)

where

$$s = \frac{2}{(1-A_i^2)}$$ (6-12)

and x_{j-1} is the previous day's x-score. The x-score for the first day is picked at random from a uniform distribution ranging from 0 to 1. Then, for day j, the x-score is selected as:

$$x_j = \beta(c,d)$$ (6-13)

The APEX code for performing this process keeps track of which x-scores are picked. If the same score is selected more than once, then the algorithm finds the closest unused score. The process laid out by equations 6-10 through 6-13 continues until x-scores for all simulation days are selected.

On very short time series (less than 30 days), the autocorrelation step has a slight effect on the resulting **D** for the population (a few percent increase).

5. Assign the selected x-score (scaled rank) values to each day in the simulation, and assign corresponding diaries from the diary pool. The result of steps 1-4 is a time series of x-score values mapped to simulation days, for example,

Jan 1   Jan 2   Jan 3

0.148   0.372   0.324

The diary pool has already been defined by APEX (typically by factors including age, gender, employment, day type, and season, and perhaps others, see Section 6.1). The pool is then sorted into rank order from lowest to highest score for the key variable, and sort order is mapped onto a corresponding x-score. The x-score reflects the behavior of an individual relative to their peer group (for example, a person with score 0.75 is above 75% of the people in the same cohort and pool, in terms of the key variable). Scores can be moved across diary pools, whereas absolute values for the key variable might not. Thus, there might be a diary with six hours of outdoor time in the Sunday pool, but no such diary in the Monday pool. But a score of 0.75 exists on all days. The use of scores also helps in ensuring that all the available diaries are collectively sampled with the correct frequency. Note that the use of scores does not destroy information. All that matters in terms of diary assembly is the ability to specify which diary should be used on a given simulation day. For this purpose, requesting the available diary nearest to score 0.38 is no different than requesting the available diary nearest to (for example) 73 minutes of outdoor time.

APEX assigns the diary whose x-score is closest to the daily x-score value to the day. No distinction is made or needed between day types, seasons, etc., because that is already taken into account. Note that any diary matching criteria such as day type, season, temperature, rainfall,

workday, holiday, etc., affect the list of diaries that belong to the pool for a given day, but have no effect on the x-scores.

6.3.2   Selecting Appropriate D and A Values For a Simulated Population

The statistic D for a population of individuals is given by

$$D = \sigma_b^2 / (\sigma_b^2 + \sigma_w^2) \qquad (6\text{-}14)$$

where σ_b^2 and σ_w^2 are the between- and within- person variances in the key variable. Note that σ_b^2 is the variance between persons in their long-term (not daily) means for the key variable. Since both variances are non-negative, it is clear that D is in the interval [0,1]. $D=0$ means that σ_b^2 is zero, or that each person has the same mean score. A small D means that σ_b^2 is substantially smaller than σ_w^2, indicating that the overall variability between people in the key diary statistic is smaller than the variability observed over days within the same person. A D near one means that σ_b^2 is much larger than σ_w^2, or that each person shows little variation over time relative to the variability between persons.

The lag-one autocorrelation A is simpler to calculate than D, because each time series can be examined independently. The first step is to determine the x-score for each day, relative to the entire time series. If there are J days in the time series, and a given day is at rank R in terms of the rank for the key variable among the J days, then the x-score for that day is (R-1/2) / J. The overall mean and variance in these scores for the time series is then calculated. Due to the properties of the discrete uniform distribution of the scores (neglecting tied scores), the mean must be 1/2 and the variance is

$$\sigma^2 = \frac{1}{12}\left(1 - \frac{1}{J^2}\right) \qquad (6\text{-}15)$$

which is very close to 1/12 for large J. The lag-one covariance is calculated by

$$COV = \frac{1}{J}\sum\left(x(J) - \frac{1}{2}\right)\left(x(J+1) - \frac{1}{2}\right) \qquad (6\text{-}16)$$

where x(j) is the x-score on day j (see for example, Box et al., 1994). The lag-one autocorrelation for the individual time series is given by the ratio of the covariance to the variance:

$$A_i = \frac{COV}{\sigma^2} \qquad (6\text{-}17)$$

This calculation is repeated for each time series, and the statistic A is the mean of these individual autocorrelations. The statistic A has a range from -1 to +1, with positive values indicating that each day has a tendency to resemble the day before. Random selection of diaries from day to day produces A values near zero. Negative A values imply dissimilarity between consecutive days.

A study of children conducted in Southern California (Xue et al., 2004) provided about 60 days of data on each of 163 children. The time series are not continuous, as the monitoring consisted

of twelve six-day periods, one per month over a year.   Furthermore, only about 40 children were measured simultaneously, as the other children were sampled in different weeks. However, a sample size of 40 is sufficient to calculate reliable rankings across persons. The number of consecutive day pairs was substantially less than the number of days, due to the gaps in the time series. However, D and A statistics were calculated for three variables directly recorded on the activity diaries (outdoor time, travel time, and indoor time), and also for a fourth variable, the physical activity index or PAI (McCurdy, 2000). The analyses were performed for all children together and for two gender cohorts. The separation into two cohorts reduces the number of children measured simultaneously to fewer than 20. Further division into more cohorts is therefore not practical, as the reliability of the scores would become very uncertain.   The results for these analyses are given in Table 6.1.

Table 6.1. D and A Statistics Derived from the Southern California Children's Study

Variable	Group	D	A
Outdoor time	all	0.19	0.22
Outdoor time	boys	0.21	0.21
Outdoor time	girls	0.15	0.24
Travel time	all	0.18	0.07
Travel time	boys	0.18	0.05
Travel time	girls	0.18	0.08
Indoor time	all	0.17	0.22
Indoor time	boys	0.21	0.2
Indoor time	girls	0.17	0.24
PAI	all	0.16	0.23
PAI	boys	0.16	0.2
PAI	girls	0.16	0.25

For all variables and each group, the standard deviation between persons for autocorrelation was about 0.20, and the standard error in the mean A was about 0.02. The values in Table 6.1 indicate that gender differences for both D and A are small, if present at all. The variance in A over the population was also examined for the four diary variables. While the absolute values of A were different across variables, it was found the variance in individual autocorrelations was very similar (approximately 0.2) in all variables. This variance was used to derive the parameters for the target A distribution (eq. 6-9) in the APEX algorithm, and thus the method returns diaries that reproduce a variance of 0.2 in the daily autocorrelation, no matter what diary variable is modeled or what absolute A value is used.

6.4   Cluster-Markov Chain Diary Assembly

The following section combines two technical memos compiled for T. Palma, S. Graham, and J. Langstaff by ICF International (Rosenbaum & Cohen, 2004; Rosenbaum, 2008).

Recently, a new algorithm has been developed and incorporated into APEX that attempts to more realistically represent the day-to-day correlation of activities for individuals. The algorithms first use cluster analysis to divide the daily activity pattern records into groups that

are similar, and then select a single daily record from each group. This limited number of daily patterns is then used to construct a long-term sequence for a simulated individual, based on empirically-derived transition probabilities. This approach is intermediate between the assumption of no day-to-day correlation (i.e., re-selection for each time period) and perfect correlation (i.e., selection of a single daily record to represent all days).

The steps in the algorithm are as follows:

- For each demographic group (age, gender, employment status), temperature range, and day-of-week combination, the associated time-activity records are partitioned into 3 groups using cluster analysis. The clustering criterion is a vector of 5 values: the time spent in each of 5 microenvironment categories (indoors – residence; indoors – other building; outdoors – near road; outdoors – away from road; in vehicle).

- For each simulated individual, a single time-activity record is randomly selected from each cluster.

- Next the Markov process determines the probability of a given time-activity pattern occurring on a given day based on the time-activity pattern of the previous day and cluster-to-cluster transition probabilities. The cluster-to-cluster transition probabilities are estimated from the available multi-day time-activity records. (If insufficient multi-day time-activity records are available for a demographic group, season, day-of-week combination, then the cluster-to-cluster transition probabilities are estimated from the frequency of time-activity records in each cluster in the CHAD data base.)

Figure 6.2 presents the Cluster-Markov algorithm in flow chart format.
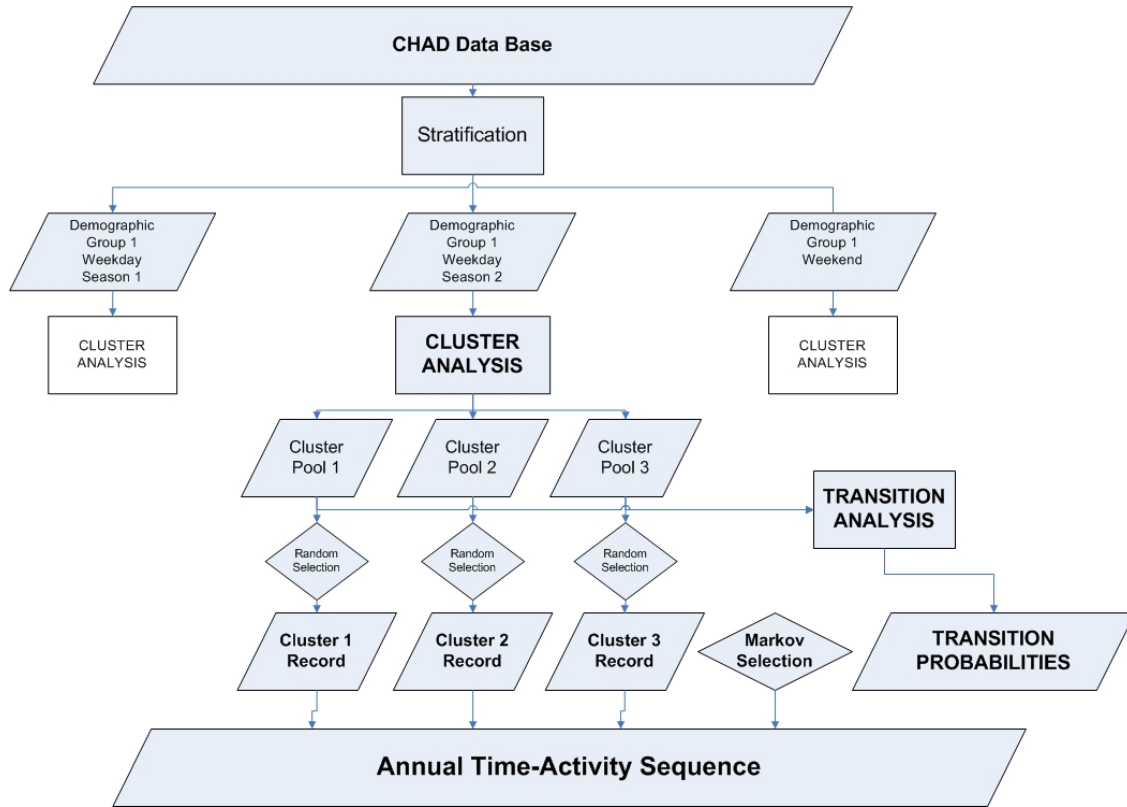
Figure 6.2. Overview of the Markov-Cluster Diary Assembly Algorithm

The algorithm above can be broken down into the following steps:

Data Preparation

Step 1: Each daily activity pattern in the CHAD data base is summarized by the total minutes in each of five micro-environments: indoors – residence; indoors – other building; outdoors – near road; outdoors – away from road; in vehicle. These five numbers are assumed to represent the most important features of the activity pattern for their exposure impact.

Step 2: All CHAD activity patterns for a given day-type and demographic group are subjected to cluster analysis, resulting in 2 or 3 cluster categories. Each daily activity pattern is tagged with a cluster category.

Step 3: For each day-type and demographic group, the relative frequency of each day-type in the CHAD data base is determined.

Step 4: All CHAD activity patterns for a given day-type and demographic group that are consecutive days for a single individual, are analyzed to determine the category-to-category transition frequencies in the CHAD data base. These transition frequencies are used to calculate category-to-category transition probabilities.

For example, if there are 2 categories, A and B, then:

P_{AA} = the probability that a type A pattern is followed by a type A pattern,

64

P_{AB} = the probability that a type A pattern is followed by a type B pattern ($P_{AB} = 1 - P_{AA}$),

P_{BB} = the probability that a type B pattern is followed by a type B pattern, and

P_{BA} = the probability that a type B pattern is followed by a type A pattern ($P_{BA} = 1 - P_{BB}$).

Activity Pattern Selection

For each day-type and demographic group in each census tract:

Step 5: One activity pattern is randomly selected from each cluster category group (i.e., 2 to 3 activity patterns)

Creating Weights for Day-type Averaging

For each day-type and demographic group in each census tract

Step 6: A cluster category is selected for the first day of the day-type sequence, according to the relative frequency of the cluster category days in the CHAD data set.

Step 7: A cluster category is selected for each subsequent day in the day-type sequence day by day using the category-to-category transition probabilities.

Step 8: The relative frequency of each cluster category in the day-type sequence is determined.

Step 9: The activity patterns selected for each cluster category (Step 5) are averaged together using the cluster category frequencies (Step 8) as weights, to create a day-type average activity pattern.

Creating Annual Average Activity Patterns

For each demographic group in each census tract

Step 10: The day-type average activity patterns are averaged together using the relative frequency of day-types as weights, to create an annual average activity pattern.

Creating Replicates

For each demographic group in each census tract

Step 11: Steps 5 through 10 are repeated 29 times to create 30 annual average activity patterns.

Evaluation against observations (Rosenbaum and Cohen 2004)

The Cluster-Markov algorithm is also incorporated into the Hazardous Air Pollutant Exposure Model (HAPEM). The algorithm in HAPEM was tested using multi-day diary data sets collected as part of the Harvard Southern California Chronic Ozone Exposure Study (Xue et al. 2005, Geyh et al. 2000). In this study, 224 children in ages between 7 and 12 yr were followed for 1 year from June 1995 to May 1996, for 6 consecutive days each month. The subjects resided in

two separate areas of San Bernardino County: urban Upland CA, and the small mountain towns of Lake Arrowhead, Crestline, and Running Springs, CA.

For purposes of clustering the activity pattern records were characterized according to time spent in each of 5 aggregate microenvironments: indoors-home, indoors-school, indoors-other, outdoors, and in-transit. For purposes of defining diary pools and for clustering and calculating transition probabilities the activity pattern records were divided by day type (i.e., weekday, weekend), season (i.e., summer or ozone season, non-summer or non-ozone season), age (7-10 and 11-12), and gender.

Week-long sequences (Wednesday through Tuesday) for each of 100 people in each age/gender group for each season were simulated.

To evaluate the algorithm the following statistics were calculated for the predicted multi-day activity patterns and compared them with the actual multi-day diary data.

- For each age/gender group for each season, the average time in each microenvironment

- For each simulated person-week and microenvironment, the average of the within-person variance across all simulated persons (The within-person variance was defined as the variance of the total time per day spent in the microenvironment across the week.)

- For each simulated person-week the variance across persons of the mean time spent in each microenvironment.

In each case the predicted statistic for the stratum was compared to the statistic for the corresponding stratum in the actual diary data. The mean normalized bias for the statistic, which is a common performance measure used in dispersion model performance and was also calculated as follows.

$$NBIAS = \frac{100}{N} \sum_{1}^{N} \frac{(predicted - observed)}{observed}$$

The predicted time-in-microenvironment averages matched well with the observed values. For combinations of microenvironment/age/gender/season the normalized bias ranges from –35% to +41%. Sixty percent of the predicted averages have bias between –9% and +9%, and the mean bias across any microenvironment ranges from -9% to +4%. Fourteen predictions have positive bias and 23 have negative bias.

For the variance across persons for the average time spent in each microenvironment, the bias ranged from –40% to +120% for any microenvironment/age/gender/season. Sixty-five percent of the predicted variances had bias between –22% and +24%. The mean normalized bias across any microenvironment ranged from –10% to +28%. Eighteen predictions had positive bias and 20 had negative bias.

For the within-person variance for time spent in each microenvironment, the bias ranged from – 47% to +150% for any microenvironment/age/gender/season. Seventy percent of the predicted

variances had bias between –25% and +30%. The mean normalized bias across any microenvironment ranged from –11% to +47%. Twenty-eight predictions had positive bias and 12 had negative bias, suggesting some tendency for over-prediction of this variance measure. The overall conclusion was that the proposed algorithm appeared to be able to replicate the observed data reasonably well. Although some discrepancies were rather large for some of the "variance across persons" and "within-person variance" subsets, about two-thirds of the predictions for each case were within 30% of the observed value.

Comparison with other algorithms (US EPA 2007)

As part of the application of APEX in support of US EPA's recent review of the ozone NAAQS several sensitivity analyses were conducted. One of these was to make parallel simulations using each of the three algorithms for constructing multi-day time-activity sequences that are incorporated into APEX.

Table 1 presents the results for the number of persons in Atlanta population groups with moderate exertion exposed to 8-hour average concentrations exceeding 0.07 ppm. The results show that the predictions made with alternative algorithm Cluster-Markov algorithm are substantially different from those made with simple re-sampling or with the Diversity-Autocorrelation algorithm ("base case"). Note that for the cluster algorithm approximately 30% of the individuals with 1 or more exposure have 3 or more exposures. The corresponding values for the other algorithms range from about 13% to 21%.

Table 2 presents the results for the mean and standard deviation of number of days/person with 8-hour average exposures exceeding 0.07 ppm with moderate or greater exertion. The results show that although the mean for the Cluster-Markov algorithm is very similar to the other approaches, the standard deviation is substantially higher, i.e., the Cluster-Markov algorithm results in substantially higher inter-individual variability.

Table 1. Sensitivity to longitudinal diary algorithm: 2002 simulated counts of Atlanta general population and children (ages 5-18) with any or three or more 8-hour ozone exposures above 0.07 ppm concomitant with moderate or greater exertion (after US EPA 2007).

Population Group	One or more exposures			Three or more exposures		
	Simple re-sampling	Diversity-Autocorrelation	Cluster-Markov	Simple re-sampling	Diversity-Autocorrelation	Cluster-Markov
General Population	979,533	939,663 (-4%)	668,004 (-32%)	124,687	144,470 (+16%)	188,509 (+51%)
Children (5-18)	411,429	389,372 (-5%)	295,004 (-28%)	71,174	83,377 (+17%)	94,216 (+32%)

Table 2. Sensitivity to longitudinal diary algorithm: 2002 days per person with 8-hour ozone exposures above 0.07 ppm concomitant with moderate or greater exertion for Atlanta general population and children (ages 5-18) (after US EPA 2007).

Population Group	Mean Days/Person			Standard Deviation		
	Simple re-sampling	Base case	Cluster	Simple re-sampling	Base case	Cluster
General Population	0.332	0.335 (+1%)	0.342 (+3%)	0.757	0.802 (+6%)	1.197 (+58%)
Children (5-18)	0.746	0.755 (+1%)	0.758 (+2%)	1.077	1.171 (+9%)	1.652 (+53%)

CHAPTER 7.   ESTIMATING ENERGY EXPENDITURES AND VENTILATION

Ventilation rates are used in APEX for

- Calculating exertion level for use in tabulating exposure summaries for the population

- Estimating dose

Ventilation does not influence the exposures for a simulated person.

Ventilation is a general term for the movement of air into and out of the lungs. Minute or total ventilation is the amount of air moved in or out of the lungs per minute. Quantitatively, the amount of air breathed in per minute (V_i) is slightly greater than the amount expired per minute (V_e). Clinically, however, this difference is not important, and by convention minute ventilation is always measured on an expired sample, V_e. Alveolar ventilation (V_a) is the volume of air breathed in per minute that (1) reaches the alveoli <u>and</u> (2) takes part in gas exchange. The ventilation rate needed for the %COHb calculation is this ventilation rate, V_a, and is derived for use in APEX based on work by Adams (1998), Astrand and Rodahl (1977), Burmaster and Crouch (1997), Esmail et al. (1995), Galetti (1959), Johnson (1998), Joumard et al. (1981), McCurdy (2000), McCurdy et al. (2000), Schofield (1985), and many others.   Only a brief description of V_A is described below; for the complete derivation, see Johnson (2002).

Ventilation is calculated on an activity event-by-activity event basis. Ventilation is derived from the energy expenditure rate (MET, given as a multiple of resting metabolic rate), associated with the diary activities. The general steps in the estimating ventilation are

- Generate the MET event time-series based on the diary activities

- Adjust the resulting MET series for fatigue and excess post-exercise oxygen consumption

- Convert the MET time-series into a ventilation rate time series

These steps are covered in the following sections.

7.1   Generating the MET Time-Series

MET—which comes from "metabolic equivalents of task"—is a dimensionless ratio of the activity-specific energy expenditure rate to the basal or resting energy expenditure rate. While different people have very different basal metabolic rates, it is generally found that the MET ratios do not exhibit as much variability. Thus, standing still might require two times the basal energy expenditure, or two MET, for most people, with relatively little variation. The basal rate is constant (it only has to be determined once per profile), while the activity-specific MET ratio is calculated for each of the activities reported on the composite activity diary.

Each possible diary activity code (see *Volume I*), is mapped to a corresponding APEX MET distribution number the *MET Mapping* input file. Each of these distributions is then defined in the *MET Distributions* file. This file (see *Volume I*) gives the properties of the MET distribution

for each type of activity, in some cases as a function of age or occupation. The distributions are defined in the standard APEX format (see Section 3.1). These distributions are based on many available data on energy expenditure, and in general should not be changed. This file is read into APEX in the **DiaryModule:ReadMETS**. In the subroutine **DiaryModule:METSEval**, APEX steps through the activity diary and assigns a MET value to each event by randomly selecting a value from the appropriate distribution as defined by the activity code and the profile. The result is consider the "raw" MET time-series, which is then adjusted to be physiologically realistic. The adjustments are covered in the next section.

7.2 Adjusting the MET Time-Series for Fatigue and Excess Post-Exercise Oxygen Consumption

As discussed in the previous section, APEX assigns distributions for MET level to each diary event, based on the reported event activity (and in some cases, age and occupation). However, these raw MET time-series do not consider the sequence of the events (i.e., the order in which they occur). It is well known that a person's capacity for work will diminish as they get tired, and in practice, this means that the upper bound on MET is lowered if events in the recent past have been at unusually high MET levels. Furthermore, once high activity levels have ended, people tend to breathe heavily even while resting, as they recover their accumulated oxygen deficit. This effect is called excess post-exercise oxygen consumption (EPOC), and results in raising the MET levels above the 'raw' values pulled from the activity-based distributions. APEX contains an algorithm for adjusting the MET time series for both of these effects. The algorithm is implemented in **ExposureDoseModule:Ventilation**.

The adjustment method is based on keeping a running total of the oxygen deficit as a simulated individual proceeds chronologically through his or her activity diary. The oxygen deficit is the amount of energy supplied to the muscles by non-aerobic systems during exercise. It reflects a need for increased post-exercise ventilation to "pay back" this energy. The oxygen deficit calculations were derived from a synthesis of numerous published studies (see below).

Oxygen deficit is measured as a percentage of the maximum oxygen deficit an individual can attain prior to deterioration of exercise performance. Limitations on MET levels corresponding to post-exercise diary events were based on maintaining an oxygen deficit below this maximum value. In addition, adjustments to MET were simultaneously made for EPOC. The EPOC adjustments are based in part on the modeled oxygen deficit and in part on data from published studies on EPOC, oxygen deficit, and oxygen consumption.

The methods are constructed in terms of reserve MET, which is the amount over the basal rate (MET=1). Furthermore, we defined M as the normalized reserve, so that M=0 at MET=1, and M=1 at maximum MET:

$$M = \frac{MET - 1}{MET_{max} - 1} \tag{7-1}$$

(Recall that MET_{max} is a profile variable assigned for each simulated profile; see Section 5.3). Using a normalized reserve assures that the method can be applied identically to the entire population of profiles, each having a unique MET_{max} value.

A number of terms will be used in the description of the algorithm. They are defined below:

- MET   Metabolic equivalent of task (unitless)

- MET_{max} Maximum achievable metabolic equivalent for an individual (unitless)

- M   Normalized MET reserve (unitless, M, bounded between 0 and 1)

- ΔM Change in M from one diary event to the next (M)

- D_{max} Absolute maximum oxygen deficit that can be obtained (M-hr)

- F   Fractional oxygen deficit (percent of individual maximum, unitless)

- t_e Duration of activity diary event (hours)

- t_r Time required to recover from an F of 1 to an F of 0 at rest (recovery time, hours)

- dF_{inc} Rate of change of F due to deficit increase (F/hr, will have a positive value)

- dF_{rec} Rate of change of F due to deficit recovery (F/hr, will have a negative value)

- dF_{tot} Total rate of change of F, $dF_{inc} + dF_{rec}$ (F/hr)

- ΔF_{inc} Increase in F due to anaerobic energy expenditure (F)

- ΔF_{rec} Decrease in F due to recovery of oxygen deficit (F)

- ΔF_{tot} Change in F due to simultaneous anaerobic work and oxygen recovery, $\Delta F_{inc} + \Delta F_{rec}$ (F)

- ΔF_{fast} Total change in F during the fast recovery phase (F)

- S_{fast} Magnitude of the rate of change in M during fast component (M/hr)

- $EPOC_{fast}$ Change in M due to fast-component EPOC (M)

- $EPOC_{slow}$ Change in M due to slow-component EPOC (M)

See Isaacs et al. (2007) for a complete derivation of the method.

7.2.1   Simulation of Oxygen Deficit

This section presents the theoretical development of the equations describing the accumulation of oxygen deficit. The method was developed using a large number of studies on oxygen consumption, oxygen deficit, and EPOC. Individual studies will be referenced below. The first two subsections below describe the equations themselves, while the last section describes the determination of the values for the model parameters.

7.2.1.1   Fast Processes

There exists a component of the accumulated oxygen deficit that is due to transition from one M level to another (McArdle et al., 2001).   This component derives from the anaerobic work that is required by sudden muscular motion. There is also a corresponding fast component of oxygen

recovery which occurs very quickly after a change from a high M level to a lower one. In the absence of any data to the contrary, it is assumed that these fast deficit accumulation and fast recovery processes occur at the same rate. These processes are illustrated in Figure 7.1. The adjustment to F is equal to the area of the triangle associated with either a positive or negative change in M, normalized by the maximum obtainable accumulated oxygen deficit (D_{max}). The normalized area can thus be calculated as:

$$\Delta F_{fast} = 0.5 \frac{\Delta M |\Delta M|}{S_{fast} D_{max}} \tag{7-2}$$

where $\Delta M = M_i - M_{i-1}$ and S_{fast} is the slope of the change in M (in M/hr). Note that this change in F will be positive if ΔM is positive, and negative otherwise.
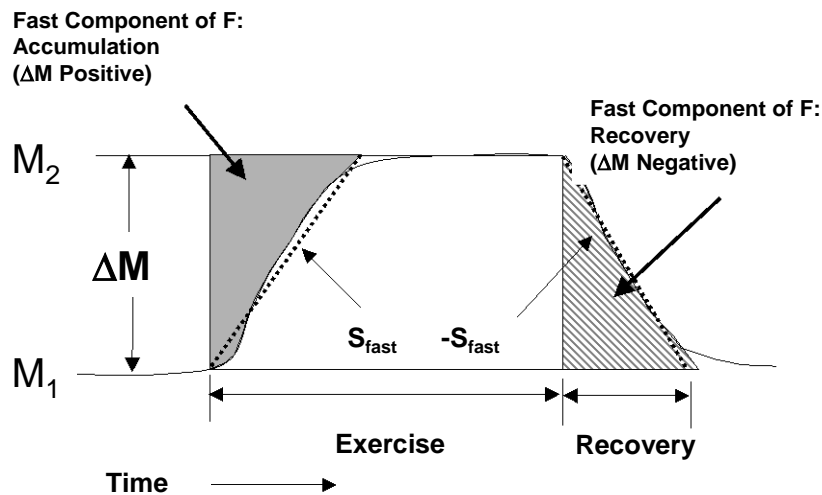
Figure 7.1. Fast Components of Oxygen Deficit and Recovery

7.2.1.2 Slow Processes

The slow component of the increase in oxygen deficit corresponds to the accumulation of deficit over a period of heavier exercise (rather than that associated with an increase in activity level). The method was derived from the analysis of a number of studies on exercise and EPOC including Bahr (1992), Bahr et al. (1987), Bielinski et al. (1985), Brockman et al. (1993), Gillette et al. (1994), Gore and Withers (1990), Hagberg et al. (1980), Harris et al. (1962), Kaminsky and Whaley (1993), and Katch et al. (1972), Maehlum et al. (1986), Sedlock (1991a,b). The following data were considered: the time it took for subjects to reach exhaustion, their accumulated oxygen deficit, their MET_{max}, the MET value at which they exercised, and the corresponding normalized reserve MET (M). (Note that the MET and MET_{max} quantities were derived from the published VO_2 and VO_{2max} measurements). The data indicated that oxygen deficit accumulates at a much faster rate when M is high. For example, an M value near 0.5 requires about 5 times longer to reach exhaustion than an M value near 0.75 (on average), indicating that F is nonlinear in M.

Let the rate of increase in F be given by dF_{inc}. The relationship between dF_{inc} and M is a power law:

$$dF_{inc} = aM^b \qquad (7\text{-}3)$$

where a and b were estimated from available data. The slow recovery of oxygen deficit must also be accounted for, as it occurs simultaneously with debt accumulation. A slow, but continual, process for recovering oxygen deficit is modeled, independent of the MET level. EPOC recovery is modeled as constant over time until the oxygen deficit is erased. Assuming this takes t_r hours, the slow recovery of oxygen deficit occurs at a rate

$$dF_{rec} = -\frac{1}{t_r} \qquad (7\text{-}4)$$

The total net rate of change in F from slow processes during an event with duration t_e is given by

$$dF_{slow} = dF_{inc} + dF_{rec} \qquad (7\text{-}5)$$

and the associated change in F is

$$\Delta F_{slow} = \left(aM_i^b - \frac{1}{t_r} \right) t_e \qquad (7\text{-}6)$$

For an individual starting with an F of 0 and exercising to exhaustion (neglecting the transitory effects), the change in ΔF is 1.0. In this case, rearranging and taking the logarithm gives

$$log\left(\frac{1}{t} + \frac{1}{t_r} \right) = log(a) + b\,log(M) \qquad (7\text{-}7)$$

This equation can be used to fit data to estimate the parameters a and b (this will be discussed in the next subsection).

The starting normalized oxygen deficit for the next event (i +1), taking into account both the fast and slow changes in F, is then

$$F_{i+1} = F_i + \Delta F_{slow} + \Delta F_{Fast} \qquad (7\text{-}8)$$

7.2.1.3 Derivation of Appropriate Values for the Model Parameters

The values of the model parameters t_r, a, and b, were derived from summaries of published data on EPOC and oxygen debt (see references listed in Section 7.2. Several of the these studies reported t_r values, however, due to variability in measurement and protocol differences, these recovery times varied from 0.5 hours to 24 hours. From a modeling viewpoint, it would be unacceptable to allow recovery to significantly carry over from one day to the next. To do so could lead to a perpetual delay in recovering an oxygen deficit, for example, by repeatedly encountering new exercise events before recovery is complete. In APEX, t_r, which is a profile

73

variable, is selected from a uniform distribution having a minimum of 8 and a maximum of 16 hours.

In APEX, a and b are modeled as a function of t_r:

$$a = 5.20 - \left(\frac{1.54}{t_r}\right) + \left(\frac{3.92}{t_r^2}\right) \qquad (7\text{-}9)$$

$$b = 3.93 - \left(\frac{3.57}{t_r}\right) + \left(\frac{3.66}{t_r^2}\right) \qquad (7\text{-}10)$$

These expressions were derived from the experimental data.

Appropriate distributions for maximum oxygen debt (MOD) in ml/kg were derived from data from a number of studies in adults (Bickham et al., 2002, Billat et al., 1996, Buck and McNaughton, 1999, Demarle et al., 2001, Doherty et al., 2000, Faina et al., 1997, Gastin and Lawson, 1994, Gastin et al., 1995, Hill et al., 1998, Maxwell and Nimmo, 1996, Olesen,1992, Renoux et al., 1999, Roberts et al., 2003, Weber and Schneider, 2000) adolescents (Naughton et al., 1998) and children (Berthoin et al., 1996, Carlson and Naughton, 1993). The studies covered multiple types of exercise protocols, some having more than one protocol per study. Normal distributions for MOD were defined for all three age groups, based on average mean and standard deviation values from the studies:

- adults (>17 yrs):   54.95±14.46 (ml/kg)
- adolescents (12-17 yrs):   63.95±21.12 (ml/kg)
- children (<12 yrs):   34.74±13.10 (ml/kg)

(These mean and standard deviations are read in from the *Physiology* file; see Section 5.3.) Values are selected from normal distributions with these characteristics. These values are constant for an individual over the simulation period. The bounds of these distributions are selected as two standard deviations from the mean; these ranges were found to be reasonable when compared to reported ranges (Olesen 1992). These values are transformed to D_{max}, via a units conversion factor and the normalization needed for use with reserve MET:

$$D_{max}\ (M\text{-}hr) = \left(\frac{MOD}{60\ METStoO_2}\right)(METS_{max} - 1)^{-1} \qquad (7\text{-}11)$$

where $METStoO_2$ is the conversion factor for ml O_2 to MET-min, 3.5 [(ml O2/min)/kg]/MET. Note that the variability in this factor is not addressed here.

A number of studies on EPOC (Almuzaini et al., 1998, Dawson et al., 1996, Frey et al., 1993, Harms et al., 1995, Kaminsky et al., 1990, Knuttgen, 1970, Maresh et al., 1992, Pivarnik and Wilkerson, 1988, Short and Sedlock, 1997, Trost et al., 1997) were used to derive S_{fast}. These were all studies in which oxygen consumption was measured relatively soon (within a few minutes) after the end of exercise and at a frequency high enough to capture the kinetics of the change in oxygen consumption. The data were found to be relatively uniform from the minimum

(0.6 MET/min) to the maximum (3.7 MET/min) slope values, and so values were selected from a uniform distribution having these bounds. Converting units and normalizing to M, one obtains:

$$S_{fast} \ (M/hr) = \frac{60 \ Uniform \ (0.6, 3.7)}{(METS_{max} - 1)}$$ (7-12)

7.2.2 Adjustments to M for Fatigue

The equations provided in the previous section describe a method for keeping a running total of the fractional oxygen deficit (F) for each diary event for an individual. These event F values are used to limit M for each event to appropriate values. Basically, the maximum M value that can be maintained for an entire event is the value that would result in an F_{i+1} (eq. 7-8) equal to 1 (i.e., the maximum value) at the end of the diary event. The approach used in APEX is to set M for each event equal to the raw MET value, and test if $F_{i+1} > 1$. If it is, then the M_i value is reduced by a predetermined amount (currently 0.01) and F_{i+1} is recalculated. The process continues until an appropriate value of M_i, called $M_{max,i}$ is found. As the exposure model marches through the events of the activity diary, the M values associated with each event are adjusted if necessary:

$$M_i = min(M_i, M_{max, i})$$ (7-13)

7.2.3 Adjustments to M for EPOC

As noted above, it has been observed in many studies that EPOC is characterized by both slow and fast components. The fast increase in oxygen consumption occurs within minutes of exercise, while the slow component may persist for many hours. Both fast and slow EPOC components were modeled.

7.2.3.1 Fast Processes

The fast EPOC component, which takes place in the first few minutes after exercise, is also characterized by the slope S_{fast}. The energy recovered during those first few minutes corresponds to the recovery triangle in Figure 7.1 and this increase in the rate of energy expenditure for a post-exercise event is modeled as the area of the triangle divided by the event duration:

$$EPOC_{fast} = 0.5 \frac{(\Delta M)^2}{S_{fast} t_e}$$ (7-14)

$EPOC_{fast}$ will thus have units of M (normalized reserve MET). The M level for the post-exercise events will be incremented by $EPOC_{fast}$.

7.2.3.2 Slow Processes

The increase in M associated with the slow EPOC component is estimated as the amount required to maintain the slow recovery of F. Since the deficit D_{max} is recovered in full in the recovery time t_r, the time-averaged adjustment to MET for the slow recovery process must be

75

$$EPOC_{slow} = \frac{D_{max}}{t_r} \qquad (7\text{-}15)$$

Every diary event with the full rate of slow recovery will have its M value adjusted upward by $EPOC_{slow}$. An appropriate fraction of $EPOC_{slow}$ is used if only partial recovery is needed to eliminate the deficit (i.e., return F to 0). The final adjusted M value for the diary event is thus

$$M_{adj} = M + EPOC_{fast} + EPOC_{slow} \qquad (7\text{-}16)$$

and the new MET value for the event is

$$METS_{adj} = M_{adj}(METS_{max} - 1) + 1 \qquad (7\text{-}17)$$

7.3 Calculating PAI and the Ventilation Rates

APEX calculates three different ventilation rates from the adjusted MET time series. These are the expired ventilation rate (V_e) the alveolar ventilation rate (V_a), and the effective ventilation rate (EVR). All three are reported for each hour in the simulation in the APEX output files. V_a is used in the CO dose calculations, and EVR is used in compiling summary exposure tables for different populations during different levels of exertion.

In addition, the final MET time-series is used to calculate a physical activity index (PAI) for each individual. Finally, an intermediate rate, oxygen consumption (VO_2), is also calculated. The equations for calculating these rates from the MET time series are given below. All of these calculations are implemented in **ExposureDoseModule:Ventilation**.

7.3.1 Calculating PAI and Energy Expenditure

Once the final MET time series is calculated, the timestep and hourly physical activity index (PAI) for each hour in the simulation for the simulated individual is calculated as the time-weighted average of MET:

$$PAI = \frac{\sum_{i=1}^{N_{events}}(METS_i)(t_i)}{t} \qquad (7\text{-}18)$$

where MET_i is the MET value for event i, t_i is the event duration in minutes, and t is the length of the timestep in minutes (or 60 minutes, if calculating hourly values). N_{events} is the number of diary events in the considered timestep or hour. These PAI values can be written to the *Timestep* or *Hourly* files. The daily PAI value is simply the average of the 24 hourly values. Finally, a median daily PAI value is calculated for each profile. The daily and median daily PAI values are saved as a profile variables (see Section 5.3). The median daily PAI value is used in the characterization of persons as "active" when creating the output exposure summary tables (see *Volume I* and Section 9.2).

The energy expenditure (kcal/min) is

$$EE = PAI \times RMR \qquad (7\text{-}19)$$

where RMR is the profile resting metabolic rate in kcal per minute. EE is calculated for both timesteps and hours, and can be written to the corresponding output files.

7.3.2 Calculating Oxygen Consumption and Ventilation Rates

The oxygen consumption rate in ml/min/kg (McCurdy, 2000), normalized to body mass, is given by

$$VO_2 = \frac{METS \times ECF \times RMR}{BM} \tag{7-20}$$

where ECF is the profile energy conversion factor in liters of oxygen per kcal and BM is the profile body mass. The alveolar ventilation rate is also calculated from MET using:

$$V_a = METS \times 19630 \times ECF \times RMR \tag{7-21}$$

where the constant 19630 is the oxygen to air conversion factor (19,630 ml of air/l of O_2).

The calculation of V_e is based on the VeSlope, VeResid, and VeInter profile variables (see Section 5.3). The calculation of those variables and the following equations for V_e comprise the V_e regression equations derived by Graham and McCurdy (2005). V_e is calculated as

$$V_e = BM\left(e^X\right) \tag{7-22}$$

where BM is the profile body mass and the exponent term X is given by

$$X = VeInter + VeSlope\left(ln(VO_2)\right) + Z\left(VeResid\right) \tag{7-23}$$

where Z is a random number pulled from a normal distribution every event. EVR is then

$$EVR = \frac{V_e}{BSA} \tag{7-24}$$

where BSA is the profile body surface area.

Using the above equations, APEX generates an event time-series for Ve and Va and EVR. Ve and Va are output on the *Events* output file. Timestep and hourly values (time-weighted timestep and hourly averages of the event values) for EVR, Va, Ve, are calculated and can be written to the *Timestep* and *Hourly* output files (see *Volume I*).

7.3.3 Calculating Ozone-Induced Changes to Forced Expiratory Volume

Studies of exposure to ozone have shown that there is a significant relationship between ozone exposure and reversible decrements in the forced expiratory volume in 1s (FEV1). Activity levels, duration of exposure, age, height and weight have also been shown to be significant factors in determining ΔFEV1. APEX uses a model developed by McDonnell, Stewart and Smith (2010) to calculate the %ΔFEV1 due to ozone for each event for the *i*th person, at the *j*th time, in the *k*th exposure protocol:

$$\%\Delta FEV1_{ijk} = e^{Ui} \left\{ \frac{\beta_1 + \beta_2 y_{ijk} + \beta_7 \, [BMI_{ijk} - 23.41]}{1 + \beta_4 \, e^{-\beta_3 \, Xijk}} - \frac{\beta_1 + \beta_2 y_{ijk} + \beta_7 \, [BMI_{ijk} - 23.41]}{1 + \beta_4} \right\} + E1_{ijk} + E2_{ijk}$$

(7-25)

Here, $\beta_1 - \beta_7$ and U are unitless fitted model parameters (see paper for details of fit), they are chosen once for each individual and remain constant throughout the simulation. $E1_{ijk}$ and $E2_{ijk}$ are terms that describe the error involved in measurements of $\%\Delta FEV1$. The error has two terms in order to model the hourly and daily variability independently. The sampling rates of these two parameters are controlled by the parameters *HourlyFEVE1* and *HourlyFEVE12* in the Control file. See McDonnell, Stewart and Smith (2007, 2010).

BMI (Eq. 5-2) is the Body-Mass Index, which is an APEX profile variable that depends on the individual's height and weight. Two models are presented in McDonnell et al. 2010, one with and one without considering *BMI*. We chose to incorporate the one that used *BMI*. However, the APEX user can use the fitted model values for the non-*BMI* model, by using $\beta_7 = 0$ to eliminate that term (see cited paper for details).

X is specified as a differential equation that depends on various time-varying factors. In APEX, because the concentration and ventilation rate are constant over an event, this equation has an analytic solution for each event:

$$X(t) = X_o \, e^{-\beta 5 t} + \frac{C}{\beta_5} \left(\frac{VE}{BSA} \right)^{\beta 6} (1 - e^{-b5t})$$

(7-26)

Here, *C* is the concentration in the microenvironment (ppm), *VE* is the instantaneous expired minute volume (L min^{-2}), *BSA* is the body surface area (m^2), and *t* is the duration of the event. In the McDonnell model formulation, *BSA* is calculated using the equation from Dubois and Dubois (1916):

$$BSA = 0.007184 \times wt^{0.425} \, ht^{0.725}.$$

(7-27)

However, APEX uses the BSA model of Burmaster (1998) (Equation 5-3) that depends on weight alone. We continue using the default formulation of BSA, rather than adopt the DuBois and DuBois (1916) method.

The *y* term is a function of the age of the individual in years. In the original equation from McDonnell et al. 2010, y is given as $[Age_{ijk} - 25]$, however this term was only fit to using data from individuals aged 18-35. APEX allows the user to specify piecewise linear equations for *y* as a function of age: $y = FEVSLP \times Age + FEVSLP$. *FEVSLP* and *FEVINT* are parameters specified in the Physiology file.

CHAPTER 8.   CALCULATING POLLUTANT CONCENTRATIONS IN MICROENVIRONMENTS

APEX calculates concentrations of all modeled air pollutants in all microenvironments at each timestep of the simulation period for each of the simulated individuals. The default APEX timestep is 1 hour (See *Volume I*). The microenvironmental concentrations are set in **MicroEnvModule:MicroConcs**. The input files and algorithms for these calculations are described in the following sections.

8.1   Defining Microenvironments

APEX gives the user great flexibility in defining the number and properties of the microenvironments (see step 4 in Figure 2-1). (Note that the term microenvironment is generally shortened to micro in the computer code and files.) Along with this flexibility, however, is the need for the user to specify a substantial amount of information about the microenvironments in the input files.

There are three input files that relate to microenvironments. The first is the *Microenvironment Mapping* file, which contains the mapping from the location categories used in the activity diaries to the APEX microenvironments. The second is the *Microenvironment Descriptions* file, which contains rules for calculating pollutant concentrations in each microenvironment. The third file is the *Profile Functions (Distributions)* file, in which profile (person) variables (such as the presence of air conditioning or a gas stove in the home) influencing the microenvironmental concentrations can be defined. See *Volume I* for a discussion of the *Profile Functions (Distributions)* file.

The *Microenvironment Mapping* file gives the user control over how many microenvironments will be modeled and what CHAD (or other activity database) locations should be grouped into each of microenvironment. The file contains one row for each CHAD location code, indicating which APEX microenvironment is to be used whenever that CHAD code is encountered.   Thus, the more than 100 location codes defined in the activity (CHAD) database are mapped into a smaller subset of user-defined microenvironments amenable to modeling. In addition, location codes are also mapped to concentration locations (Home, Work, Other, Road, Road Work, Near Home, Near Work, Last; H/W/O/R/RW/NH/NW/L), which tell APEX which set of microenvironmental concentrations to use for a particular location code. Road and Road Work are optional locations and are used in conjunction with a set of specific roadway air quality data. See Section 8.2.1 for details.

Table 8.1 lists the 115 location codes currently in CHAD and examples of microenvironments which can be assigned in the Microenvironment Mapping file.

Table 8.1. Default Mapping of CHAD Location Codes to APEX Microenvironments

CHAD Location Code	CHAD Location Description	APEX Microenv. Code	APEX Microenviroment Description	Location (see Section 8.2.1)
U	Uncertain of correct code	−1	Use previous microenvironment	U
X	No data	−1	Use previous microenvironment	U
30000	Residence, general	1	Indoors − Residence	H
30010	Your residence	1	Indoors − Residence	H
30020	Other residence	1	Indoors − Residence	H
30100	Residence, indoor	1	Indoors − Residence	H
30120	Your residence, indoor	1	Indoors − Residence	H
30121	..., kitchen	1	Indoors − Residence	H
30122	..., living room or family room	1	Indoors − Residence	H
30123	..., dining room	1	Indoors − Residence	H
30124	..., bathroom	1	Indoors − Residence	H
30125	..., bedroom	1	Indoors − Residence	H
30126	..., study or office	1	Indoors − Residence	H
30127	..., basement	1	Indoors − Residence	H
30128	..., utility or laundry room	1	Indoors − Residence	H
30129	..., other indoor	1	Indoors − Residence	H
30130	Other residence, indoor	1	Indoors − Residence	H
30131	..., kitchen	1	Indoors − Residence	H
30132	..., living room or family room	1	Indoors − Residence	H
30133	..., dining room	1	Indoors − Residence	H
30134	..., bathroom	1	Indoors − Residence	H

CHAD Location Code	CHAD Location Description	APEX Microenv. Code	APEX Microenviroment Description	Location (see Section 8.2.1)
30135	..., bedroom	1	Indoors − Residence	H
30136	..., study or office	1	Indoors − Residence	H
30137	..., basement	1	Indoors − Residence	H
30138	..., utility or laundry room	1	Indoors − Residence	H
30139	..., other indoor	1	Indoors − Residence	H
30200	Residence, outdoor	10	Outdoors − Other	H
30210	Your residence, outdoor	10	Outdoors − Other	H
30211	..., pool or spa	10	Outdoors − Other	H
30219	..., other outdoor	10	Outdoors − Other	H
30220	Other residence, outdoor	10	Outdoors − Other	H
30221	..., pool or spa	10	Outdoors − Other	H
30229	..., other outdoor	10	Outdoors − Other	H
30300	Residential garage or carport	7	Indoors − Other	H
30310	..., indoor	7	Indoors − Other	H
30320	..., outdoor	10	Outdoors − Other	H
30330	Your garage or carport	1	Indoors − Residence	H
30331	..., indoor	1	Indoors − Residence	H
30332	..., outdoor	10	Outdoors − Other	H
30340	Other residential garage or carport	1	Indoors − Residence	H
30341	..., indoor	1	Indoors − Residence	H
30342	..., outdoor	10	Outdoors − Other	H
30400	Residence, none of the above	1	Indoors − Residence	H
31000	Travel, general	11	InVehicle − Cars and Trucks	O/R
31100	Motorized travel	11	InVehicle − Cars and Trucks	O/R
31110	Car	11	InVehicle − Cars and Trucks	O/R
31120	Truck	11	InVehicle − Cars and Trucks	O/R
31121	Truck (pickup or van)	11	InVehicle − Cars and Trucks	O/R

CHAD Location Code	CHAD Location Description	APEX Microenv. Code	APEX Microenviroment Description	Location (see Section 8.2.1)
31122	Truck (not pickup or van)	11	InVehicle − Cars and Trucks	O/R
31130	Motorcycle or moped	8	Outdoors − Near Road	O/R
31140	Bus	12	InVehicle − Mass Transit	O/R
31150	Train or subway	12	InVehicle − Mass Transit	O
31160	Airplane	0	Zero concentration	O
31170	Boat	10	Outdoors − Other	O
31171	Boat, motorized	10	Outdoors − Other	O
31172	Boat, other	10	Outdoors − Other	O
31200	Non-motorized travel	10	Outdoors − Other	O/R
31210	Walk	10	Outdoors − Other	O/R
31220	Bicycle or inline skates/skateboard	10	Outdoors − Other	O/R
31230	In stroller or carried by adult	10	Outdoors − Other	O
31300	Waiting for travel	10	Outdoors − Other	O/R
31310	..., bus or train stop	8	Outdoors − Near Road	O/R
31320	..., indoors	7	Indoors − Other	O
31900	Travel, other	11	InVehicle − Cars and Trucks	O/R
31910	..., other vehicle	11	InVehicle − Cars and Trucks	O/R
32000	Non-residence indoor, general	7	Indoors − Other	O
32100	Office building/ bank/ post office	5	Indoors − Office	O
32200	Industrial/ factory/ warehouse	5	Indoors − Office	O
32300	Grocery store/ convenience store	6	Indoors − Shopping	H
32400	Shopping mall/ non-grocery store	6	Indoors − Shopping	O
32500	Bar/ night club/ bowling alley	2	Indoors − Bars and Restaurants	O
32510	Bar or night club	2	Indoors − Bars and Restaurants	O
32520	Bowling alley	2	Indoors − Bars and Restaurants	O
32600	Repair shop	7	Indoors − Other	O
32610	Auto repair shop/ gas station	7	Indoors − Other	O

CHAD Location Code	CHAD Location Description	APEX Microenv. Code	APEX Microenviroment Description	Location (see Section 8.2.1)
32620	Other repair shop	7	Indoors − Other	O
32700	Indoor gym /health club	7	Indoors − Other	O
32800	Childcare facility	4	Indoors − Day Care Centers	O
32810	..., house	1	Indoors − Residence	O
32820	..., commercial	4	Indoors − Day Care Centers	O
32900	Large public building	7	Indoors − Other	O
32910	Auditorium/ arena/ concert hall	7	Indoors − Other	O
32920	Library/ courtroom/ museum/ theater	7	Indoors − Other	O
33100	Laundromat	7	Indoors − Other	H
33200	Hospital/ medical care facility	7	Indoors − Other	O
33300	Barber/ hair dresser/ beauty parlor	7	Indoors − Other	H
33400	Indoors, moving among locations	7	Indoors − Other	O
33500	School	3	Indoors − Schools	O
33600	Restaurant	2	Indoors − Bars and Restaurants	O
33700	Church	7	Indoors − Other	H
33800	Hotel/ motel	7	Indoors − Other	O
33900	Dry cleaners	7	Indoors − Other	H
34100	Indoor parking garage	7	Indoors − Other	O
34200	Laboratory	7	Indoors − Other	O
34300	Indoor, none of the above	7	Indoors − Other	O
35000	Non-residence outdoor, general	10	Outdoors − Other	O
35100	Sidewalk, street	8	Outdoors − Near Road	O/R
35110	Within 10 yards of street	8	Outdoors − Near Road	O/R
35200	Outdoor public parking lot /garage	9	Outdoors − Public Garage / Parking	O/R
35210	..., public garage	9	Outdoors − Public Garage / Parking	O/R
35220	..., parking lot	9	Outdoors − Public Garage / Parking	O/R
35300	Service station/ gas station	10	Outdoors − Other	O
35400	Construction site	10	Outdoors − Other	O

CHAD Location Code	CHAD Location Description	APEX Microenv. Code	APEX Microenviroment Description	Location (see Section 8.2.1)
35500	Amusement park	10	Outdoors − Other	O
35600	Playground	10	Outdoors − Other	H
35610	..., school grounds	10	Outdoors − Other	O
35620	..., public or park	10	Outdoors − Other	H
35700	Stadium or amphitheater	10	Outdoors − Other	O
35800	Park/ golf course	10	Outdoors − Other	O
35810	Park	10	Outdoors − Other	O
35820	Golf course	10	Outdoors − Other	O
35900	Pool/ river/ lake	10	Outdoors − Other	O
36100	Outdoor restaurant/ picnic	10	Outdoors − Other	O
36200	Farm	10	Outdoors − Other	O
36300	Outdoor, none of the above	10	Outdoors − Other	O

All of the other properties of the microenvironments are provided in the *Microenvironment Descriptions* file. All microenvironments assigned locations in the *Microenvironment Mapping* file must be defined in the *Microenvironment Descriptions* file. More microenvironments may be described than are assigned locations, but they will not be used by APEX (since in this case simulated people will never enter the microenvironment). The total number of microenvironments described in the *Microenvironment Descriptions* file must also be indicated in the *Simulation Control* input file. (These input files are also covered in *Volume I*.)

Definition of the microenvironments using the *Microenvironment Descriptions* file is covered in Section 8.2.4.

8.2   Calculating Concentrations in Microenvironments

APEX calculates concentrations of all the air pollutants in all the microenvironments at each timestep of the simulation period for each of the simulated individuals, based on the ambient air quality data specific to the geographic locations visited by the individual. APEX provides two methods for calculating microenvironmental concentrations: the mass balance (MASSBAL) method and the simpler factors (FACTORS) method. The MASSBAL method starts with the previous timestep's concentration in each microenvironment, which is modified over time by exchange with the ambient air. The FACTORS method uses a simple equation to relate the concentration in each microenvironment to the current ambient concentration. Both methods require that a number of parameters including proximity, penetration and pollutant sources be specified over time, while the MASSBAL method uses some additional parameters, such as air exchange, volume, and decay rates. All pollutants use the same method in each microenvironment. These methods are described in the next two subsections. The user is required to specify the calculation methods for each of the microenvironments in the simulation in the *Microenvironment Descriptions* file (see *Volume I*). Microenvironments within a single simulation may use either method; mixing the methods (across micros, not pollutants) is allowed with no restrictions.

8.2.1 Microenvironmental Concentrations in Locations

APEX calculates up to six sets of microenvironmental concentrations for each person. In general, these concentrations represent the geographical locations a person moves through in a day. These seven locations are "Home" (H), "Work" (W), "Other" (O), "Roadway" (R), "Road near Work" (RW), "Near Home" (NH), and "Near Work" (NW). An either location, "Last" (L), draws from either Near Home or Near Work depending on the Last location the individual was in. (A person who is not employed has identical work and home locations.) The H and W concentrations are calculated from the air quality data in a person's home and work sectors respectively. The concentrations in the O location are calculated from a composite of set of air districts. By default, APEX uses the city-average air concentration to calculate O concentrations. However, the user can customize this average concentration using the *Control* file settings **SampleOtherLocs**, **#OtherDistricts**, and **HomeProbab** (see *Volume I*). If the user specifies roadway air quality districts, then APEX will use these AQ data to determine microenvironmental concentrations for R and RW locations. R is drawn from air concentrations near the Home location, while RW is drawn from concentrations near the work location. NH is randomly sampled from a tract within a given distance from the H location, while W is sampled near the work location. L is set to either NH or NW, depending on the last location.

Location is determined event-by-event for each simulated person. In general, APEX determines which set of concentrations to use for each event via the diary (CHAD or other) location code The *Microenvironment Mapping* file assign locations definitions to each activity database location code (see Table 8.1). However, APEX also assigns diary events with a "work" activity code to the W location. This assignment overrides the location assignment based on location code. By default, APEX assigns CHAD activity codes 10000-10300 to the work location (see Table 4-5 in *Volume I*). However, the user also has the ability to customize this setting using the *Control* file variable **CustomWork**.

APEX only defines a single set of micro parameter distributions for each micro (i.e. there are no unique distributions for the H, W, O, R, RW, NH, NW, L locations.) However, the values of the parameters themselves may differ between locations. By using the **ResampleWork** keyword in a micro parameter description, APEX will select a different value from the distribution to use for the W location (see Section 8.2.4.3 for details). If **ResampleWork** is used, then the micro parameters for the O location will be the average of the parameters for the H and W locations. If not, the H, W, and O locations will all use the same values of the parameters for the micro. In addition, if the simulated person (profile) is not employed, there is no W location, and the values of the parameters for the O location are equal to the H values. If the user specifies roadway AQ data, then APEX will use these data for all CHAD locations indicated by the R, or RW value. If the user chooses the **RoadLast** =Y option, then roadway concentrations will be chosen similar to the Last location: R or RW will be selected based on the last event to occur in either the home or work location.

8.2.2 Mass Balance Method

The mass balance method assumes that an enclosed microenvironment (e.g., a room in a residence) is a single well-mixed volume in which the air concentration is approximately

spatially uniform. The concentration of an air pollutant in such a microenvironment is estimated using the following four processes (as illustrated in Figure 8.1):

- Inflow of air into the microenvironment;

- Outflow of air from the microenvironment;

- Removal of a pollutant from the microenvironment due to deposition, filtration, and chemical degradation; and

- Emissions from sources of a pollutant inside the microenvironment.
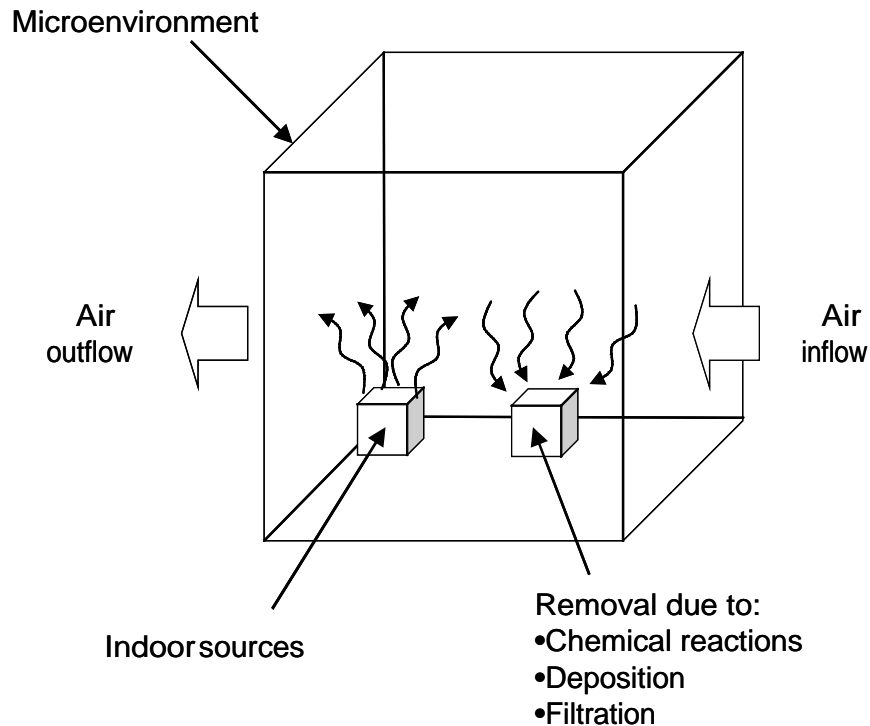
Figure 8.1. The Mass Balance (MASSBAL) Model

It is assumed that the flow of outside air into the microenvironment is equal to that flowing out of the microenvironment, and this rate is given by the air exchange rate, $R_{air\ exchange}$. $R_{air\ exchange}$ is given in units of hr^{-1}. The air exchange rate can be interpreted as the number of times per hour the entire volume of air in the microenvironment is replaced.

Considering the microenvironment as a distinct, well-mixed volume of air, the mass balance equation for a pollutant can be described by:

$$\frac{dC(t)}{dt} = \dot{C}_{in} - \dot{C}_{out} - \dot{C}_{removal} + \dot{C}_{source} \qquad (8\text{-}1)$$

where:

$C(t)$ = Concentration in the microenvironment at time t ($\mu g/m^3$)

$$\dot{C}_{in} = \text{Rate of change in C(t) due to air entering the micro}$$

$\dot{C}_{in}$ =   Rate of change in C(t) due to air entering the micro

$\dot{C}_{out}$ =   Rate of change in C(t) due to air leaving the micro

$\dot{C}_{removal}$ =   Rate of change in C(t) due to all removal processes

$\dot{C}_{source}$ =   Rate of change in C(t) due to all source terms

(Note that concentration must be in the same units as the ambient air quality data, i.e., either ppm, ppb, or $\mu g/m^3$, although throughout these equations concentration is shown only in $\mu g/m^3$ for brevity.

The change in microenvironmental concentration due to influx of air, $\dot{C}_{in}$, is

$$\dot{C}_{in} = C_{ambient} \times f_{proximity} \times f_{penetration} \times R_{air\,exchange} \qquad (8\text{-}2)$$

where:

$C_{ambient}$ =   Ambient timestep concentration ($\mu g/m^3$)

$f_{proximity}$ =   Proximity factor (unitless)

$f_{penetration}$ =   Penetration factor (unitless)

The proximity factor $f_{proximity}$ is used to account for differences in ambient concentrations between the geographic location represented by the ambient air quality data (e.g., a regional fixed-site monitor) and the geographic location of the microenvironment. That is, the outdoor air at a particular location may differ systematically from the outdoor air at the center of the air quality district. For example, a house might be located next to a busy road in which case the air outside the house would have elevated levels for mobile source pollutants such as carbon monoxide. The concentration $C_{outdoor}$ in the air directly outside the microenvironment is given by the product of the ambient concentration and $f_{proximity}$:

$$C_{outdoor} = f_{proximity} C_{ambient} \qquad (8\text{-}3)$$

For some pollutants (especially particulate matter), the process of infiltration may remove a fraction of the pollutant from the air. The fraction that is retained in the air is given by the penetration factor $f_{penetration}$. During exploratory analyses, the user may examine how a microenvironment affects overall exposure by setting the microenvironment's proximity or penetration factor to zero, thus effectively eliminating the microenvironment.

Change in microenvironmental concentration due to outflux of air is calculated as the concentration in the microenvironment C(t) multiplied by the air exchange rate:

$$\dot{C}_{out} = R_{air\,exchange} \times C(t) \qquad (8\text{-}4)$$

The third term in the MASSBAL calculation represents removal processes within the microenvironment. There are three such processes in general: chemical reaction, deposition, and filtration. Chemical reactions are significant for ozone, for example, but not for carbon

monoxide. The amount lost to chemical reactions will generally be proportional to the amount present, which in the absence of any other factors would result in an exponential decay in the concentration with time. Similarly, deposition rates are usually given by the product of a (constant) deposition velocity and a (time-varying) concentration, also resulting in an exponential decay. The third removal process is filtration, usually as part of a forced air circulation or HVAC system. Filtration will normally remove particles but not gases. In any case, filtration rates are also proportional to concentration. Change in concentration due to deposition, filtration, and chemical degradation in a microenvironment is simulated based on the first-order equation:

$$\dot{C}_{removal} = \left(R_{deposition} + R_{filtration} + R_{chemical}\right)C(t) = R_{removal} \times C(t) \tag{8-5}$$

where:

$\dot{C}_{removal}$ = Change in microenvironmental concentration due to removal processes ($\mu g/m3/hour$)

$R_{deposition}$ = Removal rate of a pollutant from a microenvironment due to deposition (1/hour)

$R_{filtration}$ = Removal rate of a pollutant from a microenvironment due to filtration (1/hour)

$R_{chemical}$ = Removal rate of a pollutant from a microenvironment due to chemical degradation (1/hour)

$R_{removal}$ = Removal rate of a pollutant from a microenvironment due to the combined effects of deposition, filtration, and chemical degradation (1/hour)

For unreactive gases like carbon monoxide, all three removal terms could be zero, in which case $R_{removal} = 0$.

The fourth term in the MASSBAL calculation represents pollutant sources within the microenvironment. This is the most complicated term, in part because several sources may be present. APEX allows two methods of specifying source strengths: emission sources (**ESource** or **ES**) or concentration sources (**CSource** or **CS**). Either may be used for MASSBAL microenvironments, and both can be used within the same microenvironment. The source strength values are used to calculate the source term $\dot{C}_{source}$, which has standard units of $\mu g/m^3/hr$.

Emission sources are expressed as emission rates in units of $\mu g/hr$. To determine the source term associated with an emission source, ES must be divided by the volume V of the microenvironment in m^3:

$$\dot{C}_{source,ES} = \frac{ES}{V} \tag{8-6}$$

Concentration sources however, are expressed in units of concentration. These must be the same units as used for the ambient concentration (e.g., $\mu g/m^3$). Concentration sources are normally

used as additive terms for microenvironments using the FACTORS method. Strictly speaking, they are somewhat inconsistent with the MASSBAL method, since concentrations should not be inputs but should be consequences of the dynamics of the system. Nevertheless, a suitable meaning can be found by determining the source strength $\dot{C}_{source}$ that would result in a mean increase of CS in the concentration, given constant parameters and equilibrium conditions, in this way:

Assume that a microenvironment is always in contact with clean air (ambient = zero), and it contains one concentration source. Then the mean concentration over time in this microenvironment from this source should be numerically equal to CS. The mean source strength expressed in ppm/hr, ppb/hr or $\mu g/m^3$/hr is the rate of change in concentration $\dot{C}_{source, CS}$. In equilibrium,

$$CS = \frac{\dot{C}_{source, CS}}{R_{air\ exchange} + R_{removal}}$$
(8-7)

$\dot{C}_{source, CS}$ can be written as

$$\dot{C}_{source, CS} = CS \times R_{mean}$$
(8-8)

where R_{mean} is the chemical removal rate. From eq. 8-7, R_{mean} is equal to the sum of the air exchange rate and the removal rate ($R_{air\ exchange} + R_{removal}$) under equilibrium conditions. In general, however, the microenvironment will not be in equilibrium, but in such conditions there is no clear meaning to attach to $\dot{C}_{source, CS}$ since there is no fixed emission rate that will lead to a fixed increase in concentration. The simplest solution is to use $R_{mean} = R_{air\ exchange} + R_{removal}$. However, the user is given the option of specifically specifying R_{mean} (see discussion of parameters below). This may be used to generate a truly constant source strength $\dot{C}_{source, CS}$ by making CS and R_{mean} both constant in time. If this is not done, then R_{mean} is simply set to the sum of ($R_{air\ exchange} + R_{removal}$). If these parameters change over time, then $\dot{C}_{source, CS}$ also changes. Physically, the reason for this is that in order to maintain a fixed elevation of concentration over the base conditions, then the source emission rate would have to rise if the air exchange rate were to rise.

Multiple emission and concentration sources within a single microenvironment are combined into the final total source term by combining equations 8-6 and 8-8:

$$\dot{C}_{source} = \dot{C}_{source, ES} + \dot{C}_{source, CS} = \frac{1}{V} \sum_{i=1}^{n_e} ES_i + R_{mean} \sum_{i=1}^{n_c} CS_i$$
(8-9)

where:

ES_i	=	Emission source strength for emission source i (μg/hour)
CS_i	=	Emission source strength for concentration source i ($\mu g/m^3$)

89

n_e =   Number of emission sources in the microenvironment

n_c =   Number of concentration sources in the microenvironment

(<u>A note on units</u>: The above equation is modified if the units of air quality are ppm or ppb rather than $\mu g/m^3$. Specifically, $1/V$ is replaced by f/V, where $f = 1/ppmFact$. The value of ppmFact is a user-supplied in the *Simulation Control* input file; it expresses the number of $\mu g/m^3$ that equate to 1 ppm. For the pollutant CO, ppmFact=1,145. The conversion factor ppmfactor could also be used to convert $\mu g/m^3$ to other units.)

Equations 8-2, 8-4, 8-5,and 8-9 can now be combined with 8-1 to form the differential equation for the microenvironmental concentration C(t). Within the time period of a timestep, $\dot{C}_{source}$ and $\dot{C}_{in}$ are assumed to be constant. Using $\dot{C}_{combined} = \dot{C}_{source} + \dot{C}_{in}$ leads to:

$$\frac{dC(t)}{dt} = \dot{C}_{combined} - R_{air\ exchange}C(t) - R_{removal}C(t)$$

$$= \dot{C}_{combined} - R_{mean}C(t) \qquad (8\text{-}10)$$

Solving this differential equation leads to:

$$C(t) = \frac{\dot{C}_{combined}}{R_{mean}} + \left(C(0) - \frac{\dot{C}_{combined}}{R_{mean}} \right)e^{-R_{mean}t} \qquad (8\text{-}11)$$

where:

C(0)   =   Concentration of a pollutant in a microenvironment at the beginning of a timestep $(\mu g/m^3)$

C(t)   =   Concentration of a pollutant in a microenvironment at time t within the time period of a timestep $(\mu g/m^3)$.

Based on eq. 8-11, the following three concentrations in a microenvironment are calculated:

$$C_{equil} = C(t \to \infty) = \frac{\dot{C}_{combined}}{R_{mean}} = \frac{\dot{C}_{source} + \dot{C}_{in}}{R_{air\ exchange} + R_{removal}} \qquad (8\text{-}12)$$

$$C_{end} = C_{equil} + \left(C(0) - C_{equil} \right)e^{-R_{mean}t} \qquad (8\text{-}13)$$

$$C_{mean} = \frac{\int_0^1 C(t)dt}{\int_0^1 dt} = C_{equil} + \left(C(0) - C_{equil} \right)\frac{1 - e^{-R_{mean}t}}{R_{mean}t} \qquad (8\text{-}14)$$

where:

t   =   length of the APEX timestep (hours)

$$C_{equil} \quad = \quad \text{Concentration in a microenvironment (}\mu g/m^3\text{) if } t \to \infty$$
$$\text{(equilibrium state).}$$

$$C(0) \quad = \quad \text{Concentration in a microenvironment at the beginning of the}$$
$$\text{timestep (}\mu g/m^3\text{)}$$

$$C_{end} \quad = \quad \text{Concentration in a microenvironment at the end of the timestep}$$
$$(\mu g/m^3)$$

$$C_{mean} \quad = \quad \text{Mean concentration in a microenvironment for timestep (}\mu g/m^3\text{)}$$

$$R_{mean} \quad = \quad R_{air\ exchange} + R_{removal} \quad \text{(1/hour)}$$

At each timestep of the simulation period, APEX uses Eqs. 8-12, 8-13, and 8-14 to calculate the equilibrium, ending, and mean concentrations. APEX reports mean concentration as the concentration for a specific timestep. The calculation continues to the next timestep by using C_{end} for the previous timestep as $C(0)$.

The microenvironmental parameters for the MASSBAL method that can be defined by the user in the *Microenvironment Descriptions* file are summarized in the Table 8.2, with their valid ranges and their corresponding names in the file.

Table 8.2. Microenvironmental Parameters

Parameter	Definition	Units	Range	Default Value	Name[a]
$f_{proximity}$	Proximity factor	unitless	$f_{proximity} \geq 0$	1	PR
$f_{penetration}$	Penetration factor	unitless	$0 \leq f_{penetration} \leq 1$	1	PE
CS	Concentration source	$\mu g/m^3$, ppb, or ppb	$CS \geq 0$	0	CS
ES	Emission source	$\mu g/hr$	$ES \geq 0$	0	ES
$R_{removal}$	Removal rate due to deposition, filtration, and chemical reaction	1/hr	$R_{removal} \geq 0$	0	DE
$R_{air\ exchange}$	Air exchange rate	1/hr	$R_{air\ exchange} \geq 0$	none	AE
R_{mean}	Mean removal rate:	1/hr	$R_{mean} \geq 0$	$R_{removal} + R_{air\ exchange}$	MR
V	Volume of microenvironment	m^3	$V > 0$	none	V

[a] Designation in *Microenvironment Descriptions* file

Not all of the possible parameters are always needed, and several of them have natural default values. Based on the above equations, the following generalizations can be made about the definition of the MASSBAL parameters in the *Microenvironment Descriptions* file:

- Air exchange rate is a critical parameter that is always needed in a MASSBAL calculation. It must always be defined in the file as it has no default value.

- Air exchange rate and volume are not pollutant-specific, and therefore are defined only once for each micro. All other parameters must be defined for each pollutant.

- Removal rate must also be user-defined in the file if not assumed to be zero. For some pollutants it can be assumed to have a natural default value of zero.

- The proximity and penetration factors must be defined in the file unless assumed to be unity, which is the natural default value for both factors that should be used in the absence of data to the contrary.

- If any emission source terms are present then volume must be defined. Volume has no default value.

- If any concentration source terms are present then the mean removal rate may be user-defined, but if appropriate, it may assume a default value of ($R_{air exchange} + R_{removal}$).

The details for specifying these input parameters in the *Microenvironment Descriptions* file are provided in the *Volume I* of this User's Guide. Further details on the options for designating these parameters are given in Section 8.2.4.

In APEX, it is assumed that the outdoor concentration and the other modeling parameters for the MASSBAL method remain constant during any timestep. Of course, recalling that the APEX default timestep is one hour, in many cases the MASSBAL parameters may not remain constant for an timestep at a time. For example, a person may enter a microenvironment and smoke a cigarette for five or ten minutes and then leave. Or, someone might enter a kitchen and cook for a few minutes using a gas stove. Or one might alter an air exchange rate by opening or closing a window. There are two reasons why it is difficult to model such events in APEX. First, there is already a large computational burden in calculating concentrations in every microenvironment for every timestep for every simulated person. This burden is substantially large if very fine time resolution were demanded. Second, most examples of fine-scale parameter variation are driven by human actions. The CHAD activity diaries generally do not contain enough detail to determine when each cigarette is lit or each time a stove is used or a window is opened or closed. Furthermore, the diaries only follow the activities of a single person. It is quite possible for these actions to be performed by other people. For example, if the activity diary follows a child, then the child's parents may be doing these things that affect the properties of the microenvironments that the child is in. Since the diaries do not reliably report such information, it was decided that a very fine time resolution could not reliably be used for the calculation of concentrations.

In a MASSBAL microenvironment, the concentration during any timestep depends on the concentration for the timestep before. Ultimately, all timesteps depend on some method for establishing initial conditions. To avoid the problem of establishing new initial conditions every time the activity diary indicates that a MASSBAL microenvironment is entered, the time series is evaluated for all timesteps in the simulation period. An extra 24 hour period is added prior to the start of the APEX simulation period by duplicating the properties from the first day of the

simulation period. It is assumed that 24 hours is sufficient so that the initial concentration becomes irrelevant. The entire simulation period is then evaluated timestep by timestep without gaps, with each timestep being used to determine the next.

8.2.3 Factors Method

The FACTORS method is simpler than the mass balance method. In this method, the value of the concentration in a microenvironment is not dependent on the concentration during the previous timestep. Rather, the method uses the following equation to calculate timestep concentration in a microenvironment from the user-provided air quality data:

$$C_{timestep} = C_{ambient} f_{proximity} f_{penetration} + \sum_{i=1}^{n_C} CS_i$$

(8-15)

where:

$C_{timestep}$ = Timestep concentration in a microenvironment ($\mu g/m^3$)

$C_{ambient}$ = Timestep concentration in ambient environment ($\mu g/m^3$)

$f_{proximity}$ = Proximity factor (unitless)

$f_{penetration}$ = Penetration factor (unitless)

CS_i = Mean air concentration resulting from source i ($\mu g/m^3$)

n_c = number of concentration sources in the microenvironment

The user may provide values for proximity, penetration, and any concentration source terms, or may allow them to assume default values (see Table 8.2); however, it is not mandatory that the user supply any values if the default values are suitable. An undefined proximity or penetration is assumed to be unity at all times. Missing (i.e., undefined) sources are assumed to be zero. Parameters are left undefined by simply omitting them from the *Microenvironment Descriptions* input file. If all parameters are missing, then the concentration in the microenvironment is always the same as the ambient concentration. All of the parameters in the above equation are evaluated for each timestep, although these values might remain constant for several hours, entire days, or even for the entire simulation. For the ambient concentration, the timestep values come from the input *Air Quality Data* file, and may be either measurements or modeled results, or may be sampled for each hour from a distribution (see *Volume I* for available formats of this file). For the other parameters, the timestep values are the result of the calculations based on the information specified in the *Microenvironment Descriptions* input file.

8.2.4 Microenvironment Parameter Definitions

The second section of the *Microenvironment Descriptions* input file contains the rules for determining the values of the parameters used in the MASSBAL and FACTORS methods. Instructions for specifying microenvironmental input parameters (those in Table 8.2) in the *Microenvironment Descriptions* file are provided in *Volume I* of this User's Guide, but further details on the options for using resampling rates, conditional variables, periodic (daily, weekly,

and monthly) groupings, and random seeds, are provided in this section. This includes an explanation of ways to specify CS terms as products of distributions.

Both of the concentration calculation methods require multiple user-defined input parameters. These microenvironmental parameters are defined by probability distributions defined in the *Microenvironment Descriptions* input file, with values being assigned to each timestep of the simulation. The file is read in **MicroEnvModule:ReadMicroData**. Any of the following distribution types in Table 3.1 can be used for microparameters.

The user may provide different distribution data for the parameter for any combination of the following temporal and spatial variables:

- Hour in a day

- Day in a week

- Month in a year (i.e., season)

- Air quality district

For example, the user can define probability distributions for a parameter that vary depending on the time of day and whether the simulated timestep is on a weekday or a weekend, or the user can define a distribution that changes with the season of the year and with the air quality district associated with the microenvironment being considered (recall that home and work sectors for each profile will be associated with a unique air quality district).

The distributions for the microenvironmental parameters may also depend on conditional variables that are a subset of the profile variables for an individual. A single microenvironmental parameter may depend on up to three of the above conditional variables. Conditional variables may change on an interpersonal, geographic, meteorological, or temporal basis, influencing the microparameters accordingly.

The rules for determining any microenvironmental parameter (MP) are unique to each microenvironment. For example, the rules for proximity for a house may differ completely from the rules for proximity for a car. Every combination of parameter, pollutant, and microenvironment is distinct (with the exception of air exchange rate and volume, which can only be defined once per micro). The order in which the MP definitions are presented is not significant to APEX, although it might help the user to group them by microenvironment, pollutant, or MP. Note that the entire definition of an MP can be omitted if its default value is acceptable, so for example if proximity is always to be unity in some microenvironment, then no MP definition is needed for proximity in that microenvironment. The example in Exhibit 8-1 shows one possibility for the proximity parameter for microenvironment #1. The actual data are only for illustrative purposes and are not intended to properly represent this MP in any real scenario.

```
Micro number      = 1
Pollutant = 3
Parameter Type    = Proximity
Hours - Block     = 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1 1
Weekday-DayType   = 1 1 1 1 1 1 1
Month-Season      = 1 1 2 2 2 3 3 3 4 4 4 1
District-Area     = 1 1 1 1 1 1
Condition #1 = 0
Condition #2 = 0
Condition #3 = 0
ResampHours = NO
ResampDays  = YES
ResampWork  = YES
RandomSeed  = 0
Block DType Season Area  C1  C2  C3   Shape      Par1   Par2  Par3 Par4  LTrunc UTrunc  ResampOut
1     1     1      1     1   1   1    Normal     1.5    1.2    .    .      0     4.0      Y
2     1     1      1     1   1   1    Point      2.0    .      .    .      .     .        .
1     1     2      1     1   1   1    Lognormal  1.2    1.5    .    .      0     10       Y
2     1     2      1     1   1   1    Lognormal  0.4    1.2    .    .      0     10       Y
1     1     3      1     1   1   1    Triangle   0      3      2    .      .     .        Y
2     1     3      1     1   1   1    Normal     2.5    1.5    .    .      .     .        Y
1     1     4      1     1   1   1    Uniform    0      3      .    .      .     .        Y
2     1     4      1     1   1   1    Lognormal  3      2      .    .      0     10       Y
```

Exhibit 8-1. Example of a Microenvironmental Parameter Description

The general format is the same for all MPs. The first three lines are mandatory and specify the microenvironment number, the pollutant (indicated by its order in the *Control* file), and the MP, or parameter type (the **Pollutant** line may be absent for AER and Vol). This combination should be unique for every MP in the input file, with the possible exception of enumerated sources (discussed later).

The parameter types are indicated using standard keywords (given in Table 8.2). Note that only the first two characters of the parameter type are checked by APEX, and the keyword is not case sensitive, so the example above could use "PR". The user may spell out the parameter types if desired, providing greater clarity.

After the microenvironment number and parameter type, any or all of the remaining lines containing an equal sign may be omitted. These indicate the settings for various options, all of which have default values. These settings may appear in any order within the description; they are recognized via the keyword that precedes the equal sign. One option, missing in the above example since it only applies to parameter types ES and CS, is the source number. See section 8.2.4.6 for an example using this option. The other seven options in this example are the mappings that determine the values for the seven indices that label each distribution. This is followed by three resampling options and a random seed initialization option. These options are covered in the following subsections.

After all the options are specified, the next line (starting with "Block") indicates that the following lines contain descriptions of distributions. At least one distribution is always required; the exact number needed depends on the settings of the seven indexing options. The shortest possible MP description (other than one completely missing) consists of five lines. Such a description would have the first four mandatory lines, the header line indicating that distributions follow, and a single distribution that applies to all timesteps of the simulation, as in Exhibit 8-2.

```
Micro number = 1
Pollutant = 1
Parameter Type = Proximity
Block DType Season Area  C1  C2  C3  Shape  Par1  Par2  Par3 Par4  LTrunc UTrunc  ResampOut
1     1     1      1      1   1   1   Normal 1.5   1.2   .    .     0      4        Y
```

Exhibit 8-2. Example of the Shortest Possible MP Description

These rules state that the proximity in microenvironment #1 is to be drawn from a normal distribution with mean 1.5 and standard deviation 1.2. If the value drawn is below zero or above 4.0 then another value is drawn, until one is found that is within bounds. This single value is then applied to all timesteps of the simulation, for that particular simulated individual, for their home air quality district. A separate single value is applied to that individual for all timesteps in their work district. Actually, a third value, the average of the first two, is applied to all timesteps in the "other" (non-home, non-work) air quality district. In effect, all the microenvironments are modeled in triplicate to account for the three different places. In the above example the three values would all be the same if an extra line "ResampleWork=NO" were added after the second line. Each simulated individual is modeled independently so new values are drawn for all parameters when starting another profile.

It is necessary that all the parameter distribution data be given in the correct units (i.e. those that are compatible with the data in the *Air Quality Data* input files.)

The motivation for the rather complex programming that defines and evaluates the MP is that the various parameters that enter the MASSBAL and FACTORS equations may have widely divergent properties. For example, a parameter like house volume should have a single value that does not change over time. Another parameter such as an air exchange rate may change every hour. Some parameters like source strengths from cooking or from traffic may show strong diurnal patterns that may repeat on a daily or a weekly basis. Parameters that relate to temperature may show seasonal variation.

There are a number of possibilities for each optional rule in the MP definitions. The options fall into the following categories:

- Time and area mappings;
- Conditional variables;
- Correlation settings;
- Resampling options;
- Random number seeds; and
- Source number specification.

Each of these are discussed in the following subsections, after which comes a brief subsection on the specification of distributions.

8.2.4.1 Time and Area Mappings

Each MP is evaluated for every timestep of the simulation period. Normally this is done by drawing a value at random from a distribution. The user may specify that different distributions

apply at timesteps within different hours of the day. Furthermore, the frequency of sampling can be controlled by the user. It is not the case that a new value must be drawn every timestep, instead values drawn for other times may be reused. The primary purpose of the time and area mappings is to specify which distribution applies to each timestep. The secondary purpose, in conjunction with the resampling options, is to establish periodic reuse of values on a daily, weekly, monthly, or geographical basis.

As an example, suppose some parameter should be sampled from one distribution during typical working hours and from another distribution at other times. This can be accomplished by defining two "blocks" and assigning each hour of the day to either block #1 or block #2. Perhaps hours 1-7 (midnight to 7 a.m.) and hours 19-24 (6 p.m. to midnight) belong to block #1, while hours 8-18 (7 a.m. to 6 p.m.) belong to block #2. Then distributions must be defined for block #1 and block #2. Hours that fall into block #1 will have their parameter values drawn from the distribution that applies to block #1, and so on. If, for example, the distribution for block #2 has the higher mean, then the daytime values for the parameter will generally be higher than the nighttime values, generating a diurnal pattern. Similarly, weekly and seasonal patterns may be generated.

The Hour-Block (HB) mapping indicates the block to which each hour of the day belongs. The mapping must contain 24 numbers (even if the time steps do not equal an hour). The first is the block number for hour 1 (midnight to 1 a.m.), and so on. All timesteps belonging to the same block use the same distribution. The block numbers range from 1 upwards; there can be anything from 1 to 24 blocks. The number of blocks (#blocks) is determined from this mapping itself. If the Hour-Block mapping is missing it is assumed that there is only one block, which implies that the parameter values for all 24 hours of the day (that is, all timesteps) are taken from the same distribution. The term "Block" might suggest that the hours belonging to a given block should be adjacent chronologically, but this is not necessary in APEX. It is also not necessary for each block to contain the same number of hours.

The Weekday-Daytype (WT) mapping is similar to the Hour-Block mapping, except that it contains seven values instead of 24. The first value is the day type for Sunday, the second is for Monday, and so on until the last which is the day type for Saturday. The seven days of the week are in the same order as on a standard calendar. Thus if day type 1 is weekday and 2 is weekend, the vector should be (2 1 1 1 1 1 2), but without the parentheses. The mapping (1 2 2 2 2 2 1) would be equivalent if the distributions presented further down were appropriately renumbered. If the WT mapping is missing in the *Microenvironment Descriptions* input file, then only one day type is assumed, that is, the default mapping is (1 1 1 1 1 1 1).

The Month-Season (MS) mapping is similar to the previous two, except that 12 numbers are needed. The first number indicates the season for January, and so on through December. Again, if this mapping is missing then a single season is assumed to apply to all months.

The District-Area (DA) mapping is similar to the others, except that the number of air quality districts is not a universal constant, but may vary from one simulation to another. If the mapping is present, the user must ensure that it contains the correct number of terms (one area assignment for each air quality district in the study area). The district indices represent the APEX air district numbers, as enumerated in the *Sites* output file.

If the user defines 2 blocks, 2 day types, 4 seasons, and 3 areas, then a total of 48 distributions (that is, 2 x 2 x 4 x 3) must be specified, one for each possible combination. The number would be even larger if any conditional variables were used. To ease the burden of data requirements the number of cases should be kept to a minimum. For example, if the seasonal dependence of this parameter were weak, one could eliminate it and reduce the number of distributions from 48 to just 12. If this is too extreme, perhaps two seasons would suffice to capture the variation. The number of seasons (or blocks, day types, or areas) can be defined differently for each MP, even ones that belong to the same microenvironment. Each MP is evaluated for all timesteps in the simulation period, independently of other MP, so there is no reason why the rules for one MP should match or correspond with the rules for any other MP.

8.2.4.2 Conditional Variables

Selected profile variables may be used to influence the parameter values in the MASSBAL or FACTORS equations. These profile variables are known as *Conditional Variables*. Conditional variables can be used to vary parameters on a profile, daily, hourly, or timestep basis. The list of variables to use for the current simulation are set in **ProfileModule: SetCVlist**. The allowable conditional profile variables are:

- *Gender*
- *Population category (Race/gender combination)*
- *Employed*
- *HasGasStove*
- *HasGasPilot*
- *AC_Home*
- *AC_Car*
- *Window_Res*
- *Window_Car*
- *SpeedCat*
- *ProfileConditional1*
- *ProfileConditional2*
- *ProfileConditional3*
- *RegionalConditional1*
- *RegionalConditional2*
- *RegionalConditional3*
- *RegionalConditional4*
- *RegionalConditional5*
- *FactorGroup*

These variables influence the parameters on a profile basis. See Chapter 5 for definition of these variables. With the exception of the first three, rules for setting these variables for each profile are defined in the *Profile Functions (Distributions*) input file. In addition to these variables, the MPs can also depend on seven meteorological variables:

- ***TempCat*** Hourly temperature, binned into categories.
- ***HumidCat*** Hourly humidity, binned into categories.
- ***PrecipCat*** Hourly precipitation category.
- ***WindCat*** Hourly wind speed, binned into categories.
- ***DirCat*** Hourly wind direction, binned into categories.
- ***MaxTempCat*** Daily maximum temperature, binned into categories.
- ***AvgTempCat*** Daily average temperature, binned into categories

The first five can influence parameters on an hourly basis, while the last 2 are daily-varying parameters.

The MPs can depend daily on 5 user-defined daily varying functions.

- ***DailyConditional1***
- ***DailyConditional2***
- ***DailyConditional3***
- ***DailyConditional4***
- ***DailyConditional5***

Finally, the MPs can depend daily on 5 user-defined functions that depend on the ambient air quality and vary with each timestep:

- ***AQConditional1***
- ***AQConditional2***
- ***AQConditional3***
- ***AQConditional4***
- ***AQConditional5***

These hourly, timestep, and daily varying variables are not profile variables. However, rules for defining them are also designated in the *Profile Functions (Distributions*) input file (see *Volume I*).

Note that Conditional Variables must be integer, since their values are used as indices to select the distribution to be sampled. In practice, the number of categories must be fairly small (generally 2 or 3) or else defining distributions for every case becomes burdensome. It should be noted that while the concentrations in various microenvironments may depend on the profile through the conditional variables, these concentrations do not depend on the activity diaries or the event structure.

The user may select up to three Conditional Variables from the list for each MP. If one is used, it does not matter whether conditional variable #1, #2, or #3 is used. If more than one is used then the order they are designated does not matter.

The conditional variable to be applied is identified by its name. For example, if a parameter were to depend on gender then it would be indicated as follows in the input file:

```
Condition # 1      = Gender
```

Note that the word "Gender" must be spelled out in full as in the above list, but it is not case sensitive. There are two ways to indicate that a conditional variable is not used. Either the line for it can be omitted, or else the variable name can be set to anything that is not on the list. The standard practice (if the line is not simply omitted) is to set the right hand side to zero:

```
Condition # 1  = 0
```

There is a complication for the user when it comes to specifying the distributions that are applicable to conditional variables. Each distribution has seven indices (four for time and area mappings and three for Conditional Variables). But the values that any index may have must be integers. Thus, if gender is used as a Conditional Variable then the user must specify distributions for gender=1 and for gender=2. The user cannot use mnemonic devices such as "M" or "F" instead. The numerical codes for the Conditional Variable are set as constants in **GlobalModule** and are as follows:

- *Gender:* 1=Male, 2=Female

- *Employed:* 1=YES, 2=NO

- *HasGasStove* 1=YES, 2=NO

- *HasGasPilot:* 1=YES, 2=NO

- *AC_Car:* 1=YES, 2=NO

- *Window_Res:* 1=OPEN, 2=CLOSED

- *Window_Car:* 1=OPEN, 2=CLOSED

For the population category conditional variable, the conditional variable value codes are integers that represent the order in which the population categories are defined in the "Population file" definitions in the *Control* file. For example, if "Native American females" is the third population file defined, then the code for that population category would be 3. The other Conditional Variables, the numerical values are provided by the user in the *Profile Functions* input file, so there are no pre-assigned ranges or interpretations. The list of conditional variables to be used in defining MPs is set in **DistributionModule:SetCVList**.

8.2.4.3 Correlation Settings

In APEX the user has the option of correlating samples for microenvironmental parameters. Such correlation would make sense, for example, when the value of the parameter is assumed to

be mainly a function of the properties of a simulated individual's home and the pollutants have similar properties (for example, are all particles). In addition, in some cases it may be that the same parameters may be correlated in different microenvironments.

APEX uses a simple method of correlation microparameters - by sampling them using the same random numbers. This results in values being selected for correlated parameters at the same percentile from the appropriate distributions. The percentiles will correspond each hour as long as the 2 (or more) parameters use the **same conditional variables, time and area mappings, and resampling rates** and thus have the same number of required distributions and samples. Otherwise the samples get out of phase and any correlation is lost. APEX checks that the conditionals, mappings, and resampling are the same when correlating parameters, and writes a warning if they are not. APEX will still run, but the user should be aware that the correlation is lost.

Correlation is handled by an optional keyword in the microparameter definition, CORRNUM. Each subset of microparameters that the user desires be correlated (sampled at the same percentile each hour) are assigned a unique integer 1-N, where N is the total number of correlated subsets. For example, assume that the user wants to correlate the penetration and decay values for residences (micro #1) for 2 pollutants. Valid MP definitions for this case are shown in

```
! PENETRATION FACTOR

Micro number       = 1
POLLUTANT = 1
CorrNum =  1
Parameter Type     = PE
Month - Season = 1 1 1 1 2 2 2 2 2 2 1 1
ResampHours        = NO
ResampDays         = YES
ResampWork         = YES
Block DType Season Area C1  C2  C3   Shape      Par1   Par2  Par3 Par4  LTrunc UTrunc  ResampOut
1     1     1      1    1   1   1    Normal     0.5  0.2  .    .     0.1    1.0     Y
1     1     2      1    1   1   1    Normal     0.8  0.2  .    .     0.1    1.0     Y

Micro number       = 1
POLLUTANT = 2
CorrNum =  1
Parameter Type     = PE
Month - Season = 1 1 1 1 2 2 2 2 2 2 1 1
ResampHours        = NO
ResampDays         = YES
ResampWork         = YES
Block DType Season Area C1  C2  C3   Shape      Par1   Par2  Par3 Par4  LTrunc UTrunc  ResampOut
1     1     1      1    1   1   1    Normal     0.4  0.1  .    .     0.1    1.0     Y
1     1     2      1    1   1   1    Normal     0.7  0.1  .    .     0.1    1.0     Y


! DECAY RATES

Micro number       = 1
POLLUTANT = 1
CorrNum =  2
Parameter Type     = DE
ResampHours        = NO
ResampDays         = NO
ResampWork         = YES
Block DType Season Area C1  C2  C3   Shape      Par1   Par2  Par3 Par4  LTrunc UTrunc  ResampOut
1     1     1      1    1   1   1    LogNormal  2.51  1.53  0    .     0.95   8.05    Y

Micro number       = 1
POLLUTANT = 2
CorrNum =  2
Parameter Type     = DE
ResampHours        = NO
ResampDays         = YES
ResampWork         = YES
Block DType Season Area C1  C2  C3   Shape      Par1   Par2  Par3 Par4  LTrunc UTrunc  ResampOut
1     1     1      1    1   1   1    LogNormal  2.51  1.53  0    .     0.95   8.05    Y
```

Exhibit 8-3. Example of Defining Correlated Microparameters

In this example, the 2 penetrations are correlated, as are the decays, but the decays and
penetration are not correlated with each other. (If for some reason this was desirable, all four
descriptions could be set to have CorrNum=1).

Note that if the same distributions are assigned to each pollutant (which is true for decay in this
example), the pollutants will use the exact same parameter values (samples) for that pollutant for
each hour.

8.2.4.4 Resampling Options

The time and area mappings indicate which cases are to have their parameter values drawn from the same distribution. However, they do not distinguish between cases when a single parameter value is to be drawn and applied to multiple timesteps and when separate values from the same distribution are to be drawn. The concept is called resampling, and the two specific cases mentioned above correspond to ResampTS=NO and ResampTS=YES.

There are four resampling options, namely for timesteps, hours, days, and work air quality district. Each may be set to either YES or NO. If ResampTS=NO and ResampleHours=NO, then all timesteps within a block on any day of the simulation will share the same value. Timesteps in different blocks have their values drawn from different distributions, so these values are never shared. If Resample TS=NO and ResampHours=YES, then only timesteps within each hour will share values. If ResampTS=YES, then each timestep in the same block on the same day will have its own value drawn, so $N_{timestep}$ values will be drawn no matter how many blocks there are. In this case the blocks serve only to determine which parent distribution is used for each particular hour. The defaults are ResampTS=NO and ResampHours=NO. If the *Control* file variable TimeStepsPerDay is equal to 24 (the APEX default), then ResampTS and ResampHours are interchangeable. If TimeStepsPerDay < 24, then the ResampHours flag has no meaning and is ignored (because the microconcentrations are only calculated for each timestep, which in this case is greater than an hour).

The second resampling option is ResampDays. If ResampDays=NO, then the same daily profile is used on all days in the same category. If ResampDays=YES, then all days have new sets of values drawn for them. The category for days is defined by the combination of day type, season, and conditional variables. An example might be all winter weekdays with windows open, if day type = weekday and season = winter and condition #1 = (WindowPos==OPEN), assuming these terms have been defined appropriately. If ResampDays=NO (which is the default) then all such days in the simulation period will share the same set of values.

The third resampling option is ResampWork. APEX normally generates different parameter values for home and work locations. However, there are cases when this is not logical. For example, if a car is defined to be a microenvironment and it uses the mass balance method, the volume of the car should be the same whether the car is at home or at work. If ResampWork=YES, then home and work always draw parameter values independently. If ResampWork=NO, then the same values are used for work as for home. Since such cases are rare, ResampWork=YES is the default, meaning that the workplace will have its values sampled independently of the home.

To summarize, the default values for ResampTS, ResampHours and ResampDays are NO, and for ResampWork it is YES. This means that the default is to draw only two values (one for home and one for work) from each distribution listed for that MP and to apply those values whenever possible. If a default is to be used then the line may be omitted from the input file, but it does not hurt to show the lines anyway for purposes of clarity.

8.2.4.5 Random Number Seeds

One of the features of the APEX model is the ability to conduct paired runs by controlling the random number seeds. In normal use the model stochastically generates random profiles, selects diaries, and generates MP values from distributions. If multiple model runs are to be independent then the main ***RandomSeed*** value in the *Simulation Control* input file should be set to zero or to different values. If model runs are to be paired, then identical streams of random numbers are desired, in which case RandomSeed should be set to the same positive number in both runs.

Creating paired runs in which everything is identical will create results that are identical as well. Thus, the usual mode of operation is to have one specific difference between the two runs and then see how much effect it has on the results. The difficulty from a programming point of view is that it is not sufficient to simply start both runs with the same random number seed. In addition, multiple random number streams are required. As an example, suppose one of the paired runs contains an extra source term, and there was only one random number stream. The first profile in both runs would be the same, as would all random numbers evaluated until values are drawn for the new source. From then on the two runs will be drawing random numbers out of phase, meaning at different points in the stream. This means that the next profile will differ between the two runs.

In APEX the solution to the problem of getting out of phase is to set up multiple random number streams. Then, for example, it is possible to generate the profile variables by sampling from one stream while generating sources from another. This ensures that even if the sources differ, the same profiles will be generated in both runs, since the random numbers used for the profiles always will stay in step. The "extra" random numbers used for the additional source are drawn from a separate stream and therefore do not affect the status of any of the other streams.

In general, paired runs using the same microparameters will stay in phase (even if the definitions for these microparameters change). However, if a different number of microparameters are defined (if, for example, a different number of sources are used for 2 different runs), then APEX will get out of phase. The solution to this is to allow a definition random number seed for each MP.

Each MP has an optional line for setting a RandomSeed specific to that MP. There are two choices. If RandomSeed is set to a positive value, then that sets an absolute starting point for the stream for that MP that can be set the same in another run. If RandomSeed = 0 (which is the default) then the seed is chosen internally. This internal seed is fixed relative to the overall model seed as defined in the *Simulation Control* file, based on the order of the MP definitions. Thus, if the first MP defined in the *Microenvironment Descriptions* input file has RandomSeed = 0, then this stream will begin at a fixed offset from the main stream for the model run. There are two cases, depending on whether the main seed has a fixed value or is set to zero. If the main seed is fixed (as for two paired runs), then the starting seed value for any MP will be the same in both runs, provided the MP are in exactly the same order in both runs. However, this is not the case unless the run with "extra" MP has them all appear in the input file after the MP that are in common to both runs. To avoid this restriction, it is better in paired runs to set each MP to have a non-zero random seed of its own. If the main seed is 0 and an MP seed is greater than 0, runs

can be generated in which: 1) the MP values are reproduced exactly and 2) all other random aspects of the model (for example, the profiles) change.

If an MP has RandomSeed = 0 and the *Simulation Control* file also has RandomSeed = 0, then the MP will have a starting seed that has a fixed offset from a randomly chosen main seed. This means that the MP will draw random numbers independently from one run to another.

In summary there are three cases. If independent, random runs are desired then set the main RandomSeed in the *Simulation Control* file to zero and for each MP either set the RandomSeed to zero or simply omit the option. If paired runs are desired and the MP are not altered between runs, then the main seed in the *Simulation Control* file should be nonzero and it does not matter whether the seeds for each MP are zero or not (although if they are not zero the seeds should be the same in both runs). If paired runs involve changes to the list of MP then all seeds should be set to positive values, matching seeds in the MP common to both runs.

8.2.4.6 Source Strength Specification

As described in the sections on the MASSBAL and FACTORS methods (Sections 8.2.1 and 8.2.3), APEX allows two types of sources to be defined. **ESource** terms are emission sources expressed in units of micrograms per hour. **CSource** terms are sources expressed in concentration units of $\mu g/m^3$ (or ppm, ppb). ESource and CSource strengths can optionally be specified as the product of two or more values drawn from different distributions.

As an example, an ESource term representing emissions from gas stoves can be constructed as the product of three terms: a binary switch for Use/Non-use for each timestep, a duration of usage term, and an emission rate per minute of usage. One advantage of separating this term into three pieces is that different rules for the time and area mappings and the resampling rate can be defined for each of the three pieces.

Each source in APEX, meaning each MP of type ES or CS, may be assigned an optional source number. This is done by adding a line to the MP definition as inExhibit 8-3:

```
Micro number   = 4
Parameter Type = ES
Source number = 2
Pollutant = 1
Block DType Season Area  C1  C2  C3    Shape      Par1   Par2  Par3 Par4  LTrunc UTrunc  ResampOut
1     1     1      1     1   1   1     Lognormal  1000   2     .    .     100    10000   Y
```

Exhibit 8-4. Use of Source Number in MP Definition

For clarity, the source number should appear right after the parameter type. It cannot appear earlier nor can it appear after the header line starting with "Block". It only applies to types ES or CS and is not relevant for other parameter types. If the source number is omitted then it is assumed to be zero, which is the catch-all category for additive source terms.

All MP of type ES or CS that share the same microenvironment number and source number are evaluated separately for all timesteps according to their own rules, then the results are multiplied together on an timestep basis. For example, if another MP has the description shown in Exhibit 8-5, then both this MP and the previous one are evaluated for each timestep and then the results are multiplied together, timestep by timestep.

```
Micro number  =  4
Parameter Type=  ES
Source number = 2
Pollutant = 1
Hours - Block = 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 1 1 1 1
Block DType Season Area  C1  C2  C3   Shape      Par1  Par2  Par3 Par4  LTrunc UTrunc  ResampOut
1     1     1      1     1   1   1    Normal     10    10    .    .     0      60      Y
2     1     1      1     1   1   1    Point      45    .     .    .     .      .       .
```

Exhibit 8-5. Second MP Definition with Source Number 2.

Since the first MP was not resampled, only one value is generated per person and that value remains constant over the simulation. The second MP is resampled every hour (although the timesteps using the Point distribution will all return the same value).

It is possible to have a large number of terms sharing the same microenvironment and source numbers, in which case all terms are evaluated separately and the timestep results are multiplied. Note that all terms sharing the same microenvironment and nonzero source numbers must also share the same parameter type; one cannot mix ES and CS types since it does not make sense to multiply them together. APEX will generate an error message if this is attempted. It is possible for some sources to be ES while others are CS, even in the same microenvironment, as long as they are not assigned the same nonzero source numbers.

Once the product is evaluated, the result is treated exactly the same as any additive sources for that microenvironment. All ESource terms are added together timestep by timestep, whether each resulted from a product or was a separate term by itself. The same applies to all CSource terms in the same microenvironment. In effect there is no change at all to either the MASSBAL or the FACTORS equations, there is simply a change in how the ESource and CSource terms are determined.

When defining product terms, a line must be added to the *Simulation Control* input file indicating the largest source number used in the run for each pollutant. This line has the keyword *#SOURCES* and it might appear as in the pollutant parameters section of the *Simulation Control* file as shown in Exhibit 8-6.

```
Pollutant  = CO

DoDose      = YES
InputUnits  = ug/m3
OutputUnits = ug/m3
#Sources    = 3
```

Exhibit 8-6. Use of #sources Setting in the Pollutant Parameters section of the *Simulation Control* File.

This value reported here (3 in this case) is echoed to the *Log* file after "#microenvironments" and it is called "#Enumerated sources". Actually, like #microenvironments, this value is only used to allocate array space, and APEX will run correctly as long as #sources is large enough to accommodate the source numbers used in the *Microenvironment Descriptions* input file. If #sources is larger than is needed, no error occurs although job execution will be slightly less efficient. This line can only be omitted from the *Simulation Control* file if no source numbers are assigned to any MP.

106

Not all sources need be expressed as products. These sources can either be left without source numbers or can explicitly have source number of zero, or may even have a positive source number. If there is only one MP with a given microenvironment number and source number, then it essentially constitutes a product with only one term. If only source numbers = 0 are used (i.e. only additive terms are defined), then #Sources may be set to 0 in the control file or omitted.

8.2.4.7 Specification of Distribution Data

The number of distributions that the user must supply for each MP is the product of these numbers:

$$N_{Distributions} = N_{blocks} \text{ x } N_{daytypes} \text{ x } N_{seasons} \text{ x } N_{areas} \text{ x } N_{C1} \text{ x } N_{C2} \text{ x } N_{C3} \qquad (8\text{-}16)$$

Here N_{C1}-N_{C3} are the number of possible responses for conditional variables #1-#3. If a conditional variable is not used, then it has one possible value (its index is always equal to 1). The number of possible responses varies from one conditional variable to another. All preset Conditional Variables have two values. Population Category has as many values as population files are defined in the *Control* file. For other Conditional Variables the number is determined from the definition supplied by the user in the *Profile Functions (Distributions)* input file.

Each distribution occupies one line in the *Microenvironment Descriptions* input file. Every combination of the seven indices must have a distribution defined, even if that specific combination never occurs during the simulation. For example, if a winter season exists then it must have a set of distributions defined, even if the simulation period only covers the summer. The reason is that the distributions are stored in an array with room for all possible combinations of index values, and this array is checked once for gaps (missing data) before the first profile is begun. This is more efficient than checking to see if a distribution exists every time it is called, as a model run can contain millions or even billions of calls to distributions. The price is that distributions that ultimately are never called must still exist in the array.

The user does not need to number the distributions, this is done internally by the program. The distributions are assigned index numbers in standard Fortran order (the block index changes fastest, and Condition #3 changes slowest). Thus, distribution#1 is for (1,1,1,1,1,1,1), and if there is more than one block then distribution#2 is for (2,1,1,1,1,1,1), etc. In the input file the distributions can appear in any order, but the standard order is preferred for consistency.

Each line describing a distribution contains the following information First, the seven indices are listed; block, day type, season, area, c1, c2, and c3. The seven indices must all appear explicitly in the set order. Any superfluous indices must be given a value of one. Thus if a conditional variable such as c3 is not used then the c3 index number is 1 for all distributions for that MP.

After the seven indices comes the distribution definition in standard APEX distribution format (Section 3.1). Any of the APEX distributions can be used; the available shapes and their parameters are given in Table 3.1.

CHAPTER 9.   CALCULATING EXPOSURES

Below is a description of how the microenvironment concentrations and other information are used by APEX to estimate exposure (see step 6 in Figure 2-1), and how the model then presents and summarizes the exposure results. Exposures are calculated in **ExposureDoseModule:Exposure**.

9.1   Estimating Exposure

For inhaled pollutants such as the ones APEX models, exposure is defined as the time integrated concentration of the pollutant in the breathing zone of a person. We refer to the concentration to which a person is exposed as the *exposure concentration*. This concentration is assumed to be approximately spatially uniform within each microenvironment and also approximately temporally uniform for the duration of any one activity event (at most one hour). A time series of exposure concentrations can be constructed by following the sequence of microenvironments and locations (e.g. "Home," "Work," or "Other") visited according to the composite activity diary assembled for the target profile.

As an example, assume the activity diary indicates that the first 40 minutes of the simulation are spent in microenvironment #3 ("Home"), the next 20 minutes in microenvironment #2 ("Other"), and the next 60 minutes in microenvironment #5 ("Work"), and so on. Then the exposure time series has its first 40 minutes at the concentration for hour 1 in microenvironment #3 in location "Home," the next 20 minutes at the concentration for hour 1 in microenvironment #2 for location "Other," and the next 60 minutes at the concentration for hour 2 in microenvironment #5 for location "Work," and so on. The exposure itself depends neither on the activities that the person is performing nor on any personal physiological properties.

The user may select the units for reporting the exposure output. Either ppm, ppb, or $\mu g/m^3$ may be chosen. This applies both to concentration and to exposure. It also applies to the levels used as cutpoints in the various exposure tables. The parameter ***OutputUnits*** in the *Simulation Control* file controls this; if set to PPM then parts per million (ppm) are used, if set to PPB, then parts per billion (ppb) are used, otherwise micrograms per cubic meter ($\mu g/m^3$) are used.

APEX calculates exposure as a time series of exposure concentrations that a simulated individual experiences during the simulation period. APEX calculates the exposure by identifying the concentrations in the microenvironments visited by the person according to the composite activity diary. In this manner, a time-series of event exposures are found. Then, the timestep exposure concentration at any clock hour during the simulation period is calculated using the following equation:

$$C_i = \frac{\sum_{j=1}^{N}\left(C_{timestep,j}t_j\right)}{T} \qquad (9\text{-}1)$$

where:

C_i = Exposure concentration at hour i of the simulation period ($\mu g/m^3$, ppm, or ppb)

N	=	Number of events (i.e., microenvironments visited) in timestep i of the simulation period.
$C_{timestep\ (j)}$	=	Timestep concentration in microenvironment j ($\mu g/m^3$, ppm, or ppb)
$t_{(j)}$	=	Time spent in microenvironment j (minutes)
T	=	Length of timestep (minutes)

From the timestep exposures, APEX calculates time series of 1-hour, 8-hour and daily average exposures that a simulated individual would experience during the simulation period. APEX then statistically summarizes and tabulates the timestep, hourly, 8-hour, and daily exposures. Note that if the APEX timestep is greater than an hour, the 1-hour and 8-hour exposures are not calculated and the corresponding tables are not produced. Exposures are calculated independently for all pollutants in the simulation.

9.2   Exposure Summary Statistics

The exposure time series provides a wealth of detail on the exposure experienced by each profile. However, it is difficult to analyze since the number of events differs for each profile and even the number of events on any given calendar day is unpredictable. Also, a model run may consist of thousands of profiles, so it is not practical to retain the exposure time series for all profiles in memory. For output tables and for analysis, summaries of the exposure time series are required.

Exposure summary statistics are calculated for each pollutant in the simulation, and are written to pollutant-specific output files: the *Micro Summary* file, the *Micro Results* file, and the *Tables* file. Each exposure metric in this section is thus calculated for each pollutant, and the *Control* file keywords listed below are pollutant-specific. (See *Volume I*).

The first step in summarizing exposure is to calculate the time series of event-level, timestep-level, and hourly average exposures for the profile. The event exposures for all pollutants are written to the *Events* output file (if the *Simulation Control* file setting **EventsOut** = YES), while the timestep values are written to the *Timestep* output file (if the *Simulation Control* file setting **TimestepOut** = YES). Daily averages and maxima for each pollutant can be written to the *Daily* output file as well. The timestep values are used to derive most of the other exposure summary statistics.

There are two exposure time series reported on an hourly basis, namely the series of 1-hour averages and running eight hour averages. These are stored in other vectors. For the first seven hours of the simulation the averages are taken over fewer than eight values, otherwise it is always the current hour and the previous seven hours. These hours may cross day, month, or even yearly boundaries. The 1-hour and 8-hour averages are not calculated for timesteps greater than 1 hour (ie. when the *Control* file variable TimestepsPerDay is less than 24).

There are three exposure statistics calculated on a daily basis. The first is the daily average exposure or **DAvgExp**. This is this arithmetic mean of the 24 values of hourly exposures that fall on a given calendar day. Note that all days contain 24 hours in APEX; the effect of Daylight Savings Time is removed from the model. The daily average exposure is then binned into levels according to the cutpoints provided by the user in the *Simulation Control* file. For example, the input line

```
DAvgExp  = 2, 5, 8, 12, 20
```

indicates that the first bin for daily average exposure extends from 0.0 to 2.0 (ppm, ppb, or µg/m^3), and the second bin from 2.0 to 5.0, et cetera. The final or sixth bin in this example contains all values over 20.0. The number of days at each level is recorded for each profile.

The second daily exposure statistic is the maximum timestep average for each calendar day, or **DMTSExp** in the code (for Daily Maximum Timestep Exposure). It is the highest of the timestep values on each day. Like DAvgExp, these are also converted to bins or levels using cutpoints from the *Simulation Control* input file. The number of days at each level is recorded for each profile.

The third daily exposure statistic is the maximum 1-hour average for each calendar day, or **DM1HExp** in the code (for Daily Maximum 1-Hour Exposure). It is the highest of the 24 hourly values on each day. Like DAvgExp, these are also converted to bins or levels using cutpoints from the *Simulation Control* input file. The number of days at each level is recorded for each profile.

The final daily summary statistic for exposure is **DM8HExp** which is the Daily Maximum 8-Hour Exposure. It is the largest of the 24 8-hour running averages for each calendar day. As for the other daily statistics, it is also binned into levels and recorded for each profile.

The average exposure over the entire simulation period is also calculated. As for the daily summary statistics, the average exposure is binned using the cutpoints designated in the *Simulation Control* input file by **SAvgExp**.

In addition to the exposure statistics described above, there are a few others that are derived directly from the event-based exposure time series. The variable **TimeExp** represents the number of minutes spent in each bin in each micro, based not on hourly averages but on the original event exposures. Again, the cutpoints for the TimeExp bins are provided by the user in the *Simulation Control* input file.

The user can also set a threshold exposure level in the *Simulation Control* file. This variable is called **AlertThresh**. If the exposure time series exceeds AlertThresh for any event then the following three things occur. First, the count of high exposure events for this profile is incremented by one. Second, the total duration over the threshold exposure is incremented by the duration of this event. Third, the exposure is checked to see if it exceeds the maximum exposure previously experienced by this profile. These results are reported in the *Log* file for the model run for each profile that exceeds the threshold.

9.3 Exposure Summary Tables

APEX writes out up to 130 different exposure summary tables for the statistics described above. The content and interpretation of these tables (including examples) are covered in *Volume I*. There are 11 basic types of tables; the tables are written to the *Tables* files (one for each pollutant) and optionally the *Log* file in **ExposureDoseModule:Output:**

1.   Minutes in each Exposure Interval by Microenvironment (**TimeExp**)

110

2. Minutes at or above each Exposure Level by Microenvironment (*TimeExp*)
3. Person-Days at or above each Daily Maximum 1-Hour Exposure Level (*DM1HExp*)
4. Person-Days at or above each Daily Maximum 8-Hour Exposure Level (*DM8HExp*)
5. Person-days at or above each Daily Maximum Timestep Exposure Level (*DMTSExp*)
6. Number of Simulated Persons with Multiple Exposures at or above each Daily Maximum 1-Hour Exposure Level (*DM1HExp*)
7. Number of Simulated Persons with Multiple Exposures at or above each Daily Maximum 8-Hour Exposure Level (*DM8HExp*)
8. Number of Simulated Persons with Multiple Exposures at or above each Daily Maximum Timestep Exposure Level (*DMTSExp*)
9. Number of Simulated Persons with Multiple Exceedances (in the Simulation) of the Threshold Timestep Exposure Levels (*TSExp*).
10. Person-Days at or above each Daily Average Exposure Level (*DAvgExp*)
11. Persons at or above each Overall Average Exposure Level (*SAvgExp*)

The levels written to each table are given by the *Simulation Control* file keywords in parentheses. The definition of terms in the titles of these tables are as follows:

- **Person-day**: A single simulated day for one simulated individual. A 100-day simulation of 10 persons contains 1000 person-days, as does a single-day simulation of 1000 persons. APEX in general counts exposures in Person-days. Multiple exposures (at a single level) during single day are counted as one Person-day of exposure.

- **Multiple Exposures**: Multiple exposures for the same person on different simulation days. This term refers to multiple person-days of exposure in a simulation corresponding to the same profile. Multiple exposures (at a single level) during single day are counted as one Person-day of exposure.

- **Multiple Exceedances**: Multiple exposures for the same person on different timesteps of the simulation. Multiple exposures during the same day (at a single level) DO count as different exceedances.

Table types 1, 2, 10, and 11 are generated only once, for the entire population. Table types 3 to 9 are generated for six population subgroups, under three exertion levels. The six population subgroups are as follows:

1. All Persons. The table statistics are based on the entire population.

2. Children. The table statistics are based on the population of children, as defined by the age range given by the *Control* file settings **ChildMin** and **ChildMax**.

3. Active Persons. The table statistics are based on the population of people having a median Physical Activity Index (PAI, mean MET) over the whole simulation period that exceeds the value designated by the *Control* file setting **ActivePAI**.

4. Active Children. The table statistics are based on the population of active children, as determined by the *Control* file settings **ChildMin**, **ChildMax**, and **ActivePAI**.

5. Ill Persons. The table statistics are based on the population of ill people. The population is determined by the probabilities given in the *Prevalence* file. This population is only considered if the input variable **Disease** is set in the *Control* file.

6. Ill Children. The table statistics are based on the population of ill people. The population is determined by the probabilities given in the *Prevalence* file and the *Control* file settings **ChildMin and ChildMax**. This population is only considered if the input variable **Disease** is set in the *Control* file.

The three exertion levels are:

1. All Exertion Conditions. The table statistics are based on exposures experienced by the population subgroup under any ventilatory conditions.

2. Moderate Exertion. The table statistics are based on exposures experienced by the population subgroup only during periods in which their average equivalent ventilation rate (EVR) is in the "moderate" range. The period of time during which EVR is averaged is either 1 hours or 8 hours, based on the table being generated. The "moderate" EVR ranges are defined by the *Simulation Control* file settings **ModEVR1** (for timestep exposures), **ModEVR1** (for 1-hour exposures) and **ModEVR8** (for 8-hour exposures). An individual's EVR is in the moderate range if it is greater than or equal to the **ModEVR#** setting and less than the **HeavyEVR#** setting for the exposure period.

3. Heavy Exertion. The table statistics are based on exposures experienced by the population subgroup only during periods in which their average equivalent ventilation rate (EVR) is in the "heavy" range. The period of time during which EVR is averaged is either 1 hours or 8 hours, based on the table being generated. The "heavy" EVR ranges are defined by the *Simulation Control* file settings HeavyEVRTS (for timestep exposures), **HeavyEVR1** (for 1-hour exposures) and **HeavyEVR8** (for 8-hour exposures). An individual's EVR is in the heavy range if it is greater than or equal to the **HeavyEVR#** setting for the exposure period.

The exertion level statistics are calculated in the following manner: For each day in the simulation, the mean EVR level during every timestep, one hour, and running eight hour time period is calculated. If the mean timestep, 1-hour or 8-hour EVR is higher then the EVR levels indicated (in the *Simulation Control* file) for moderate or heavy exertion, then the exposure during the same time period is compared with the levels given in the *Simulation Control* file, and the statistics and tables are updated if the exposure exceeds the level.

NOTE: Many of the tables can include statistics at the 0.0 exposure level, if it is indicated on the *Simulation Control* file. This can be used to obtain some useful statistics (such as total final study area of the subpopulation population), since all persons will have exposures equal to or exceeding 0.0 level exposures on all person-days. However, use caution in examining these "0.0" level statistics in the case of the exertion-level tables. If a simulated person has no timestep, 1-hour or 8-hour periods at Moderate or Heavy EVR, then they will NOT have an exposure in that table for the 0.0 level, and the 0.0 level statistics will not correspond to the entire subpopulation.

CHAPTER 10. CALCULATING DOSE

APEX contains algorithms for estimating pollutant doses. The term "dose" refers to some measure of the amount of pollutant in the body of the target person. The situation is not as clear as for exposure since there are numerous specific definitions of dose that are used in various contexts. For an airborne pollutant, dose could refer to the amount inhaled, or the amount currently in the lungs, or the amount crossing from the lungs to the body, or the total amount in the body, or the total in some specific target organ, or a number of other things. Dose may be more useful or accurate than exposure for evaluating the effects of air pollutants because it accounts better for differences in pollutant uptake resulting from (1) the variation in physiology and activities across populations and (2) the variation in physiological responses to activities within an individual. In APEX, dose is generally defined at the amount inhaled. APEX contains a special algorithm for the pollutant CO, in which the model calculates the percent of carboxyhemoglobin (%COHb) in the blood. Carboxyhemoglobin is hemoglobin that has carbon monoxide instead of the normal oxygen bound to it. In addition, APEX contains algorithms to estimate the deposited lung dose in the case of particulate matter (PM). When the APEX model is extended to other pollutants, it will likely require the development of specific dose algorithms for each new pollutant, or at least for each class of pollutant.

The simple algorithm for calculating inhaled dose is discussed in the next section, followed by the algorithm for the %COHb calculation. The final topic relating to dose is the explanation of the summary statistics for reporting dose. Doses are calculated in **ExposureDoseModule:Dose.**

10.1 Inhaled Dose Calculation

Currently, for all pollutants other than CO, APEX calculated inhaled dose. Inhaled dose is simply the amount of pollutant inhaled over the course of a specified time period. In APEX, inhaled dose for each timestep is calculated as

$$D_i = V_e C_i \qquad (10\text{-}1)$$

where

C_i = Timestep exposure concentration at timestep hour i of the simulation period ($\mu g/m^3$, ppm, or ppb)

V_e = Expired ventilation rate (ml/min)

The calculation of the expired ventilation rate V_e is discussed in Section 7.3. The exposure C_i is discussed in Section 9.1. From the timestep doses, APEX calculates time series of 1-hour, 8-hour and daily average dose that a simulated individual would experience during the simulation period. APEX then statistically summarizes and tabulates the hourly, 8-hour, and daily doses. Note that if the APEX timestep is greater than an hour, the 1-hour and 8-hour dose are not calculated and the corresponding tables are not produced. Doses are calculated independently for all pollutants in the simulation.

10.2 Carboxyhemoglobin (COHb) Calculation

The calculation of CO dose is complex. It starts with the exposure time series, which indicates the pollutant concentration in the inhaled air at each moment in time. It also requires the ventilation rate which is activity dependent, knowledge of a number of physiological parameters, and the %COHb level depends not only on current conditions but on recent history as well. The discussion of physiological parameters is in the chapter on personal profiles. In APEX, dose is the delivered dose of CO as measured by the biotransformation product carboxyhemoglobin (COHb)—specifically %COHb—in the blood.

Conceptually, APEX uses a number of factors, in particular a time series estimate of alveolar ventilation rate V_a (which is activity and physiology dependent) and a time-series estimate of exposure (which indicates the pollutant concentration in the inhaled air for specific moments in time), to calculate %COHb. The ventilation rate algorithm is discussed in Section 7.3 and the %COHb algorithm is discussed in the following subsections. For other factors and additional detail, see Johnson (2002).

The %COHb calculation in APEX uses the time series for exposure to CO and the time series for alveolar ventilation rate, V_A, as inputs (among other factors). The dose calculation is based on the solution to the non-linear Coburn, Forster, Kane (CFK) equation, as detailed in Johnson (2002). As pointed out by that report, the CFK equation does not have an explicit solution, so an iterative solution or approximation is needed to calculate the %COHb. An iterative solution, however, was determined to be unsuitable because of the model execution time necessary (a typical model run of one calendar year represents roughly 14,000 events per person and several thousand people, or tens of millions of diary events). Therefore, the CFK equation is solved using a modified Taylor's series method in which the event duration is restricted in time (if necessary) to ensure convergence with only a few terms. This method avoids the dangers of non-convergence that arise in some other methods.

As the mathematical derivation in the above report is very detailed, only the main results are presented here. First, it should be noted that the literature discusses two forms of the CFK equation, namely a linear and a non-linear form. The linear form itself is an approximation that allows an explicit solution, but is not accurate under all conditions. The non-linear form is considered to be more correct and is the one being discussed here.

Restricting %COHb(t) to between 0 and 100 (percent), the CFK equation takes the form of the following differential equation:

$$\%COHb'(t) = C_0 - C_1 \times \frac{\%COHb(t)}{100 - \%COHb(t)} \qquad (10\text{-}2)$$

where C_0 and C_1 are constants over the duration of one event that depend on physical and physiological parameters, including V_a and the CO exposure. C_0 is given by

$$C_0 = \frac{Endgn + P_{CO}/B}{RHB_0 + Blood} \qquad (10\text{-}3)$$

where Endgn and Blood are physiological profile variables (Section 5.3). P_{CO} is the partial pressure of CO (torr)

$$P_{CO} = P_{gases} \times Exposure \times 10^{-6} \qquad (10\text{-}4)$$

where Exposure is the event CO exposure concentration and P_{gases} is the partial pressure (torr) of dry gases at the study altitude (EPA, 1978):

$$P_{gases} = 760e^{-0.0000386Altitude} - 47 \qquad (10\text{-}5)$$

where altitude is in feet. The variable RHB_0 is the total reduced blood hemoglobin level (ml O_2 or ml CO per ml blood), adjusted for altitude (as in EPA, 1978)

$$RHB_0 = 1.39 \times 0.01 \times 0.995 \times Hmglb\left(1 + \frac{2.76e^{0.0001429Altitude}}{100}\right) \qquad (10\text{-}6)$$

where Hmglb is the profile variable for hemoglobin density. The factor B is given by

$$B = \frac{1}{DIFF} + \frac{P_{gases}}{V_a} \qquad (10\text{-}7)$$

Va is the event alveolar ventilation (see Section 7.3) and DIFF is lung CO diffusivity (ml/min/torr) adjusted for ventilation rate

$$DIFF = Diff + 0.000845V_a - 5.7 \qquad (10\text{-}8)$$

where Diff is the CO diffusivity profile variable (which corresponds to a baseline ventilation).

The constant C_1 is given by

$$C_1 = \frac{1 + 0.32 \times PO_2}{69.76 \times RHB_0 \times Blood} \qquad (10\text{-}9)$$

where PO_2 is the partial pressure of oxygen in the lungs (torr)

$$PO_2 = 0.209P_{gases} - 49 \qquad (10\text{-}10)$$

See Johnson (2002) for a detailed derivation of the above equations for C_1 and C_2.

Time zero represents the start of the current event. The concentration *%COHb(0)* (at time zero) is assumed to be known. The first derivative, *%COHb'(0)*, can easily be found from the above equation. The solution *%COHb(t)* is a smoothly varying function of time without sudden discontinuities or changes in slope. It therefore can be expanded in a Taylor's series about $t = 0$, which should converge fairly rapidly. One simplification is to rescale the time variable to the unitless parameter z:

$$z = \frac{(C_0 + C_1) \times t}{(100 \times D_0 \times D_0)}$$

(10-11)

where

$$D_0 = \frac{1 - \%COHb(0)}{100}$$

(10-12)

The Taylor's series up to the fourth order term is:

$$T_4(z) = \%COHb(0) + 100 \times D_0 \times Dz - \frac{100 \times A_1 \times D_0 \times Dz^2}{2} +$$

$$\frac{100 \times A_1 \times D_0 \times D \times (A_1 - 2D) \times z^3}{6} +$$

$$\frac{100 \times A_1 \times D_0 \times D \times (A_1^2 - 8DA_1 + 6D^2) \times z^4}{24}$$

(10-13)

where

$$A_1 = \frac{C_1}{C_0 + C_1}$$

(10-14)

$$D = D_0 - A_1$$

(10-15)

For typical values for the constants C_0, C_1, and %COHb(0), convergence occurs for z<1. For z values below this limit but still close to one, the convergence is slow, so the terms beyond fourth order would be needed if high accuracy were desired. It is found that z<1 generally corresponds to %COHb(0) values below 40 to 50% for one-hour events.

The z value is proportional to t. In APEX, an event can have a duration of no more than one hour. For one hour events there are conditions where z is close to one and convergence of the Taylor's series may require more than four terms. However, it is not necessary to evaluate the entire hour in one step. By dividing the event into shorter subevents, each will have a smaller z value. For example, if a one-hour activity diary event has initial conditions that correspond to z=0.9, then by dividing this into three 20 minute subevents, each will have a z value around 0.3. Actually, the first subevent will have exactly z=0.3. The others will be slightly different as the initial conditions for those subevents will have changed slightly. In practice, a dimensionless subevent duration is used, and all the subevents have equivalent length. An accumulated dose is calculated as the running sum of the average %COHb level over the subevents. At the end of all subevents, the average dose is this accumulated dose divided by the number of subevents while the final value of the dose is simply the final value of COHb itself. These values are saved and the next diary event is processed.

10.3 Calculating PM Dose

In APEX PM dose is modeled as the mass of PM depositing in the entire respiratory system, including the extrathoracic regions (mouth, nose, and oropharynx) and the lungs. The PM dose algorithm was developed from the empirical lung deposition equations of the International Commission on Radiological Protection's Human Respiratory Tract Model for Radiological Protection (ICRP 1994).

The algorithm calculates the deposition fraction (f) in each of 9 filters (see Figure 10.1) and determines the PM mass deposited in each for each event. The 9 filters correspond to the following regions of the respiratory system: 1. Nose (inhalation, f_N) 2. Oropharynx (inhalation, f_O) 3. Tracheobronchi (inhalation, $f_{TB,i}$) 4. Bronchioles (inhalation, f_B), 5. Alveoli (f_A), 6. Bronchioles (exhalation, f_B), 7. Tracheobronchi (exhalation, $f_{TB,e}$) 8. Oropharynx (exhalation, f_O) and 9. Nose (exhalation, f_N). The f values determine the fraction of the particle mass entering the region that deposits. Only the fraction in the Tracheobronchial filters differs for inhalation versus exhalation, for the other filters the value of the fraction is the same in both cases. Deposition via both aerodynamic and thermodynamic (diffusive) mechanisms are estimated for each filter.
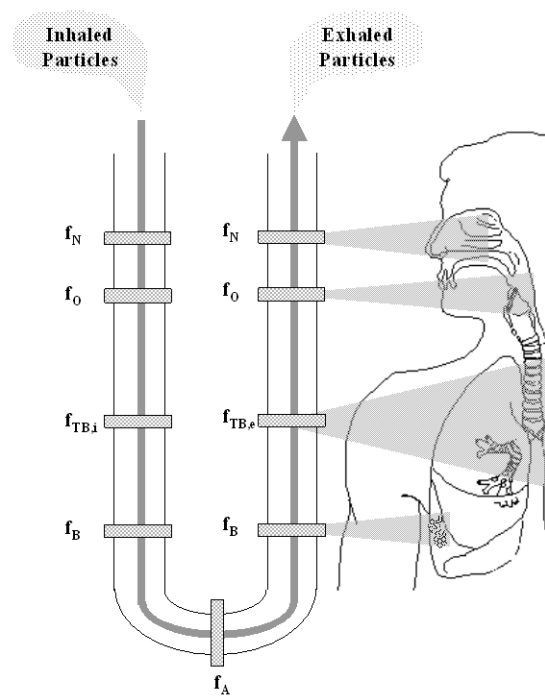

Figure 10.1 Structure of the ICRP Deposition Model.

The fractions f and the resulting deposited doses are calculated for each particle size considered. The size-specific mass are summed to get the mass deposited in each filter. The deposited filter masses are then combined into 4 deposited masses corresponding to total PM dose in the entire

respiratory system and in the extrathoracic (ET, nose + oropharynx), tracheobronchial (TB), and pulmonary (Pulm, bronchiole + alveoli) regions.

10.3.1 Particle Sizes, Inhalability, and Diffusion Coefficient

The particle size used by the ICRP algorithm is the aerodynamic diameter. Aerodynamic diameter (d_{ae}) is the property of particles measured by the majority of particle samplers, and the EPA designations of PM2.5 and PM10 are based on aerodynamic diameter. The aerodynamic diameter is provided to the model in the *Control* file using the pollutant-specific keyword *Size* (see *Volume I*).

Particle inhalability is defined as the fraction of the ambient particles that are inhaled. This fraction is calculated as:

$$f_{inh,i} = 1 - 0.5(1 - [7.6 \times 10^{-4} d_{ae,i}^2 + 1]^{-1})$$
(10.16)

The particle diffusion coefficient D_i is also required to calculate the deposition fractions. D_i is calculated using Equation 10.17:

$$D_i = \frac{C_C(d_{th_i})kT}{3\pi\mu d_{th,i}} \qquad (cm^2\,s^{-1})$$
(10.17)

where k is the Boltzmann's constant 1.38×10^{-16} g cm2 s^{-1} K^{-1}

$d_{th,i}$ is an equivalent thermodynamic diameter of particle size i

T is absolute temperature (Kelvin)

μ is the absolute viscosity of air (1.82×10^{-4} g cm^{-1} s^{-1})

and C_C is the Cunningham correction factor, given in Equation 10.18:

$$C_C(d_{th,i}) = 1 + \frac{2\lambda}{d_{th,i}}[1.257 + 0.4\ exp(-\frac{1.1*d_{th,i}}{2\lambda})]$$
(10.18)

where λ is the mean free path of air, 6.5×10^{-6} cm.

The thermodynamic diameter is calculated from the aerodynamic diameter:

$$d_{th,i} = \sqrt{\frac{\rho}{1.5}\frac{C_c(d_{ae,i})}{C_c(d_{th,i})}} \qquad (microns)$$
(10.19)

where ρ is the particle density in g/cm^3. The value of $d_{th,i}$ is found by recursively solving this equation using an initial guess of $d_{ae,i}(\rho)^{-1/2}$.

10.3.2 The ICRP Deposition Equations

As described above, the ICRP model considers the respiratory system as a system of 9 filters corresponding to the particles deposited in the nose (N), oropharynx (O), trachea/bronchi (TB), bronchioles (B), and alveoli (A) during inhalation and exhalation. The ICRP equations considers fractions for both aerodynamic (ae) and thermodynamic (th) deposition processes in each region. These fractions in each filter j are exponential functions of 3 empirical coefficients a, R, and p, as shown in Equations 10.20 and 10.21.

Aerodynamic Deposition Fraction

$$f_{ae,j} = 1 - exp(-a_{ae,j} R_{ae,j}^{p_{ae,j}})$$ (10.20)

Thermodynamic Deposition Fraction

$$f_{th,j} = 1 - exp(-a_{th,j} R_{th,j}^{p_{th,j}})$$ (10.21)

There is an a, R, and p coefficient for each filter for both aerodynamic and thermodynamic mechanisms. The coefficients may be constant or may be functions of parameters describing the respiratory system physiology and activity level of the individual being modeled. The coefficients, which may also be a function of the mode of breathing (nasal or oral), are given in Table 10.1.

Table 10.1 The values of a, R, and P for each filter for oral and nasal breathing

	Nose (N)	Oropharynx (O)	Tracheobronchial (TB)	Bronchioles (B)	Alveoli (A)
Aerodynamic Deposition					
a	0.0003	nose breathing: 0.000055 oral breathing: 0.00011	inhalation: 0.00000408 exhalation: 0.00000204	0.1147	$0.146 S_3^{-0.98}$
R	$d^2 \dot{V}_n (S_1)^3$	nose breathing: $d^2 \dot{V}_n (S_1)^3$ oral breathing: $d^2 (\dot{V})^{0.6} (V_T)^{-0.2} (S_1)^{1.4}$	$d^2 \dot{V} (S_1)^{2.3}$	$0.056 + t_B^{1.5} d^{t_B^{-0.25}}$	$d^2 t_A$
P	1	nose breathing: 1.17 oral breathing: 1.4	1.152	1.173	0.6495
Thermodynamic Deposition					
a	18	nose breathing: 15.1 oral breathing: 9	$22.02(S_1)^{1.24} \times [1 - 100e^{-[\log_{10}(100+\frac{10}{d^{0.9}})]^2}]$	$-76.8 + 167 S_2^{0.65}$	$170 + 103 S_3^{2.13}$
R	$D \dot{V}_n S_1^{-0.25}$	nose breathing: $D \dot{V}_n S_1^{-0.25}$ oral breathing: $d^2 (\dot{V})^{0.6} (V_T)^{-0.2} (S_1)^{1.4}$	Dt_{TB}	Dt_B	Dt_A

p	0.5	nose breathing: 0.538 oral breathing: 0.5	0.6391	0.5676	0.6101

As indicated in the table, several of the a, R, and P coefficients are a function of a number of physiological variables, including lung volumes, inspiratory flow rates, and residence times. These are described below.

10.3.2.1 Lung Volumes and Age Scaling Factors

The ICRP Publication provides reference values for the required lung volumes as a function of subject age and gender. The volumes are: (1) the dead spaces for the entire lung (V_d), and for the ET, TB, and B regions ($V_{d,ET}$, $V_{d,TB}$, $V_{d,B}$) and (2) the functional residual capacity (FRC).   The ICRP model also makes use of three scaling factors to adjust some of the a and R model coefficients as a function of age. Physiologically, these factors represent ratios of specific airways of a modeled person to those of a reference adult male. S_1 gives the ratio for the trachea, S_2 for the 9th airway generation, and S_3 for the 16th airway generation. Both the volumes and the scaling factors are modeled in APEX based on the reference values, using an equation of the form:

$$P=Ah^2+Bh+C \qquad (10.22)$$

The variable P is the volume or scaling factor of interest and h is the individual's height (in cm). The values of the A,B,C coefficients for the different parameters for males and females were calculated by fitting eq 10.22 to the ICRP parameters; they are given in Table 10.2.

Table 10.2 Coefficients for the Lung Volumes and Scaling Factors

	A	B	C
Volumes			
Male			
FRC	0.0002	-0.0279	1.0353
V_d	0.0078	-0.7135	29.316
$V_{d,ET}$	0.0031	-0.3175	10.907
$V_{d,TB}$	0.0026	-0.2392	9.7143
$V_{d,B}$	0.0023	-0.2119	11.375
Female			
FRC	0.0002	-0.0265	0.96

V_d	0.0079	-0.7403	30.381
$V_{d,ET}$	0.0029	-0.2861	9.5306
$V_{d,TB}$	0.0022	-0.1523	5.9635
$V_{d,B}$	0.0029	-0.3225	16.098
Scaling Factors			
Male			
S_1	1.1354E-04	-4.0700E-02	4.6711
S_2	2.3020E-05	-1.1168E-02	2.2567
S_3	7.8360E-05	-3.2100E-02	4.2381
Female			
S_1	1.2800E-04	-4.3542E-02	4.7975
S_2	2.3200E-05	1.1225E-02	2.2597
S_3	8.0500E-05	-3.2543E-02	4.2585

10.3.2.2 Tidal Volume and Activity Level

Tidal volumes (V_t) were calculated as a function of age, gender, and activity level. The starting point for the V_t calculations are the ICRP reference values for men and women of reference ages for four different activity levels: sleep, sitting, light exercise, and heavy exercise. Other ages are interpolated from the values at the reference ages. After age 30, the values are assumed to be constant with increasing age. The correct V_t for each event is determined as a function of age, gender, and activity level. Activity level is determined by the event METS values for the individual being studied. Activity level was based on normalized METS (M), defined in Equation 10.23.

$$M = \frac{METS - 1}{METSmax - 1} \qquad (10.23)$$

METSmax is the maximum obtainable MET value for the person. If M was less than or equal to 0, then activity level was assumed to be "sleep." If M was greater than 0, then the activity level was assigned as follows:

M ≤ 0.333   : activity level = sitting

0.333 < M ≤ 0.667   : activity level = light exercise

121

M > 0.667   : activity level = heavy exercise

10.3.2.3 Inspiratory Ventilation

Several of the model parameters are a function of the inspiratory ventilation. This flow rate was calculated as

$$\dot{V} = 2V_e \qquad \text{(ml/s)} \qquad (10.24)$$

where V_e is the exhaled ventilation rate.

10.3.2.4 Residence Times

The residence times in the lungs are required to calculate deposition via diffusive mechanisms. Residence times are a function of the flow rate, the dead spaces, FRC, and V_t. The residence times in the tracheobronchial, bronchial, and alveolar regions are given by:

$$t_{TB} = \frac{V_{d,tTB}}{\dot{V}}\left(1 + \frac{0.5V_t}{FRC}\right) \qquad \text{(s)} \qquad (10.25)$$

$$t_B = \frac{V_{d,B}}{\dot{V}}\left(1 + \frac{0.5V_t}{FRC}\right) \qquad (10.26)$$

$$t_A = \frac{V_t - V_{d,ET} - [V_{d,TB} + V_{d,B}]\left(1 + \frac{V_t}{FRC}\right)}{\dot{V}} \qquad (10.27)$$

10.3.2.5 Final Deposition Fractions and Deposited Masses

The total deposition efficiency for filter j is:

$$f_j = \sqrt{f_{ae,j}^2 + f_{th,j}^2} \qquad (10.28)$$

The total mass deposited in each filter j is:

$$m_j = (m_{inh} - \sum_{k=1}^{j-1} m_k)f_j \qquad (10.29)$$

The variable m_{inh} is the total inhaled PM mass that is calculated for each event, Equation 10.30.

$$m_{inh} = f_{inh} * VE * minutes * C_{PM} \qquad (10.30)$$

C_{PM} is the microenvironmental PM concentration for the event, VE is the exhaled ventilation, and minutes is the event duration.

The mass deposited in each region of the respiratory tract can be calculated by summing the mass deposited by the inhalation and exhalation filters associated with that region. The total deposited mass is given by

$$m_{tot} = \sum m_j \qquad\qquad (10.31)$$

10.4 Definition of Dose Summary Statistics

A flag called **DODOSE** is available in the *Simulation Control* file. The default is DODOSE = YES. If DODOSE = NO then the dose calculation in APEX is skipped.

If the dose calculation is performed, the initial result is the dose level for each event in the simulation. Unlike exposure, there are actually three doses calculated per event. The first is the time-average dose over the event. The second is the running 8-hour average of event doses. The third is the final instantaneous dose at the end of the event. For CO, The final dose is found directly using the series $T_4(z)$ given in the previous section. The average dose is easily found since $T_4(z)$ is a polynomial in time and therefore can be integrated without difficulty. For all other pollutants, the instantaneous end-of-event dose has no meaning and is simply equal to the value calculated in Eq. 10-1.

Most of the summary statistics for dose are analogous to those for exposure. The average dose values over an event and the instantaneous dose at the end of the event are written to *Events* output file (if it exists). Timestep and hourly-average dose time series are created by taking appropriate duration-weighted averages of dose over the events in each clock hour. These doses may be written to the *Timestep* and *Hourly* output files. A vector of instantaneous dose at the end of each hour (FDose) is also saved, for the calculation of a daily statistic for maximum end-of-hour dose (see next section). This is not an average, but simply a subset of the values of the event-end dose corresponding to the events that end on a clock hour. For pollutants other than CO, this end-of-hour dose is simply the dose on the last event of the hour.

There are five daily summary statistics for dose. The first is **DAvgDose** (Daily Average Dose) which is the average of the 24 hourly average dose values that fall on the same calendar day. The result for each day is binned according to the levels defined by the cutpoints set in the *Simulation Control* file. The second summary statistic is **DMTSDose** (Daily Maximum Timestep Dose), the largest dose over all the timestep values for the day. The third summary statistic is **DM1HDose** (Daily Maximum 1-Hour Dose) which is the largest of the 24 hourly dose values for a day. The fourth is **DM8HDose** (Daily Maximum 8-Hour Dose) which is the largest of the 24 8-hour running dose averages. The fifth is **DMEHDose** (Daily Maximum End-of-Hour Dose), which is the largest of the 24 values of the instantaneous dose level at the end of each clock hour on a day. All four daily summaries are binned according to the appropriate set of cutpoints in the *Simulation Control* file. Finally, there is the average dose over the entire simulation period, **SAvgDose**. It too is binned and tabulated according to cutpoints set in the *Simulation Control* file.

123

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